

Ion Sourcery

Optimization of a Cesium-Sputter Ion Source for use in Accelerator Mass
Spectrometry

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Abstract

Accelerator Mass Spectrometry (AMS) is a sensitive technique for the analysis of rare isotopes. Optimizing the output of the cesium-sputter ion source is a fundamental method for improving measurement precision, efficiency, and reliability. Several strategies for improving the ion source are discussed and lead to an understanding of the electrodynamics within the ion source to inform further improvement in design and operating parameters.

At the André E. Lalonde Accelerator Mass Spectrometry Laboratory (Lalonde AMS), the High Voltage Engineering Europa (HVEE) SO-110C ion source was modelled using Integrated Engineering Software (IES)'s Lorentz-2E ion trajectory simulation software. Lorentz-2E incorporates the mutual space-charge interaction between the positively charged cesium ion beam and the sputtered negative ion beam.

A critical component of this work was the development of the Rijke code. Rijke communicates with Lorentz-2E to initiate, generate, and run varied sequences of simulations, as well as analyze and record the input and output data in formats convenient for timely analysis. This software and its interconnection with Lorentz-2E is described in extensive detail for a prospective user.

Initial simulation work examined the effects of modifying various electrode geometries within the source such as the extraction cone, the target aperture, a simple cratered sample model as well as examining the effects of varying the cesium ion current. The self-repulsion of cesium was found to be important at currents of $250\ \mu\text{A}$ and above. At high enough cesium currents, the expansion of the cesium beam is such that parts of it impinge outside the extents of the sample material. Through both simulation and experiment, it was demonstrated that this effect can be mitigated by either recessing (translating along the axis of symmetry away from the ionizer) the target holding the sample or by adjusting the potential difference

between the target and ionizer.

Experimentally, at routine settings (6 kV target to ionizer potential, 115 °C cesium oven temperature, and 35 keV output energy), a target recess of 1 mm gave the most stable and sustained output of ^{12}C from graphite blanks. While the peak current was less than the unrecessed case, the total measured charge from the recessed target was higher. Cesium currents at these routine settings were found to be below the theoretical space-charge limited maximum.

Using ^{10}Be standards, a multi-dimensional experimental study examined the effects of increasing the cesium current, adjusting the target-ionizer potential from 4 to 11 kV, while also examining target recesses of 0 to 4 mm. Multiple combinations of these settings produced enhanced currents of $^9\text{Be}^{2+}$, measured at the high-energy offset Faraday cup, as high as $13.5\ \mu\text{A}$. This was higher than previously observed, resulting in the most precise measurement of ^{10}Be performed to date at Lalonde AMS.

The electrodynamics within the ion source can be characterized as three competing processes: a) a strong locus of positive space charge located at the centre of the sample, depending primarily on the focusing of the cesium beam, which draws negative ions across the axis of symmetry; b) a bulk positive space charge external to the negative ion beam, depending primarily on the magnitude of the cesium current, draws the outer-most negative ions away from the axis; and c) the raw field from the electrode potentials and geometry which is mainly defocusing for negative ions. These effects are mitigated the most when the cesium beam is distributed across the entire sample surface with the additional critical benefit of maximizing the sample material accessed for sputtering.

This thesis work has demonstrated that both the mutual and self space-charge interaction of the cesium and negative ion beams were critically important and that the use of the simulation software can inform both improved design and operation settings of the ion source.

Dedication

To the family and friends who believed in me

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List of Acronyms

Lalonde AMS André E. Lalonde Accelerator Mass Spectrometry Laboratory

AMS Accelerator Mass Spectrometry

IES Integrated Engineering Software

VBA Visual Basic for Applications

API automated programming interface

HVEE High Voltage Engineering Europa

BEM boundary element method

FEM finite element method

ESA electrostatic analyzer

GIC gas ionization chamber

NEC National Electrostatic Corporation

FSI fast sequential injection

ARC Advanced Research Complex

DREAMS Dresden Accelerator Mass Spectrometry

ROI region of interest

ODE ordinary differential equations

T-I P target-ionizer potential

MICADAS MIni CArbon DAting System

Chapter 1

Introduction

1.1 Accelerator Mass Spectrometry (AMS)

AMS is an ultrasensitive technique for the analysis of low abundance isotopes used in dating and tracing measurements. The field was born in 1977, when Purser et al. [1] verified that the isobar of ^{14}C , ^{14}N , which is ubiquitous on Earth, does not form stable negative ions. Shortly following, theirs and another lab published the first measurements of ^{14}C [2, 3] with an accelerator. Prior to this, ^{14}C dating had been performed exclusively by radioactive decay-counting. Instead of inferring the age by counting decays of ^{14}C , the atoms of a sample could be counted directly by mass. The advantages of ^{14}C dating by AMS became quickly apparent. As Litherland [4] points out, a gram of modern day carbon will give about 15 counts per minute via decay counting, while a milligram of that same carbon will produce about 15 counts per second in the detector of an accelerator mass spectrometer. The disparity between the two methods increases with the age of the sample. Despite both methods being destructive to the sample, AMS allowed for much smaller sample sizes and higher sample throughput which made it an attractive method in archaeology, geology, and biomedical applications. Nuclear physics laboratories around the world, many already using negative ion sources, quickly adjusted their accelerators to begin making ^{14}C measurements.

1.1.1 Relevant isotopes

While ^{14}C is the primary “workhorse” isotope of many AMS labs, the field has grown to include an ever expanding roster of isotopes used in geological, environmental, archaeological, astrophysical, medical, and nuclear waste management studies. The routine isotopes studies at Lalonde AMS [5], where this research took place, are ^{14}C , ^{10}Be , ^{26}Al , ^{129}I , and ^{236}U [6, 7, 8]. Developments to measure new isotopes such as ^{41}Ca [9, 10], Pu and Am [11, 12], Ra and other actinides [13], ^{125}I [14], ^{90}Sr , ^{90}Y , and ^{90}Zr [15], ^{99}Tc [16], ^{210}Pb [17], and ^{135}Cs [18] have been, and continue to be, a focus of research at Lalonde AMS. Expanding the list of measurable isotopes as well as refining the existing ones allows for the continued expansion of applications.

While these studies may be positively impacted by this work, the focus will be on the two routine isotopes at Lalonde AMS described below.

^{14}C

Half-life: 5730 a [19]

Electron affinity: 1.263 eV [20]

Typical negative ions extracted: $^{14}\text{C}^-$ [20]

Notable atomic isobars: ^{14}N

Method of isobar suppression: Negative ion source; ^{14}N does not form stable negative ions.

^{10}Be

Half-life: 1.387 ± 0.012 Ma [21] [19]

Electron affinity: 0.195 eV [20]

Typical negative ions extracted: $^{10}\text{BeO}^-$ [20]

Notable atomic isobars: ^{10}B

Method of isobar suppression: Differential stopping power through a degrader foil followed by energy filtration in the high-energy electrostatic analyzer (ESA).

1.2 Context of ion source development

The cesium-sputter negative ion source, based on Middleton’s design [22], has been the source of choice at most AMS facilities. Multiple reviews papers [23, 24, 25], including one by Middleton [26] agree on the following criteria as critical for the performance of the ion source used for AMS:

- High, stable current
- Low emittance
- High ionization efficiency
- Fast sample changing
- Low memory effects

High currents allow faster sample throughput and reduced measurement times while the stability minimizes systematic uncertainties. A low emittance, described in greater detail in Chapter 3.2, is required to maximize the number of negative ions transmitted from the ion source to the detector. The ionization efficiency, meaning the fraction of sample atoms that are sputtered and become usable negative ions relative to those emitted as neutral atoms, is important for maximizing the number of atoms analyzed from the available sample mass, and hence the precision of the measurement. Memory effects refers to cross contamination between consecutive samples (short-term memory) and over the course of many samples (long-term memory). This results from sample material adsorbed onto surfaces in the ion source being re-sputtered and transmitted into the accelerator. Minimizing memory effects increases the time the source can be operated between source cleaning while also reducing measurement uncertainty. Finally, a convenient method to measure and switch between multiple samples autonomously, without breaking vacuum is important for optimizing measurement time and minimizing instabilities in electromagnetic and vacuum conditions.

The Middleton-type ion source addressed most of these criteria. With it, Middleton also created the “Negative Ion Cookbook” [20]. It supplemented existing

electron affinity data for most known elements with the nominal outputs of negative ions achieved with his source. It also includes recommendations for the species (atomic or molecular) best suited for their emission. While on the whole, the anion formation in the ion source is complex, in general, the ionization efficiency is limited by the electron affinities of the species of interest.

For some isotopes with low electron affinities (e.g., Be) molecular anions (e.g., BeO^-) are more efficiently ionized and extracted. This is not always advantageous. In the case of ^{26}Al , a higher current could be extracted with molecular anions, but then so too would its isobar, ^{26}Mg for which the atomic species does not form negative ions. Investigation of the sputtering dynamics and the process of competitive ionization at the sample surface are ongoing [27, 28].

Methods for rapid and reliable sample changing have already been established by the three foremost AMS manufacturers: HVEE developed the 200-sample SO-110 carousel [29, 30], Ionplus developed a 40 target magazine on the MIni CARbon DAting System (MICADAS) [31], and National Electrostatic Corporation (NEC) developed a 134 sample holder in the multi-cathode source of negative ions by cesium sputtering (MC-SNICS) [32, 33]. In addition, all three manufacturers have developed gas-fed ion sources, such as the one on the MICADAS [34], which has expanded the versatility of samples that can be processed.

Radiohalides like ^{36}Cl and ^{129}I , with their high electron affinities, efficiently produce high currents of negative ions when sputtered with cesium. In this case, emphasis shifts to other criteria like reducing memory effects. In the works of Pavetich et al. [35, 36], the HVEE SO-110A ion source at the DREAMS lab was modified to better address memory effects. A more open space design was implemented for efficient pumping of neutral atoms, reducing residual gas in the source from sample to sample. To address the deposition of neutral atoms on surfaces near the target that could be accessed and re-sputtered by cesium, a new target design was made. In this design, the sample holder face area was increased (to about a 20 mm diameter compared to the typical 6 mm design). The copper target was also well cooled to promote the adsorption of neutral sample atoms on its face that would be removed from the source upon sample change. This model reduced the memory effect problems at DREAMS; however, the issue of neutral cesium depositing on and

electrically shorting ceramic insulators remains a challenge.

In an effort to address both the high, stable current and low emittance requirements, computer simulations have been employed to attempt to model the ion source. Such simulations require the uncommon capability to account for space charge interactions between the positively charged cesium ions and the negatively charged sputtered ions.

IES's Lorentz-2E simulation software combined the boundary element method (efficient for calculating field distributions from the electrodes in the spaces between them) as well as the finite element method (used to account for space charge deposited in defined spaces) [37]. The finite element mesh breaks down the space into triangular subareas. According to Asi [38], "Each triangular subarea contains three Gauss points. When a particle trajectory crosses a subarea, it will deposit appropriate amount of charges on these Gauss points based on the relative positioning of these Gauss points with respect to the crossing trajectory."

Asi demonstrated Lorentz-2D could be used to model the General Ionex Corporation's 846 Cs sputter ion source at the Center for Accelerator Mass Spectrometry (CAMS) [38]. These simulations affirmed that the design improvements made by Brown et al. [39] were shown to be favourable in simulations as well. This successful application of Lorentz-2D inspired the purchase of the software Lorentz-2E (See Section 1.2.1 for discussion of "2E") at Lalonde AMS, eventually resulting in this work.

Brown et al. [39] had made their own simulations using NEDLab which similarly included space charge interactions. Using this, they modified their source to include a flat face target rather than recessed cone geometry. They changed the existing target shield aperture into an immersion lens at a slightly raised potential relative to the sample-containing target. This lens was also designed to protrude closer to the ionizer, increasing the field strength at the surface to better extract cesium ions. A "halo" of cesium deposition on the target was observed both experimentally and in simulations to originate from the corner of the ionizer. Using this new design, they were able to increase the output of C^- by about a factor of two.

1.2.1 Lorentz-2E name convention

In the previous paragraphs, the names Lorentz-2D and Lorentz-2E were used. Integrated Engineering Software offers several software packages. Some include Electro[™], Magneto[™], Lorentz[™] which handle electrostatic fields, magnetostatic fields, and ion trajectory simulations respectively. They can be combined depending on the requirements of the user's model – which can be in 2 or 3 dimensions. Lorentz-2E represents the ion trajectory simulation software Lorentz using a 2-D geometry and incorporating the electric field simulation from Electro. Lorentz-2E is the software version that was used for this thesis work. Lorentz-2D, mentioned in Asi's paper [38] preceded this naming convention and is synonymous with Lorentz-2E.

1.3 Thesis Overview

1.3.1 Aim

Of the design criteria listed above, the two given priority in this work are that of high, stable current and low emittance. By using the Lorentz-2E simulation software, the SO-110C ion source was modelled. The geometry and electric potentials were altered to seek improved design and operational parameters that were then tested by experiment.

1.3.2 Outline

This section provided the context of design criteria for ion sources with a brief overview of work done at various labs to improve these aspects.

Chapter 2 provides an overview of the the Lalonde AMS facility including special emphasis on the ion sources used in the past 6 years.

Chapter 3 presents the relevant theory upon which much of this work is based.

In Chapter 4, an overview of the Rijke code developed by this author to interface and automate the operation of Lorentz-2E simulations is provided. The functioning of this code from start to finish, including the intercommunication between Rijke and Lorentz-2E is detailed. In addition, the optimization of critical parameters in

the operation of Lorentz-2E is discussed.

Chapter 5 provides the notable simulations and experiments performed using the Rijke software as applied to the SO-110C ion source. The chapter is organized in chronological order, exploring the evolution of the understanding of the source and the implementation of the code from beginning to end.

The main results are summarized in Chapter 6 and avenues for continued development are suggested.

Chapter 2

André E. Lalonde Accelerator Mass Spectrometry Laboratory (Lalonde AMS)

2.1 Overview

The André E. Lalonde Accelerator Mass Spectrometry Laboratory (Lalonde AMS) was installed in 2014 in the Advanced Research Complex (ARC) at the University of Ottawa and replaced IsoTrace at the University of Toronto as the only AMS facility presently in Canada. A wide-angle overview of the completed accelerator mass spectrometer can be found in Figure 2.1 while a schematic diagram is presented in Figure 2.2.

This chapter is designed to provide sufficient context for the ion source's role in an AMS measurement while simultaneously serving as a high level reference on how the spectrometer works for present and future physics graduate students at Lalonde AMS. Extra attention will be given to Section 2.2 which details the HVEE SO-110 ion source, which is the focus of this work.



Figure 2.1: A panoramic view of the Lalonde AMS accelerator.

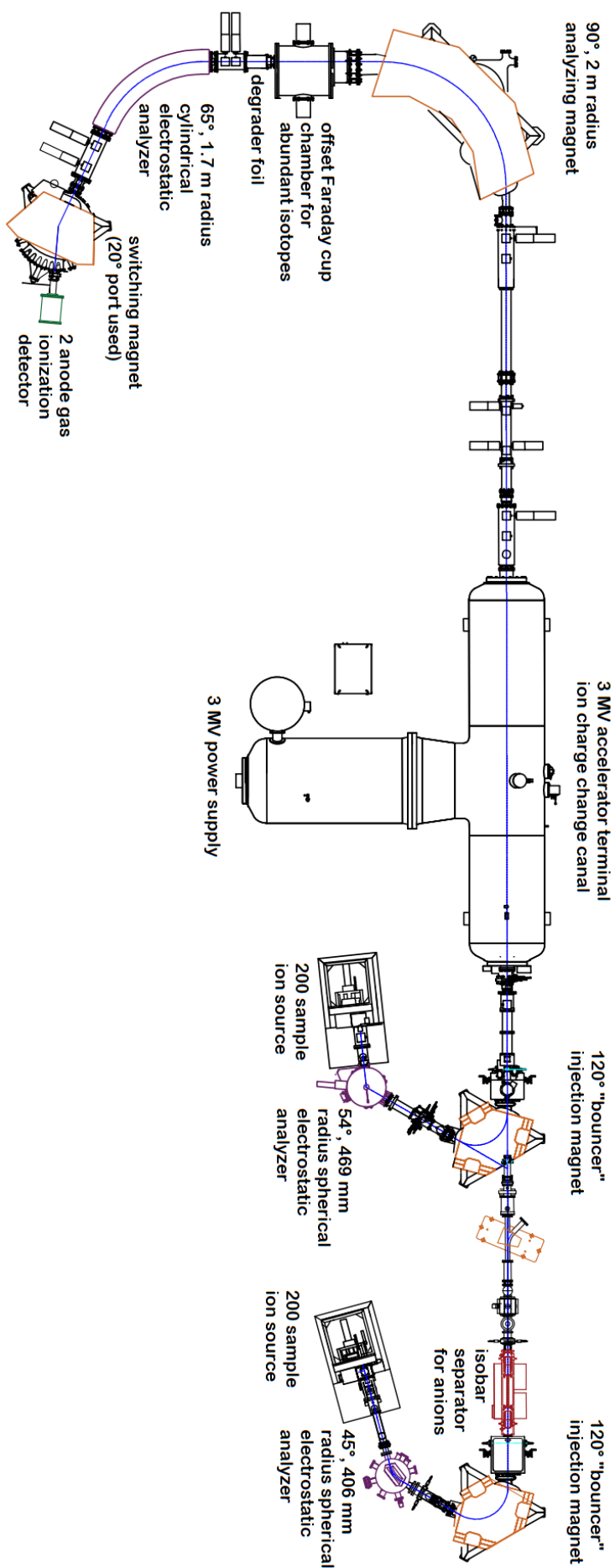


Figure 2.2: A schematic overview of the Lalonde AMS accelerator.

2.2 Ion source

2.2.1 Targets and sample wheel

AMS is a multi-disciplinary field. A large fraction of the samples are collected by geologists, chemically prepared by radiochemists, and analyzed by physicists with frequent overlap and collaboration between them. Once chemically prepared, the samples are pressed into a target (often referred to as cathode in other literature), which is screwed onto a paramagnetic stainless steel base. The bases are then inserted into a 200 sample wheel. Each receptacle in the wheel has an adjacent magnet to keep the samples from falling out. The sample wheel is mounted in the carousel as shown in Figure 2.3. Once sealed, the carousel is evacuated with vacuum pumps. Once the vacuum is sufficient (typical base pressure is about 3×10^{-8} mbar), the samples are injected one at a time into the ion source with a pneumatic piston. The tip of the piston is also magnetic to keep the bases from falling off. The carousel may be rotated to switch between four concentric circular rows of fifty samples.

2.2.2 Ion source description and operation

At the time of writing, there are three primary manufacturers of accelerator mass spectrometers: NEC, HVEE, and Ionplus. Since the beginning, Lalonde AMS has operated with a 3 MV accelerator mass spectrometer manufactured by HVEE; thus, discussion will primarily revolve around their “flagship” SO-110 series of ion source.

When this work began, Lalonde AMS was using an HVEE SO-110B type ion source [29]. Partway through this work, Lalonde AMS upgraded to the new SO-110C version [30]. A comparison of the two is presented in Section 2.2.3. Following this upgrade, tests using the B version were no longer possible. Thus, the simulations detailed in Chapter 5 primarily deal with the C version. However, other AMS facilities, for example the DREAMS lab, still use the older SO-110A model. DREAMS has modified one of their SO-110A sources and developed a new SO-

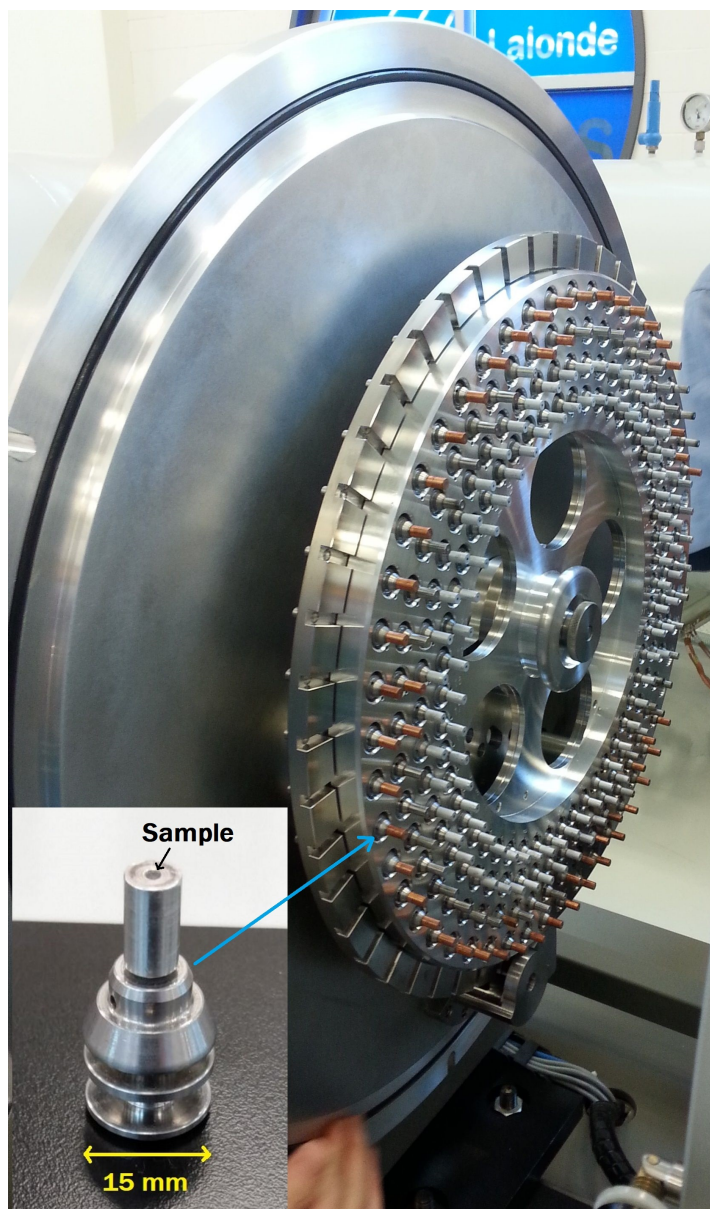


Figure 2.3: Samples are pressed into the target which is mounted on a base and loaded into a 200 sample carousel.

110V3 low-memory source for volatile samples like ^{36}Cl and ^{129}I [36, 35]. While the V3 model significantly reduces memory effects by way of pumping and thermal control, the geometry relevant to the electrostatic field is identical to its predecessor. Thus, it will not be expanded upon in this work.

Figure 2.4 shows a cross section view of the ion source. Due to confidentiality, exact dimensions are not presented. A Cs reservoir outside the source heats Cs to a vapour that is injected into the shroud. The shroud has equispaced holes that spray Cs atoms onto the ionizer. The hot molybdenum ionizer ionizes the Cs and the resulting Cs^+ ions are accelerated by a potential difference towards the target. The

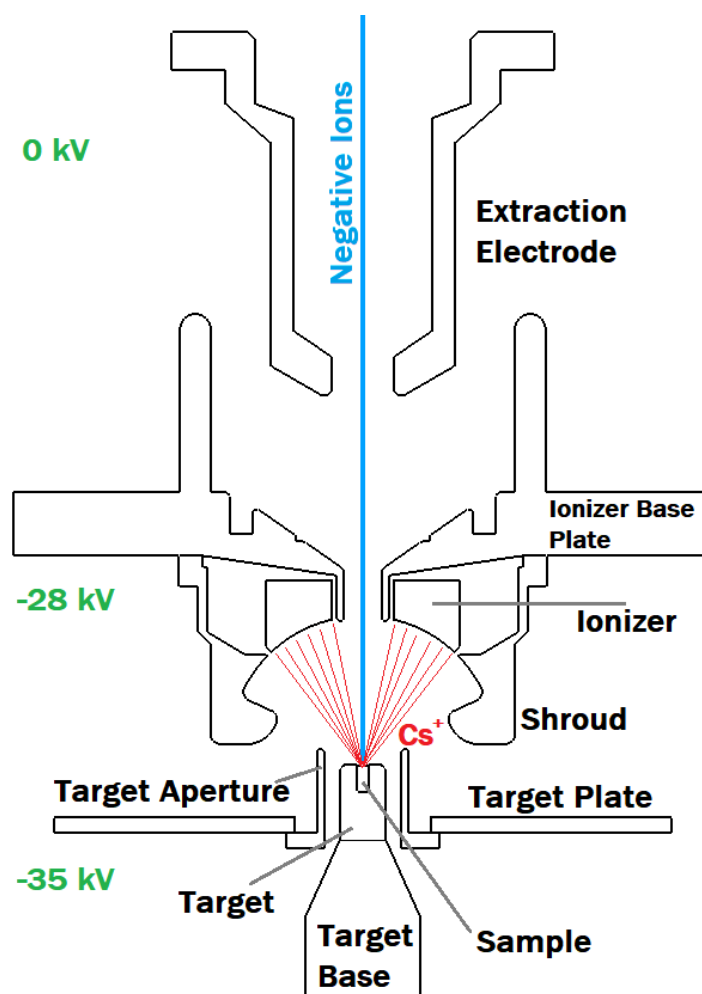


Figure 2.4: A cross section view of the SO-110C. Cs^+ ions ionized at the ionizer bombard the sample and the resulting negative ions are extracted and injected into the accelerator. The blue line represents the axis of polar rotational symmetry as well as the desired path of the negative ions.

Cs^+ ions bombard the sample and negative ions are liberated (along with a spectrum of neutral particles and electrons). The negative ions are accelerated along the axis of symmetry and the electrons are returned to components at the target potential by a moderate magnetic field perpendicular to the beam axis. Once they pass the ionizer base plate, the ions are further accelerated by another potential difference and injected into the accelerator.

With the exception of the target and the spherical ionizer, all electrostatically-relevant parts in the source are made of stainless steel. The ionizer is made of molybdenum by choice of the manufacturer. Its high work function allows for a high ionization efficiency of cesium. Typical target materials are copper and aluminum. The bombarding Cs creates a significant amount of heat at the target. Copper tar-

gets, due to their higher thermal conductivity, are used for volatile samples, like iodine, where lower target temperatures are desirable. The conical “shoulder” of the target base fits snugly into a cooling block. Both this block and the ionizer base plate are cooled with a silicone-based coolant, SylthermTM, which is in turn cooled by the main water cooling system via a heat exchanger. For volatile samples, special bases with copper shoulders are used for better heat dissipation. For practical reasons, ^{10}Be and ^{26}Al samples are also measured using copper targets. Aluminum targets were chosen for carbon measurements due to their high purity, though other labs have reported improved sputter yields using aluminum over copper [27].

The ionizer assembly (ionizer, shroud, and ionizer baseplate) is typically held at -28 or -29 kV while the target assembly (target, target base, target plate, and target aperture) is typically held at -35 kV. Both are relative to the extraction electrode which is at ground potential. Thus, the kinetic energy of the ions leaving the source is 35 keV. This results in a target-ionizer potential (T-I P) of 7 kV and an extraction potential difference of 28 kV. While these were the routine settings for the SO-110B version, routine operation of the SO-110C version have switched to a T-I P of 6 kV.

A constant challenge in AMS is the exposure of insulators to atomic cesium that can deposit and leak current across insulators. With each design iteration of the SO-110 series ion source, HVEE has made continual improvements to the protection of insulators from cesium.

2.2.3 Brief summary of previous SO-110 models

As seen in Figure 2.5, the SO-110B [29] ion source improved upon the SO-110A source by making a more open geometry for better pumping of neutral particles. This reduced the tendency for electric discharge as well as the sputtered neutral particles’ residency near the sample, lowering cross contamination between samples. The shielding of insulator components was greatly improved. This lengthened the time between source cleaning, reducing down time.

The SO-110C [30] ion source, shown in Figure 2.6, further improved the insulator shielding, allowing for higher accelerating potentials for both ion beams. The ionizer alignment was made simpler and more reproduceable. The power supply now

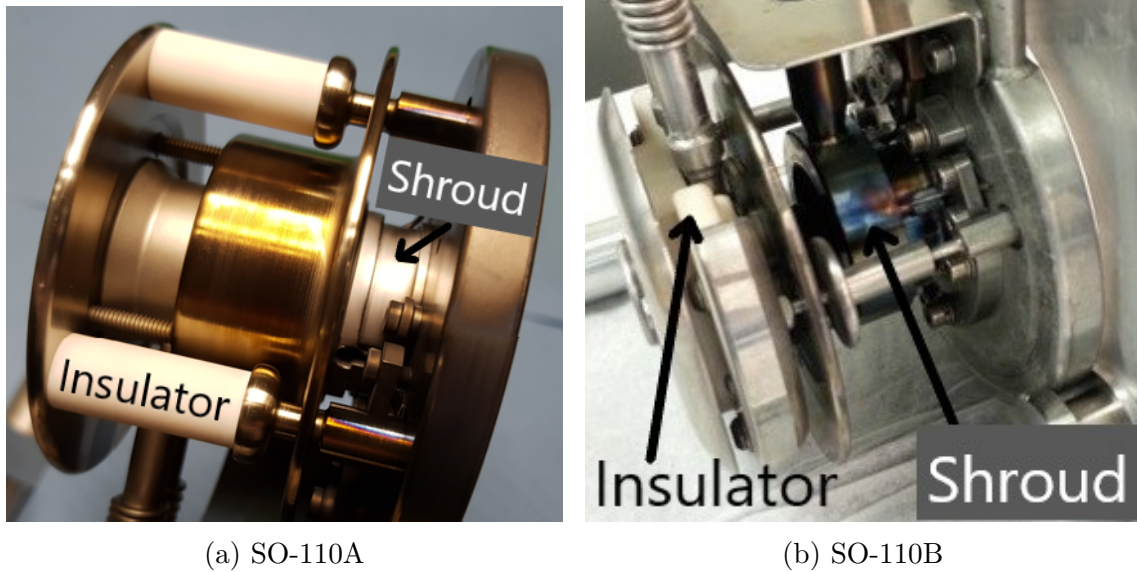


Figure 2.5: A comparison of the SO-110 A and B versions.

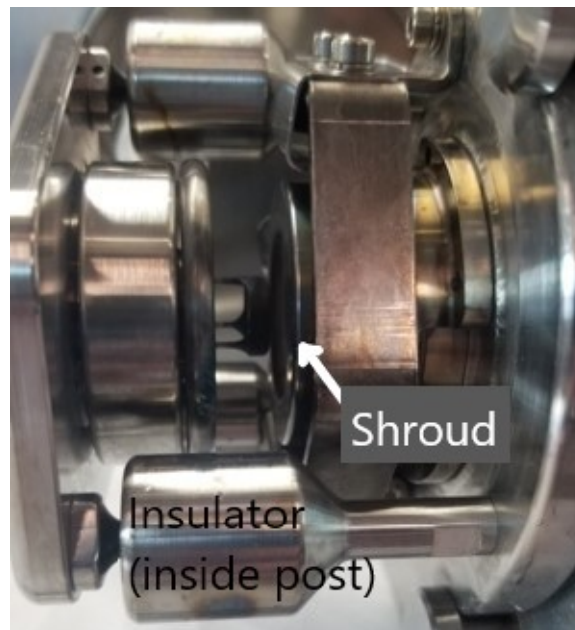


Figure 2.6: A side view of the SO-110C

supported up to 12 kV T-I P and can withstand higher currents across electrodes.

2.2.4 Beam quality post ion source

If one defines the electric potential of the target relative to ground as V_S , the atomic mass (or molecular mass in cases like $^{10}\text{BeO}^-$) of the negative ion of interest as M , and the negative charge state as q_- , the kinetic energy immediately following

the ion source, K_1 is given as:

$$K_1 = V_S q_- . \quad (2.1)$$

While a q_- of -2 is academically interesting and occasionally searched for, doubly negatively charged particle yields from the ion source have not been relevant to typical sample analysis by AMS. Thus, q_- is fixed at -1. At Lalonde AMS, the typical operating source potential is $V_S = -35$ kV. Thus, K_1 is almost always 0.035 MeV.

2.3 Low-energy mass spectrometer

An enlarged image of the low-energy mass spectrometer is found in Figure 2.7. It is responsible for filtering the output of the ion source by mass and energy before injecting the beam into the accelerator. A number of electrostatic lenses, electrostatic steerers, apertures, beam limiting slits, and removable Faraday cups are distributed along the path of the beam for tuning purposes. The major filtering components are the ESA and the bouncer magnet.

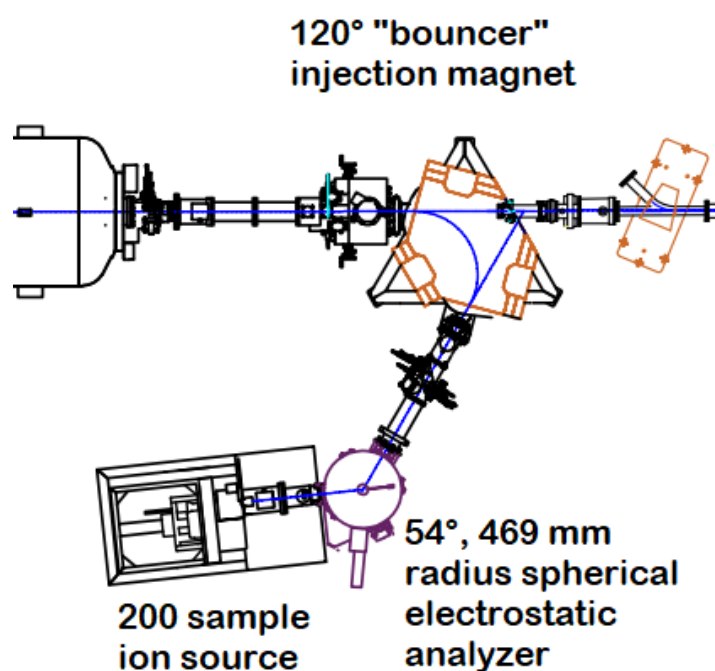


Figure 2.7: A zoom in on the low-energy side of the accelerator.

The ion source, like most ion accelerating components, outputs a spectrum

of energetic particles. Immediately following the ion source is an einzel lens, which focuses the beam through the spherical 54° ESA to a waist at the entrance slits of the magnet.

2.3.1 54° ESA

The ESA acts as an energy filter, transmitting a sharp-peaked energy spread centered on kinetic energy, K_1 . The existing spherical ESA has a radius of curvature, ρ of 469 mm, a plate separation, d , of 53 mm, and an energy resolution ($E/\Delta E$) of 850. By using the kinetic energy, the requisite centripetal acceleration, and the Lorentz Force Law, one can calculate the necessary electric potential difference across the plates, V_{LE-ESA} , as follows:

$$V_{LE-ESA} = \frac{2dK_1}{\rho q_-}. \quad (2.2)$$

To minimize the absolute voltage needed to be applied to either plate, as well as reduce aberrations from the fringe field effects at the entrance/exit, typically the inner plate is held at $+\frac{1}{2}V_{LE-ESA}$ while the outer plate is held at $-\frac{1}{2}V_{LE-ESA}$.

The plates of the ESA can be manually rotated using an external lever which allows switching the input to a second ion source port. At the time of writing, only a single port is currently installed at Lalonde AMS.

Once the beam has been filtered by energy, it is injected into the bouncer magnet for mass separation.

2.3.2 120° bouncer injection magnet

As the beam enters the injection magnet, all particles have kinetic energies of K_1 , but different momenta depending on their mass. The magnet disperses the beam by momentum and injects one isotope mass at a time into the accelerator. Fast switching, combined with gated data recording is desirable to avoid wasting target material while also facilitating higher precision measurements that are less susceptible to uncertainties from ion current drift. One challenge during the development of AMS systems was that magnetic fields change slowly and suffer from hysteresis, making them unreliable as a mechanism for timely isotope switching in

routine analyses. Electrostatic fields, on the other hand, are quick and reproducibly changeable.

The magnet is tuned to allow one particular isotope mass through the reference path. For carbon this “reference isotope” is typically ^{13}C . To transmit lower momentum particles, an electrostatic field at the entrance to the magnet accelerates the particles to the requisite momentum and then a second electrostatic field at the exit of the magnet decelerates the particles back to the original kinetic energy they had upon entry. In a similar fashion, higher momentum particles are decelerated, bent along the reference path of the magnet, and then reaccelerated upon exit. This rapid switching is referred to as fast sequential injection (FSI), more colloquially called “bouncing,” and is described in more detail by Klein et al. [40].

The feedback circuitry within the power supplies for these entrance and exit acceleration electrodes cannot manage the stable ^{12}C beam bombarding their surface when set at 0 V to allow ^{13}C through the reference path. Thus, the magnet is set to allow ^{13}C but with at a slight voltage bias on the entrance and exit electrodes to mitigate this issue.

The bouncer magnet at Lalonde AMS, described in [41] has a reference path radius of curvature of $\rho = 455$ mm, a gap of 62 mm, and a mass resolution ($M/\Delta M$) of 1050. The requisite magnetic field of the reference isotope can be calculated using the following equation:

$$\left| \vec{B} \right| = \frac{\sqrt{2MK_1}}{\rho q_-}. \quad (2.3)$$

Following the magnet are a series of steerers to correct beam divergences and an einzel lens that focuses the beam into the accelerator.

2.3.3 Beam quality post low-energy mass spectrometer

The ions are injected into the accelerator with kinetic energy, K_1 as laid out in Equation 2.1. The beam is ideally focused to a waist located at the centre of the accelerator. Depending on which mass is selected by the bouncer magnet, particles with the same magnetic rigidity are injected into the accelerator. This includes the isotopes of interest as well as any atomic and molecular isobars.

2.3.4 A comment on the ion source output

At Lalonde AMS, the bouncer magnet was calibrated by running a large graphite target and measuring a mass spectrum at the pre-accelerator Faraday cup. The results of this study are reproduced with permission (X. Zhao, private communication). The most intense currents are given in Table 2.1.

Power Supply Output	Hall Probe Reading [T]	Intensity Relative to Mass 12	Intensity Relative to Whole Beam	Mass [amu]	Probable Ions
0	0.00029				
32.17	0.16898	100.0 %	44.2 %	12	$^{12}\text{C}^-$
33.5	0.176	1.2 %	0.5 %	13	^{13}C , $^{12}\text{CH}^-$
34.778	0.18276	0.00036 %	0.00016 %	14	$^{13}\text{CH}^-$, $^{12}\text{CH}_2^-$
45.462	0.23959	80.8 %	35.7 %	24	$^{12}\text{C}_2^-$
46.412	0.24466	2.4 %	1.1 %	25	$^{12}\text{C}^{13}\text{C}^-$
55.679	0.2939	11.5 %	5.1 %	36	$^{12}\text{C}_3^-$
64.294	0.33953	12.8 %	5.7 %	48	$^{12}\text{C}_4^-$
71.881	0.37973	1.5 %	0.7 %	60	$^{12}\text{C}_5^-$
78.755	0.4161	5.8 %	2.5 %	72	$^{12}\text{C}_6^-$
90.961	0.48074	1.9 %	0.8 %	96	$^{12}\text{C}_8^-$
125.103	0.66082	1.5 %	0.7 %	181	$^{133}\text{Cs}^{12}\text{C}_4^-$
133.229	0.70347	1.9 %	0.9 %	205	$^{133}\text{Cs}^{12}\text{C}_6^-$

Table 2.1: A mass spectrum from a large graphite target measured after the bouncer magnet during magnetic field calibration. Cs temperature at the ion source was 95°C. Bouncer voltage off. Current intensities were measured at the pre-accelerator Faraday cup using a Keithley 610B electrometer. The 12 amu signal was measured to be approximately 7.8 μA . With the exception of 14 amu, only currents from other mass species exceeding 1 % the relative current of mass 12 are presented.

As expected, ^{12}C is the dominant species. However, the ^{12}C dimer is nearly as intense. Together, they represent nearly 80 % of the ion current output of the ion source. This means that when running carbon simulations the dimer at least must be taken into account for space charge effects of the negative ion beam. The next most intense species are the quadrumer and the trimer but represent less than 6 % each of the total current. Mass 14 is presented to show its insignificant contribution to the overall current. This table will be important to discussions of simulation setup of the negative ion beam discussed in Chapter 5.

2.4 3 MV terminal

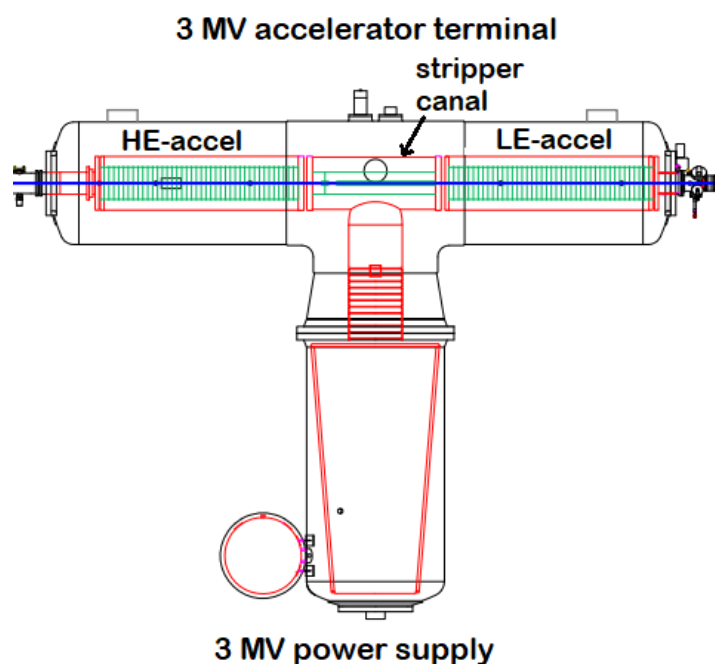


Figure 2.8: A zoom in on the accelerator. The beam path is shown in blue. Negative ions enter from the right, are accelerated from low energies (LE-accel) by a potential difference of up to 3 MV into the stripper canal. The negative ions are stripped to positive ions within the canal and are accelerated to high energies (HE-accel) by the same potential difference before exiting out the opposite end of the accelerator. More details are found in the text.

The accelerator accelerates the anions, strips electrons from them creating positive ions, and then accelerates them again to the high-energy beam line. This process destroys molecular isobars which cannot survive losing many electrons without dissociating due to the unbalanced coulomb forces within the molecule.

The 3 MV accelerator, schematically shown in Figure 2.8, is comprised of a stripper canal at its centre. Within the lower part of the “T” shape is the voltage generator that brings the electric potential of the canal up to as much as 3 MV. Forming the top of the “T” and connecting both the high and low energy beam lines to the canal are approximately 80 titanium electrodes separated by glass insulators with pumping holes on the side and a tilted centre hole for the beam. The tilted hole is rotated along the flight path so electrons are deflected (reducing X-rays) while heavier ions stay on track. Divider resistors are attached to these electrodes to make sure that an even voltage gradient is present in the tube as it steps down from high

potential to ground. The tubes and stripper canal assembly and the power supply column are located in a pressure vessel which is filled with SF_6 gas at a pressure of 6 bar. This gas prevents electrical discharge with the grounded accelerator housing.

Within the canal is a stripper gas which is kept localized by differential pumping with turbomolecular pumps. At the time of writing, argon is the stripper gas of choice, however, a planned upgrade will allow for both argon and helium to be used in the future. The momentum of the negative ions, arriving from the low-energy side of the accelerator, carries them through the equipotential canal. As they collide with the stripper gas within the canal, the electrons are stripped from the ions, leaving them positively charged. The stripping yield of a given charge state is dependent on the velocity of the incident particle, the species of the stripper gas, and the stripper gas pressure [42]. These will be optimized to maximize the yield of a desired charge state. If a sufficiently high charge state is chosen, molecular isobars that make it into the accelerator from the low-energy side ($^{12}\text{CH}_2^-$ vs ^{14}C for example) will be unable to maintain their molecular bonds and dissociate. They will then be filtered out by the high-energy mass spectrometer and eliminated as an isobaric interference. Very rarely, small molecules with a charge state of +3 have been observed [25].

The dependence of the stripping yield on the incoming species introduces a source of fractionation (^{12}C and ^{14}C are not stripped equally at a given energy). This is one of many reasons why AMS labs run standards of known isotopic ratios in every batch of unknown samples. Since they are all measured in the same way, the standard allows the correction of such fractionation effects through normalization.

Once the stripped ions exit through the other side of the canal they are accelerated again by the second gradient field and injected into the high-energy mass spectrometer.

2.4.1 Beam quality post the 3 MV terminal

In the ideal case, where an incoming negative ion is accelerated into the terminal, stripped to a desired positive charge state, q_+ , and then accelerated through the second gradient, there are three kinetic energy transformations of note. If V_T is

the terminal potential, the kinetic energy after the first acceleration, K_2 is given by:

$$K_2 = V_T q_- + K_1. \quad (2.4)$$

When accelerating molecular negative ions, like BeO^- , the molecule will dissociate into its subcomponents and the atom of interest, Be, will carry a fragment of the energy proportional to its fraction of the molecular mass. If the ingoing molecule has a mass ‘M’ and the mass of the outgoing species is denoted as ‘m,’ then the kinetic energy of the outgoing species, K_3 , is given by:

$$K_3 = \frac{m}{M} K_2. \quad (2.5)$$

Finally, this positive ion is accelerated and the final kinetic energy leaving the accelerator, K_4 is given by:

$$K_4 = V_T q_+ + K_3. \quad (2.6)$$

Which when written out fully is:

$$K_4 = V_T q_+ + \frac{m}{M} (V_T q_- + V_S q_-). \quad (2.7)$$

As with all accelerating components, and especially due to multiple scattering within the terminal, a spectrum of particle energies exits the accelerator with a sharp peak at K_4 but with energy no higher than $(q_{+,max} + 1) V_T + V_S q_-$ where $q_{+,max}$ is the maximum attainable positive charge state. This process is described in greater detail by Litherland et al. [25]. Thus, further filtration is necessary on the high-energy side.

2.5 High energy mass spectrometer

Now that the ion beam has been accelerated and molecular isobars have been removed, the high-energy side of the accelerator, enlarged in Figure 2.9, removes any remaining molecular fragments, filters the beam, and measures the isotopic ratios of rare and abundant isotopes. The beam first passes through steerers and then is focused into the high-energy magnet by an electric quadrupole lens.

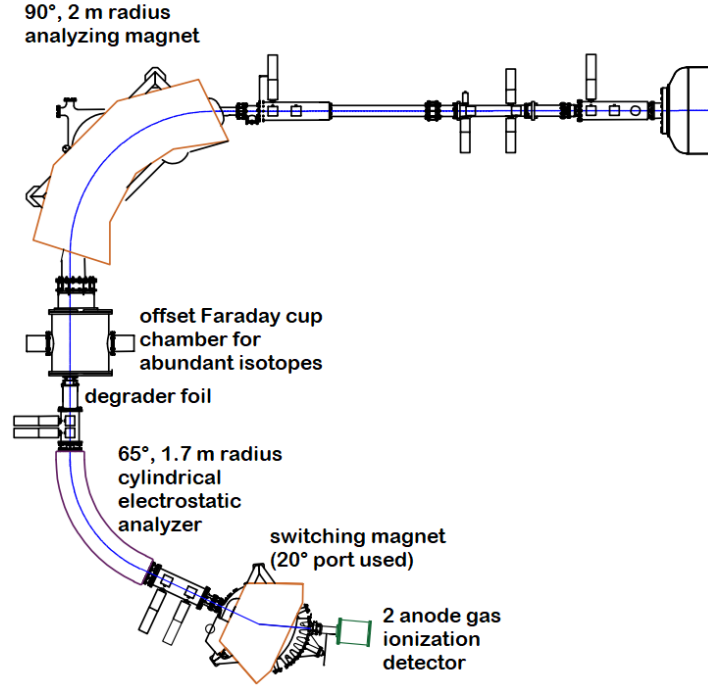


Figure 2.9: A zoom in on the high-energy side of the accelerator.

2.5.1 90° High-Energy Magnet

The high-energy magnet disperses the beam by mass/momentum again, however this time the rare isotope (of mass m_{rare}) passes through the reference path with a radius of curvature $\rho = 2000$ mm. The gap is 36 mm and the mass resolution ($M/\Delta M$) is 2600. The magnetic field strength necessary to bend the rare isotope beam is calculated as:

$$|\vec{B}| = \frac{\sqrt{2m_{rare}K_4}}{\rho q_+}. \quad (2.8)$$

NOTE: In cases, like with BeO^- , where the ion source emits a molecular beam, the value of K_3 and therefore K_4 for both the abundant isotope (i.e. ^9Be) and rare isotope (i.e. ^{10}Be or ^7Be) will be different from their stable counterparts due to the differences in masses before and after stripping. It is important to take this into account for the calculation of K_4 used in Equation 2.8.

The rare isotope is bent the full 90° towards the high-energy ESA for further processing while the abundant isotope(s) are dispersed to different angles within the Faraday cup chamber.

2.5.2 Faraday cup chamber

In the Faraday cup chamber, there are two movable Faraday cups at positions that can be adjusted manually from outside the chamber via mechanical rotary feedthroughs. The Faraday cups are optimized during tuning to the positions where the magnet disperses the abundant isotope(s). In the case of carbon, these would be optimized to collect the dispersed ^{13}C and ^{12}C beams. The Faraday cups measure and record the current of these isotopes which are used to calculate the isotopic ratios of the samples.

In addition to the high stability provided by the generating voltmeter in the terminal, these Faraday cups add an alternative corrective layer to the beam quality, which is critical to the success of the FSI method in cases where the AMS hosting facility cannot provide sufficiently stable conditions of room temperature/humidity and cooling water temperature/pressure. They are equipped with twin slits that measure current of the beam separately. If the tandem voltage drifts higher or lower, the energy of the beam and thus the position of the dispersed ions will drift off centre. When one of the slits reads more current than the other, it will send feedback to the accelerator to correct the generated voltage and recenter the beams. The output of these slits is gated in coordination with the bouncing magnet's injection of each isotope mass. By using the abundant isotopes for this slit-error stabilization during a repetition cycle (of ^{12}C , ^{13}C , and ^{14}C), one can be assured that the rare isotope position does not drift off course during the data collection. These slits are designed to maintain the beam position to within 0.1 mm which corresponds to a terminal voltage stability of ± 100 V [5]. The slit-error stabilization method does not work well for blank targets producing weak ion beams.

Although the slit stabilization method is employed to great success at other facilities, due to the excellent facility stability at Lalonde AMS, the generating voltmeter (GVM) within the accelerator housing is relied on exclusively for maintaining a stable terminal voltage.

2.5.3 Degradar foil

The degrader foil is the first part of the rare isotope line. At this point, if their parent negative ions are created in the ion source, the only isobaric interferences remaining are atomic. In the case of carbon, this was already dealt with at the ion source because ^{14}N did not form negative ions. In the case of ^{10}Be , its isobar and decay product, ^{10}B has yet to be filtered out. A 500 nm thick Si_3N_4 degrader foil is used in conjunction with the high-energy ESA to separate out this interference. As both species pass through the foil, they lose energy due to collisions within the foil, proportional to the square of the proton number, Z , of the nucleus. The kinetic energy, K_5 of the outgoing beam depends on the stopping power of the foil on the ions. This has been modeled by HVEE using the program SRIM (**S**topping and **R**ange of **I**ons in **M**atter) - a reliable simulation package for calculating interactions of energetic particles in matter [43, 44].

$^{10}_5\text{B}$ loses more energy than $^{10}_4\text{Be}$ as they pass through the foil and is bent to hit the inner plate of the high-energy ESA while the ^{10}Be is transmitted along the reference path [25, 45].

2.5.4 65° high-energy electrostatic analyzer

After the foil is the cylindrical high-energy ESA sandwiched between two electric quadrupole lenses that maintain the focus of the beam. The ESA operates in the same manner as on the low-energy side. The radius of curvature, $\rho = 1700$ mm, the plate separation, $d = 40$ mm, and the energy resolution ($E/\Delta E$) is 3000. The potential difference between the plates is given by:

$$V_{HE-ESA} = \frac{2dK_5}{\rho q_+}. \quad (2.9)$$

When the foil is not used, $K_5 = K_4$ from Equation 2.7. Otherwise, it can be determined via stopping power calculations mentioned in the previous subsection.

2.5.5 Switching magnet

The switching magnet is the final filter. It further minimizes the background while also allowing the switching between up to nine different detection ports [5]. At present, only the 20° port is used for the GIC. In the future, the remaining ports may lead to detectors with varying entrance window thicknesses for convenient switching between light and heavy isotope analysis.

2.6 Detection systems

After being bent by the switching magnet, the beam passes through a 75 nm thick Si_3N_4 foil window and into the GIC detector, as depicted in Figure 2.10. The window keeps the chamber, which is filled with isobutane gas, isolated from the vacuum of the accelerator and further attenuates the energy of the beam upon entry. As ions enter the GIC, they ionize the gas via multiple scattering and the resulting electron shower is collected on two separate anodes.

The pressure in the gas chamber is set such that all of the ions of interest will

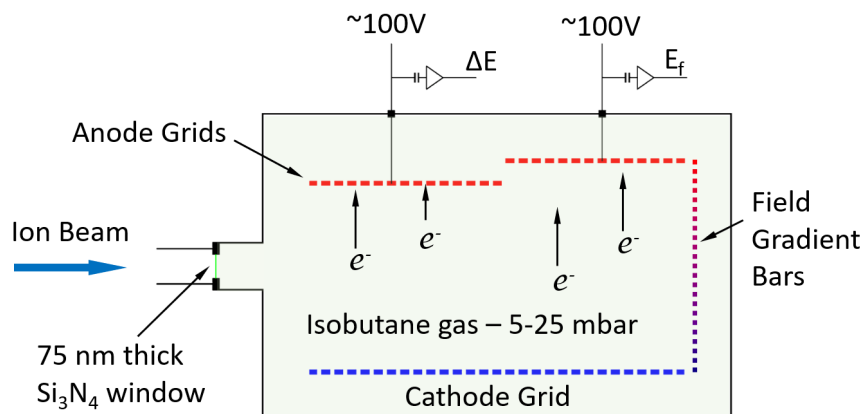


Figure 2.10: In the gas ionization detector GIC, the ion beam enters through a thin foil window and is stopped by the isobutane gas. A particle entering the GIC slows down through collisions with the gas, producing ion-electron pairs. The electrons, which are more mobile than the ions, are collected at the anode grids in amounts proportional to the energy loss of the particle that generated them.

be stopped in the gas before reaching the end of the second anode. The requisite pressures for various isotopes are as described by the operation manual prepared by HVEE. Some other labs (for example, DREAMS which uses a 4 anode GIC for

extra discrimination) use SRIM to determine a suitable pressure and predict the expected energy signature. This is of particular use when pioneering new isotope capabilities.

Collisions with the isobutane gas produce electron and positive-ion pairs.

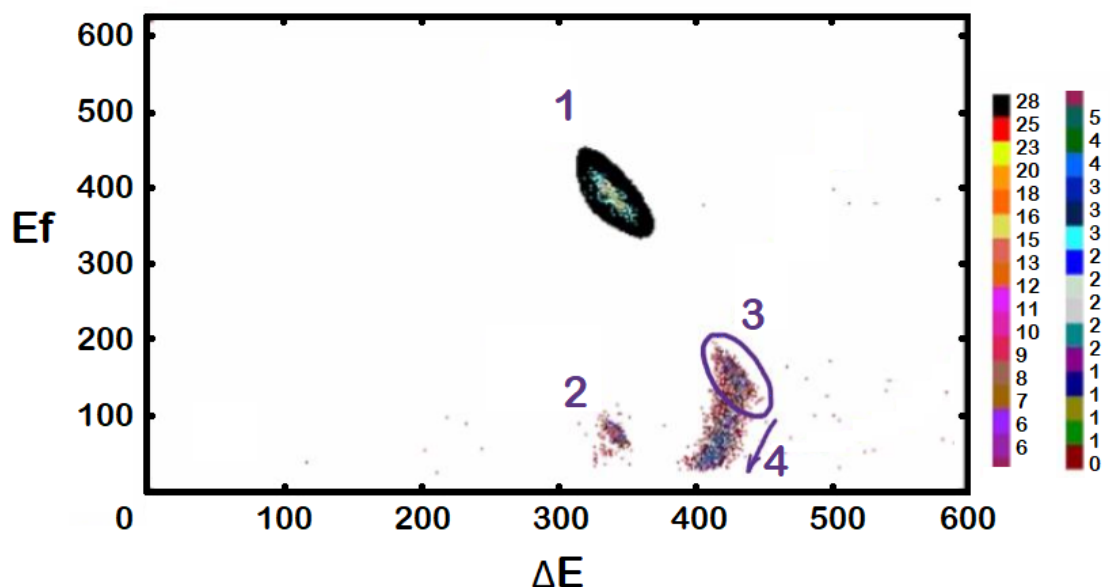


Figure 2.11: A sample $\Delta E/E_f$ 2D energy spectrum generated by the GIC for ^{10}Be , using HVEE’s MPANT software. Both axes are binned into 1024 channels (only channels 600 by 600 are shown for viewing convenience). The black background represents the region of interest corresponding to the characteristic energy signature exhibited by the species of interest. Data points within this region are counted while the rest are disregarded. Numbered features are described in the text.

Due to their higher mass, the positive ions have low mobility and are quickly neutralized by the gas. The electrons are quickly accelerated towards, and collected by, the positively biased anodes. The number of electrons collected at each anode corresponds to the energy lost by the incoming ions.

The plot in Figure 2.11 shows a sample energy spectrum taken from the experiment with ^{10}Be detailed in Chapter 5.10. In this case, the isobutane pressure was 24 mBar, the highest for all isotopes presently measured at Lalonde AMS. The energy measured on the first anode is ΔE and the energy measured on the final anode is E_f . Using HVEE’s proprietary software, one can delineate a region of interest (ROI), denoted as the black background. The program considers only those particle signatures that fall within the ROI when counting the incoming rare isotope ions. Particles with energy signatures outside of this region are considered part of the background

- either internally scattered ions that somehow make it into the detector or external cosmic rays that penetrate the chamber - and are excluded.

The individual features in Figure 2.11 are as follows:

1. **$^{10}\text{Be}^{4+}$ ions:** $^{10}\text{BeO}^-$ stripped to $^{10}\text{Be}^{2+}$ in the accelerator, then stripped to $^{10}\text{Be}^{4+}$ after the degrader foil.
2. **$^9\text{Be}^{4+}$ ions:** $^9\text{BeOH}^-$ stripped to $^9\text{BeH}^{2+}$ in the accelerator, then stripped to $^9\text{Be}^{4+}$ after the degrader foil.
3. **$^{10}\text{B}^{4+}$ ions:** $^{10}\text{BO}^-$ stripped to $^{10}\text{B}^{2+}$ in the accelerator, then stripped to $^{10}\text{B}^{4+}$ after the degrader foil.
4. **$^{10}\text{B}^{4+}$ ions:** $^{10}\text{BO}^-$ stripped to $^{10}\text{B}^{2+}$ in the accelerator, then stripped to $^{10}\text{B}^{4+}$ after the degrader foil but suffering scattering from ESA plates to have a lower energy continuum.

The rare isotope is counted one by one and a ratio of rare to abundant isotope (measured earlier in the movable Faraday cup chamber) is reported by the software. This ratio is used for determining the concentration of the rare isotope in the sample. In some cases (i.e. ^{12}C), the age of the sample material can be inferred from this value. Samples are run together with a blank and a known standard to perform background subtraction and correct for fractionation effects that may have occurred during the measurement process. Such calculations, while critical to AMS, are beyond the scope of this work.

2.7 ^{14}C and ^{10}Be AMS

To prepare the reader for the experiments conducted in Sections 5.8 and 5.10, here follows a brief review of how the above-described systems are used to analyze ^{14}C and ^{10}Be at Lalonde AMS.

Figure 2.12 details a typical ^{14}C measurement setup. The negative ions are emitted from the ion source, suppressing ^{14}N , which does not form stable negative ions. The ions passed through energy and momentum filtration on the low energy side of the accelerator. The three isotopes of carbon are sequentially injected into

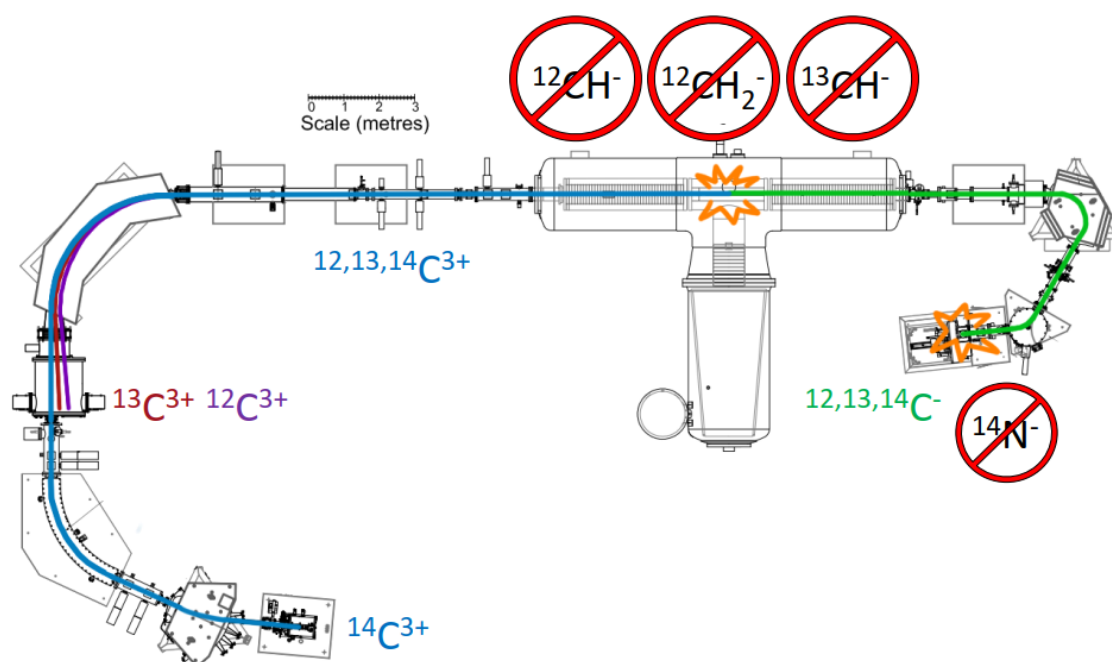


Figure 2.12: Isobaric interferences are suppressed in the ion source and accelerator stripping canal. ^{13}C and ^{12}C are collected in offset Faraday cups. ^{14}C is collected in the GIC.

the accelerator via the bouncer magnet and accelerated by a terminal voltage of 2.5 MV. In the stripping canal, the ions are stripped of electrons with the 3+ charge state being the dominant species [42]. Here, molecular isobars are suppressed. The high energy magnet is tuned to allow $^{14}\text{C}^{3+}$ down the reference path to the GIC. $^{12}\text{C}^{3+}$ and $^{13}\text{C}^{3+}$ are measured in the high-energy offset Faraday cups.

Figure 2.13 provides a simplified drawing of how a ^{10}Be AMS measurement is conducted. Beryllium oxide has a better sputtering efficiency than atomic beryllium [20], so the oxide is frequently the species of choice when performing AMS studies on beryllium. ^{10}Be beta decays into ^{10}B ; therefore, ^{10}B is an unavoidable isobar in the sample. It readily forms oxides which also form negative ions. Molecular interferences are suppressed in the stripping canal. The terminal voltage is set to 3.0 MV resulting in the 2+ charge state as the dominant species. $^9\text{Be}^{2+}$ is measured in one of the high-energy offset Faraday cups. Both $^{10}\text{B}^{2+}$ and $^{10}\text{Be}^{2+}$ are guided by the magnet to the rare isotope path where they encounter the degrader foil. Within the foil, they are stripped to a variety of charge states and lose energy proportional to the square of their proton number. The high-energy ESA is tuned to the expected energy and charge state of $^{10}\text{Be}^{4+}$, suppressing but not eliminating the $^{10}\text{B}^{4+}$. Final

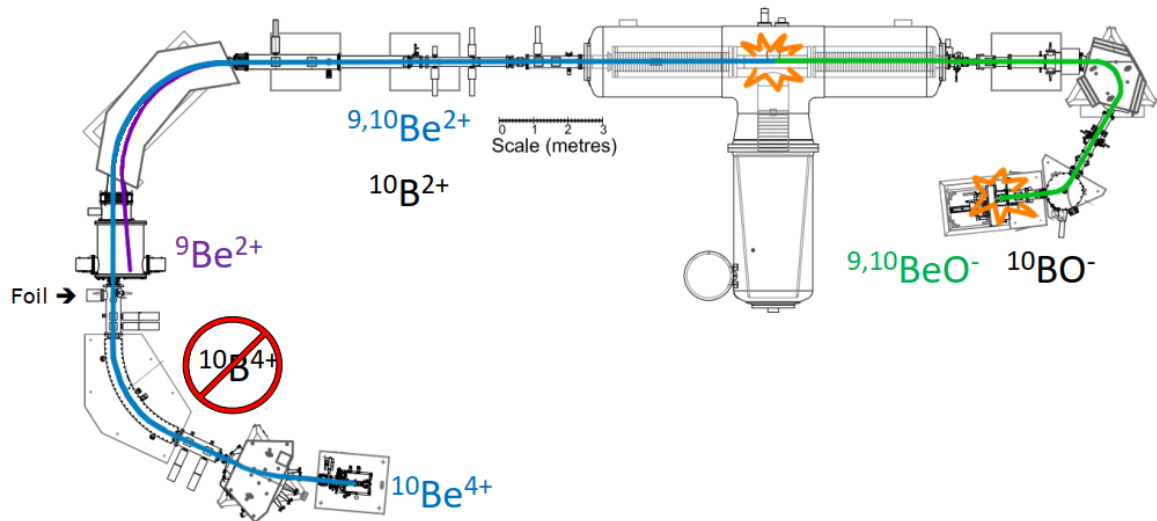


Figure 2.13: Beryllium oxide is emitted from the ion source, stripped once in the accelerator stripping canal and a second time in the degrader foil. ^{10}Be is separated from ^{10}B by differential energy loss in the degrader foil.

separation of scattered species is achieved by examining the energy signature within the GIC as detailed in Figure 2.11.

Chapter 3

Theory

3.1 Ionization and Sputtering

3.1.1 Positive ionization

The first ionization occurs when cesium atoms spray from holes in the shroud onto a hot molybdenum ionizer and become positively charged. The ionizer is estimated to be heated between 1200 and 1400 K. According to a quick Lorentz-2E plot absent of space charges, the raw electric field strength near the surface of the ionizer, as shown in Figure 3.1, is about $7\text{-}10 \times 10^4$ V/m.

According to Kaminsky's *Atomic and ionic impact phenomena on metal sur-*

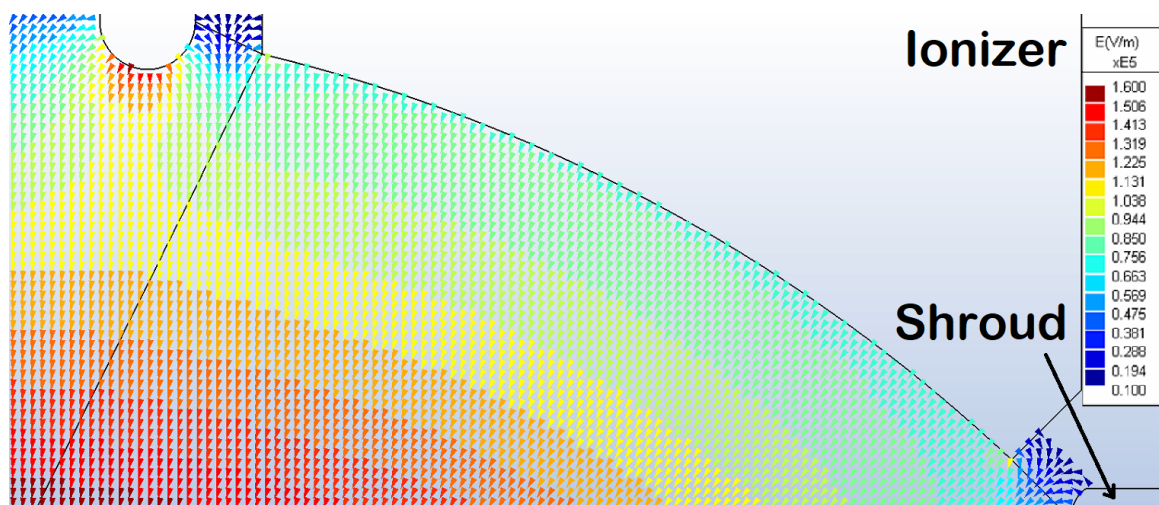


Figure 3.1: A plot in Lorentz-2E of the electric field strength near the ionizer surface.

faces [46], when atoms of first ionization potential, eI , impinge on a metal surface of

work function, $e\phi$, and temperature, T , the degree of ionization, α , which represents the ratio of ionized vs neutral particles, N_{ion}/N_{atom} , leaving the surface, is given by the Saha-Langmuir equation:

$$\alpha_+ \propto \frac{g_+}{g_0} \exp \left[\frac{e(\phi - I)}{kT} \right] \exp \left[\frac{e(k_{coulomb} q_e \varepsilon)^{\frac{1}{2}}}{kT} \right], \quad (3.1)$$

where g_+/g_0 represents the statistical weights for the ions/atoms which is 1/2 for alkali metals. k and $k_{coulomb}$ are the Boltzmann and Coulomb constants respectively. e is the electron unit of charge to ensure the numerator is in units of eV. ε is the electric field strength (in V/m) and q_e is the electron charge (C). Corrections for excited states, reflection coefficients, and electric field strengths above 10^6 V/m are found in the text [46], but are neglected in this discussion. The second exponential is referred to as the Schottky term which accounts for the presence of an external electric field. When the exponential arguments are combined, the Schottky term can make the difference between the argument being positive or negative resulting in either a high or low efficiency mode.

The ionization efficiency, β , is the fraction of the impingent atoms that leave the surface in an ionized state. It is given by:

$$\beta = \frac{\alpha}{1 + \alpha}. \quad (3.2)$$

Table 3.1 gives the work functions of various surfaces as well as the first ionization potentials (relevant for positive ionization) and electron affinities (relevant for negative ionization) of common species of interest. If one considers the ionization of alkali metals as they impinge on the molybdenum ionizer, like the one used at Lalonde AMS, only the first ionization potentials of cesium, rubidium, and potassium are lower than the work function of molybdenum. This ensures a positive argument in the first exponential of equation 3.1, resulting in a high efficiency mode, even before the Schottky modifier. When an electric field of 10^5 V/m is applied - like the one shown in Figure 3.1 - the Schottky term adds a small 0.012 eV to the $e(\phi - I)$ argument. Thus, at the typical field strengths used in the ion source, the Schottky term plays a minimal role.

Equation 3.1 is only valid above a threshold temperature (about 1000-1200 K)

Element/ Species	Electron Affinity [eV]	First Ionization Potential [eV]	Work Function [eV]	Ref
Be	0.29099(10)			[47]
BeO	2.1741(19)			[48]
Al	0.43283(5)			[49]
I	3.059037(10)			[50]
C ₂	3.269(6)			[51]
C	1.262119(20)	11.2602880(11)		[52, 53]
Li		5.391719(4)		[54]
Na		5.139076(4)		[54]
K		4.340663(9)		[54]
Rb		4.1771266(4)		[54]
Cs		3.89390572743(17)	2.14(5)	[55, 56]
Mo			4.60(15)	[57]
Cesiated W*			1.3+	[58]

Table 3.1: The relevant first ionization potentials and electron affinities of various elements and molecules from the literature are presented. Work functions relevant to the ion source surfaces are also present. As an example, 3.269(6) eV means 3.269 ± 0.006 eV

* Chou et. al. calculated that the minimum work function of cesiated tungsten could reach nearly as low as 1.3 eV depending on the thickness of cesium deposited on its surface.

that differs for each surface. At surface temperatures below this threshold, adsorption processes dominate, subsequently lowering the work function and further suppressing ionization [46]. Nevertheless, in the range of 1200-1400K that is the estimated temperature used in the molybdenum ionizer at Lalonde AMS, above the adsorption threshold, the theoretical ionization efficiency is already above 90% according to the Saha-Langmuir Equation. This implies there is minimal room for improvement of the cesium ionization efficiency.

One final note is that the first ionization potential of carbon is much greater than the work function of molybdenum. Thus, the positive ionization and subsequent acceleration of neutral carbon impinging on the surface of the ionizer is unlikely.

3.1.2 Negative ionization

The production of negative ions is a staple in ion source operation for AMS. Kaminsky gives an analogous degree of ionization equation for negative ionization:

$$\alpha_- \propto A \exp \left[\frac{e(S - \phi)}{kT} \right] \exp \left[\frac{e(k_{coulomb} q_e \varepsilon)^{\frac{1}{2}}}{kT} \right], \quad (3.3)$$

where A is a constant representing the ratio of the statistical weights of negative ion and neutral atom species. eS is the electron affinity of the incident atoms which, combined with the Schottky term, must exceed the work function of the surface, $e\phi$, to be in a high ionization efficiency mode.

3.1.3 Sputter yields

The formalism of negative ionization described in the previous section alone is not adequate to describe the extraction efficiency in the ion source because it does not consider momentum-transfer collisions. Additionally, the work function of the surface is subject to change in the presence of cesium bombardment. Krohn [59] observed that the yield of sputtered negative ions from various metal targets increased as neutral Cs was sprayed onto the target surface while simultaneously bombarding a sample with Cs^+ . The yields were well above those predicted by the Saha-Langmuir equation. It appears that a thin layer of cesium on metal surfaces can reduce the effective work function below that of both cesium and the metal on which it is coated, thus facilitating improved ionization conditions [60]. Chou et. al. used density functional theory to model the work function as a function of cesium coverage (in atoms/cm²) for various single-element transition metal surfaces. The lowest work function achieved was cesiated tungsten which reached nearly as low as 1.3 eV. This effect of lowering the work function would facilitate better negative ion efficiencies.

Conventional wisdom concerning the cesium-sputter ion source simplifies the interaction into two processes - first cesium collides with the surface and liberates bound atoms, molecules, and clusters of sample material. The ionizing interaction with the surface quickly follows as they leave the target medium. As described by

Litherland: “Electrons then tunnel back and forth from the ‘solid’ surface to the receding sputtered atom finally leaving some of the atoms converted into anions” [25].

Pachuta and Cooks [61] wrote an extensive review of sputtering and ionization as relevant for Secondary Ion Mass Spectrometry (SIMS), illustrating numerous models of sputtering. While some general observations of atomic sputtering yields were presented, secondary ion emission is much less well understood. An observation from atomic sputtering that may be useful in ionic studies, but more specifically as an initial parameter for simulations in this work, is that the sputtered ion energies tend to be about 1-10 eV on average, increasing weakly with primary ion energy.

Due to the complexity and lack of quantitative theories of ion sputter yields, further theoretical considerations are neglected. In this work, the electrodynamics of ion beams are considered taking for granted the empirically observed ion currents observed during routine operation of the ion source at Lalonde AMS.

3.2 Beam Kinetics

Unless otherwise stated, the beam kinetics described here are paraphrased from Banford’s *The transport of charged particle beams* [62].

3.2.1 Phase Space

In order to know the kinetics of a beam, one must know the position and direction of travel for each of the particles. The particle is specified by a six dimensional vector (x, y, z, p_x, p_y, p_z) of position and momentum data. The six dimensional space through which this vector propagates is referred to as phase space. [62]

When considering a cylindrically symmetric beam propagating along the y-axis, as is the case in this work, one can simplify this vector to two dimensions, r and r' where r is the radius and r' is the angle the ray makes with the axis. Lorentz-2E instead uses x and x' to denote the same thing - this notation will be used moving forward.

3.2.2 Emittance

The formalism of RMS emittance used by Lorentz-2E is based on the contents of Chapter 3 of Humphries' *Charged Particle Beams* [63] but modified to include a beam current weighting within the summation of the rays.

$$\varepsilon_{RMS} = \sqrt{\langle x^2 \rangle \langle x'^2 \rangle - \langle xx' \rangle^2} \quad (3.4)$$

Where:

$$\begin{aligned} \langle x^2 \rangle &= \sum \frac{I_i}{I_{total}} (x_i - x_c)^2 \\ \langle x'^2 \rangle &= \sum \frac{I_i}{I_{total}} (x'_i - x'_c)^2 \\ \langle xx' \rangle &= \sum \frac{I_i}{I_{total}} (x_i - x_c) (x'_i - x'_c) \end{aligned}$$

x_i and x'_i are the radial displacement and angular deviation relative to the axis of symmetry respectively. Typically, these equations would use the x_i and x'_i for each particle contained within a beam. However, because Lorentz-2E uses rays carrying a fixed current representing many particles per ray, these equations include the current weighting factor of I_i/I_{total} that would not be present in these equations for the particulate case. I_i is the current carried by the i 'th ray where I_{total} is the total current carried by the beam.

x_c and x'_c represents the centroid of the radial and angular distributions respectively which are both 0 in the case of rotational symmetry - as is the case in simulations performed in this work.

The Twiss (or transport) parameters, which define the beam ellipse in phase

space, are given by the following

$$\begin{aligned}\alpha &= -\frac{\langle xx' \rangle}{\varepsilon} \\ \beta &= \frac{\langle x^2 \rangle}{\varepsilon} \\ \gamma &= \frac{\langle x'^2 \rangle}{\varepsilon}.\end{aligned}$$

Using these, a phase space ellipse can be drawn according to the following equation:

$$\gamma x^2 + 2\alpha x x' + \beta x'^2 = \varepsilon. \quad (3.5)$$

When $\alpha = 0$, the beam is at its waist. The emittance represents the area of this ellipse in phase space divided by π . Provided particles do not collide with each other and are not undergoing acceleration, the emittance remains constant during beam transport. The shape of the ellipse, however, will change as the beam undergoes drifts and lens transformations.

3.2.3 Acceptance

An analogous quantity to emittance is that of acceptance. The acceptance refers to the phase space area within which an ion's radial displacement and angular divergence are suitable for transmission through the beam-line. Ideally, the phase space of the emitted beam should fit within this area for maximal transmission. One should also ensure any and all changes to this shape by ion-optics transformations keep the beam confined within this area. Unfortunately, the acceptance of the 3 MV accelerator at Lalonde AMS has not been specified. In lieu of this, minimizing the emittance via simulation is the best strategy for ensuring a maximum number of extracted ions reach the detector.

3.3 Child's Law of limited emission

Lorentz-2E makes use of the Child-Langmuir Law of limited emission to estimate an upper bound on ion emission in a given field and geometry [64]. The

equation is given by:

$$J = -\frac{4\varepsilon_0}{9} \sqrt{\frac{2q}{m}} \frac{V^{\frac{3}{2}}}{d^2} \quad (3.6)$$

Derived initially from the Poisson equation by Child [65] and further expanded by Langmuir [66], Equation 3.6 describes the maximum allowed current density, J , of ions of mass, m , and charge q , initially at rest travelling across an evacuated gap, d , between two infinite parallel plates with a potential difference, V . ε_0 is the vacuum permittivity.

While the geometries simulated in this thesis are not infinite planes, this equation provides an approximate upper bound for the emission of ions from various surfaces in the ion source.

3.4 Runge-Kutta Algorithm

To facilitate the calculation of ODEs on a computer, which uses discrete numbers, Lorentz-2E uses the 4th order Runge-Kutta (RK4) algorithm to approximate the trajectories of the ions. Provided a suitably small time-step is chosen, the program will iterate each step, recalculating the ion dynamics based on the fields/forces present at that point.

The RK4 algorithm is applied in the following steps:

$$\begin{aligned} k_1 &= hf'(x_n, y_n) \\ k_2 &= hf'(x_n + \frac{h}{2}, y_n + \frac{k_1}{2}) \\ k_3 &= hf'(x_n + \frac{h}{2}, y_n + \frac{k_2}{2}) \\ k_4 &= hf'(x_n + h, y_n + k_3) \end{aligned}$$

Supposing one knows the initial position (x_n, y_n) as well as the $(\frac{dy}{dt})$ derivative at that point, denoted by $f'(x_n, y_n)$, one can choose to step along x by a fixed amount, h :

1. The RK4 method expands on Euler's Method by first calculating the position of y_{n+1} at $x_{n+1} = x_n + h$ using the slope, $f'(x_n, y_n)$, times the step size. The

result is k_1 .

2. k_2 is then y_{n+1} re-evaluated using the derivative at the halfway point of $(x_n + \frac{h}{2}, y_n + \frac{k_1}{2})$

3. This is again repeated to find k_3 .

4. Finally, k_4 is y_{n+1} found using the slope evaluated at the end point, $(x_n + h, y_n + k_3)$.

5. At the end, the average of the four is computed, giving following:

$$y_{n+1} = y_n + \frac{1}{6} (k_1 + 2k_2 + 2k_3 + k_4) + O(h^5) \quad (3.7)$$

Lorentz-2E is equipped with additional, higher order, ODE solvers, including the RK5 method which can increase or decrease the time step density depending the local variation in the solution. For the purposes of this work, the RK4 method with a suitably low time step was sufficient. Additional details may be found in the Particle Trajectory Guide for Lorentz-2E [64].

Chapter 4

Rijke Automated Programming Interface and the Functionality and Optimization of Lorentz-2E

4.1 Overview

Lorentz-2E is an electromagnetic field and ion trajectory simulation software produced by Integrated Engineering Software (IES). The program allows the user to use either the finite element method (FEM) or boundary element method (BEM) to determine the electric potential generated user-defined charge distributions. The electric potential and user-defined emission settings of the ions are used to determine the dynamics of those ions. The program then recalculates the electric potential incorporating the charge present in the ion beams and re-iterates the emission and trajectory calculations until a steady state or user-defined termination state is achieved. Due to the complexity of this endeavour, automation of the setup and result logging was essential.

Rijke is the name given to the API written by this author in Microsoft Excel ® and Microsoft Excel Visual Basic for Applications (VBA) ®. It is named after Dr. Pieter Rijke who oversaw the education of Dr. Hendrik Lorentz. The Rijke software uses accessor functions (coded functions in one software that communicate and direct the operation of another) made available by IES for VBA to oversee and direct simulations in Lorentz-2E from start to finish and output relevant data in a

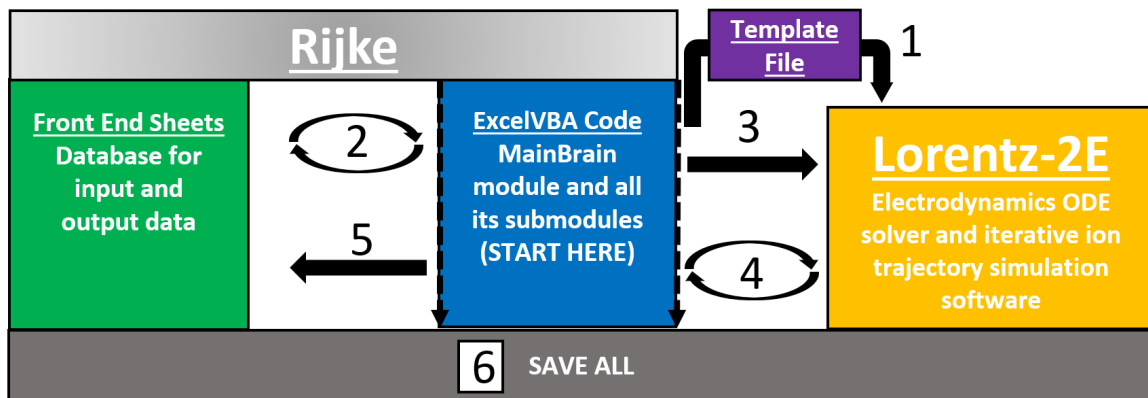


Figure 4.1: A simple block diagram illustrating the Rijke-Lorentz-2E program interface. Steps are numbered. Straight arrows represent unidirectional commands while circular arrows denote an exchange of information between software components.

manageable fashion.

Figure 4.1 gives the basic layout of the Rijke-Lorentz-2E interconnection. Rijke is housed within a single macro-enabled Microsoft Excel document. The entire operation can be represented by three columns: the front end sheets that house the input and output data, the Lorentz-2E simulation software package for executing ion optics and trajectory simulation solvers, and the Excel VBA code, “MainBrain,” controlling the flow of information between the other two as well as computing all requisite calculations to ensure simulations are run according to the user’s specifications. Once the Template File is loaded (Arrow 1, Figure 4.1), MainBrain is capable of iterating Lorentz-2E simulations (Arrows 2, 3, 4, and 5) through a range of setup parameters stored in the Excel sheet.

Section 4.2 gives a more detailed high-level overview of the Rijke-Lorentz-2E program interface. This is followed by a discussion in Section 4.3 of the MainBrain module and its ability to initiate, operate, and complete an entire self-contained simulation from start to finish. A brief discussion of batch processing follows in Section 4.4, whereby the MainBrain module is used sequentially, interspersed with changes to input parameters, to run autonomous series of simulations. This chapter then concludes (Section 4.5) with a review of important parameters and convergence criteria for the operation and reliability of Lorentz-2E simulations. A number of critical settings are mentioned here that give deeper insight into the operation of Lorentz-2E and how it is managed by Rijke.

4.1.1 Important nomenclature

Before further details are provided, some important nomenclature is required for consistency. A **workbook** is a single instance of Microsoft Excel open at any time. The workbook is organized into various **sheets** (MAIN, EMITTERS, etc) that house cells full of data relevant to their function. They can be accessed via tabs at the bottom of the screen. When referring to the numerous self-contained blocks of the underlying VBA code, the word **module** will be used. Due to the somewhat complex interconnection between the sheets and modules that, combined, make up the whole of Rijke, this distinction should clarify which is being described. The entire process begins when the user clicks the “Run” button on the MAIN sheet which calls the MainBrain module.

In addition to this, Lorentz-2E has two modes of operation: Electric and Trajectory. **Electric mode** includes everything relevant to generating and calculating the electric potential distribution and **Trajectory mode** includes everything relevant to generating charged particles and simulating their transport. To set parameters, one must be in the appropriate mode.

4.2 Rijke: high-level description

What follows is a detailed, high-level description of the Rijke API built for this doctoral research. Figure 4.2 gives a flow chart representation of how Rijke is operated. Rijke is composed of two pillars:

1. The “front-end” database sheets: The MAIN sheet contains most of the procedural information on how the simulation will run. Some of these sheets (SO-110C, SO-110B, SO-110A, DREAMS-LMS, ELECTRIC, and EMITTERS) behave as databases of input parameters containing all of the relevant geometries and physics for various ion sources to be run in Lorentz-2E. The remaining sheets (RESULTS, LOG, CsANALYSIS, CExitANALYSIS, CsBATCH, and CExitBATCH) are reserved for outputting data from Lorentz-2E in a format that is convenient for graphing and analysis.

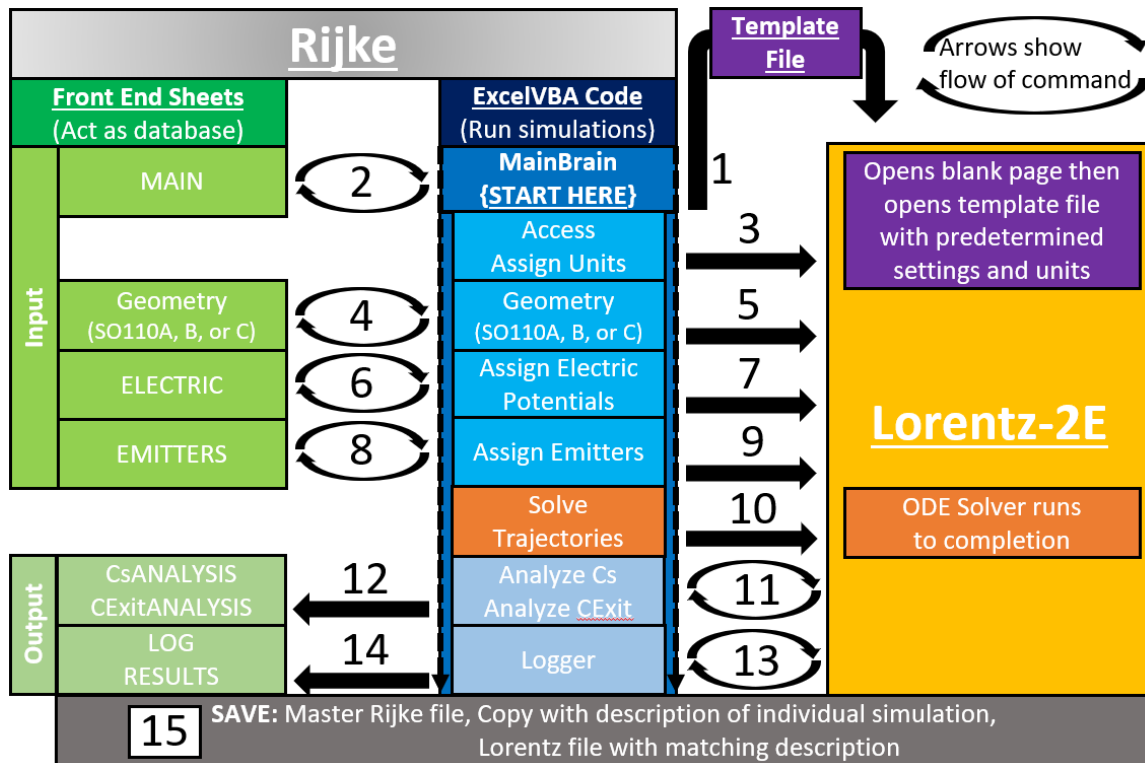


Figure 4.2: An flow chart illustrating the flow of command starting with the Main-Brain module from start to end of a complete simulation. Circular arrows indicate an exchange of information while solid arrows imply a unidirectional command or deposit of information and are numbered in sequential order. Green tiles represent the input and output database sheets, violet the template file, and orange the independent operation of Lorentz-2E

2. The underlying Excel VBA code: The MainBrain module communicates between the input database sheets and Lorentz-2E, executing commands and calculations to generate the requisite parameters. Once set up, the MainBrain initiates the Solve Trajectories protocol at which point Lorentz-2E independently runs its built in ODE solvers to simulate the behaviour of ions within the ion source. Lorentz-2E first calculates the electric fields present and then solves for the trajectories of the ions. This process is iterated repeatedly until a termination condition is met. Upon completion, control is returned to the MainBrain and the flow of information reverses. Data from the completed simulation are extracted and stored in a convenient format in the output sheets, ready for analysis. At the end, the master file, a copy with an appropriate description of the simulation in its file name, and an identically named Lorentz-2E file are saved.

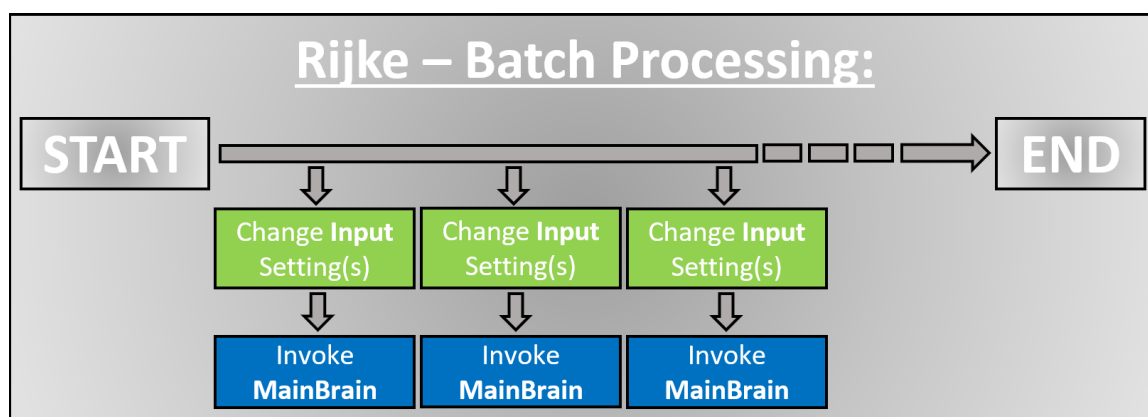


Figure 4.3: A block diagram of how the MainBrain is sequenced for automated batches of simulations.

The MainBrain module (coupled with the database sheets) contains all of the commands to initiate, run, and post-process an entire simulation from start to finish. As illustrated in Figure 4.3, a Batch code can be run at a higher level, which sequentially sets and changes input parameters according to the user’s needs and invokes the MainBrain module each time to run the self-contained simulation for each setting. Autonomous batches can conveniently be run unattended for several days and nights as needed.

While the flow charts give a simplified overview, the following chapter describes the individual sheets and modules in greater detail for a prospective user.

4.3 MainBrain module

Clicking the “Run” button on the MAIN sheet calls the “MainBrain” module. This is the central module of the program that calls on the many sub-modules to set-up, run, and analyze an entire simulation in one self-contained routine. This conveniently allows the Main Brain to be called by an overarching batch code which will be described later in Section 4.4. The sub-modules were created to make the code more manageable by compartmentalizing similar functions to be called by the MainBrain module and to minimize redundant code. Communicating between modules is achieved using global variables and function arguments.

4.3.1 Globals

Before the MainBrain module begins, the global variables are initialized. Most of these are identifiers for important segments on the ion source geometry (e.g. recording where the cesium ions and negative ions are emitted). Since each major component or cluster of connected components (like the shroud, ionizer, and ionizer baseplate) are contained in single modules, any segments drawn to connect these components must be handled using global coordinates. These global variables eliminate issues of scope when communicating between modules.

4.3.2 Preamble

Once begun, the MainBrain module runs the “Application.DisplayAlerts = False” command. Because the Lorentz-2E simulation takes an amount of time to implement functions that are above the typical time frames expected by Excel, it is inclined to generate pop ups informing the user of the supposed anomaly. This line of code disables such pop-ups because they halt the progression of the program.

Following this, the program initializes an instance of Lorentz-2E or accesses an existing one. After a number of variable declarations and initializations, the MainBrain logs the starting time. Once the entire program runs, the end time is logged and the total elapsed time is presented to the user. In case there is already an existing instance of Lorentz-2E (for example during a batch of simulations), a command deletes all existing geometry and trajectory solutions from a previous run.

At this point, the MainBrain module acquires the user-specified simulation description from the MAIN sheet. It also formats the starting time into string format and combines that with the user description to make the file name. By using the start time specified to the nearest second, accidental overwriting of existing files is avoided. Simulations always take more than a second, so each file name should be unique. For additional tracking during development, the file name also includes the version of Rijke that was used as well as which ion source model was simulated. Each time the program is run, it saves a copy of the entire workbook and the resulting Lorentz-2E file with the same name to their respective folders. The file path for those folders is defined by the user in the MAIN sheet.

4.3.3 The template file and setting units

While the API and the compilation of functions available is extensive, there are a number of parameters in Lorentz-2E that do not have associated accessor functions. As a work-around, Rijke opens a pre-generated Lorentz-2E template file with these parameters already set. Most of them affect the solver setup for both the electric field and the trajectory solvers. Details on those functions will be deferred to Section 4.3.8. The parts that are relevant now are:

1. In Electric mode of Lorentz-2E, the global geometry configuration can be set. As seen in Figure 4.4, the y-axis ($x = 0$) is set to be the axis of polar symmetry.
2. Figure 4.5 shows the General tab of the Trajectory mode Solver Setup. The ion trajectory rays are set to pass through the axis of symmetry and the intermediate beams for space charge iteration are saved before launching the next set. Allowing rays to cross over the axis (rather than reflecting them) makes tracking overfocused rays more intuitive during data analysis. Saving the simulated rays in each iteration allows the user to examine the behaviour of the beam across all iterations as they approach a steady state distribution (or not) and to track any anomalous behaviours that may have skewed the results.

4.3.4 Geometry

The units are set to millimetres via an accessor function. Then the program checks the MAIN sheet to see which source model is to be simulated. At present, there exists three viable options: SO-110A, SO-110B, and SO-110C. Depending on which model is chosen, the program will call a series of submodules to build the pieces individually. Each submodule is named denoting the source to which it corresponds and is responsible for building the geometry of a single component or cluster of components. For example the ionizer, shroud, and ionizer baseplate are built together in a single module because they are all connected physically and share surfaces.

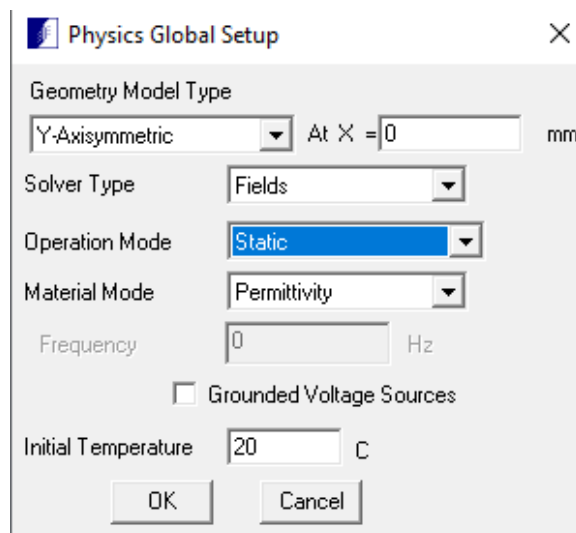


Figure 4.4: Lorentz-2E → Electric Mode → Physics Global Setup. Here the y-axis is set to be the axis of symmetry.

Each of these submodules acquires the necessary dimensions for the various components from either the SO110A, SO110B, or SO110C sheets (note: the omission of the hyphen in the sheet names is intentional so as not to break the code). On each of these sheets, a simplified drawing of each component is presented with labelled dimensions as seen in Figure 4.6. Next to the drawing is a table which compiles all of the dimensions necessary to draw the source in Lorentz-2E. The first column, “Index,” lists the dimensions by their corresponding letter as seen in the diagram. The second column, “Base [mm],” contains the base dimensions provided by the manufacturer in millimetres. The user should never tamper with this column. The third column, “Add [mm],” includes a user-specified modifier that will add or subtract from the base dimension. Above these columns is the “Scale Factor” that, if set to anything other than 1, will scale all components by the same multiplicative factor. The fourth column, “Dimensions [mm],” takes the base dimensions and computes a final dimension specified as follows:

$$\text{Dimensions} = \text{Base} \times \text{Scale Factor} + \text{Add}$$

This fourth column contains the dimensions that are used by the program modules to draw the source in Lorentz-2E. Modifying dimensions without changing them ensures the base dimensions are never overwritten. During batches, the Add or Scale Factor values can be changed incrementally between consecutive simulations. The

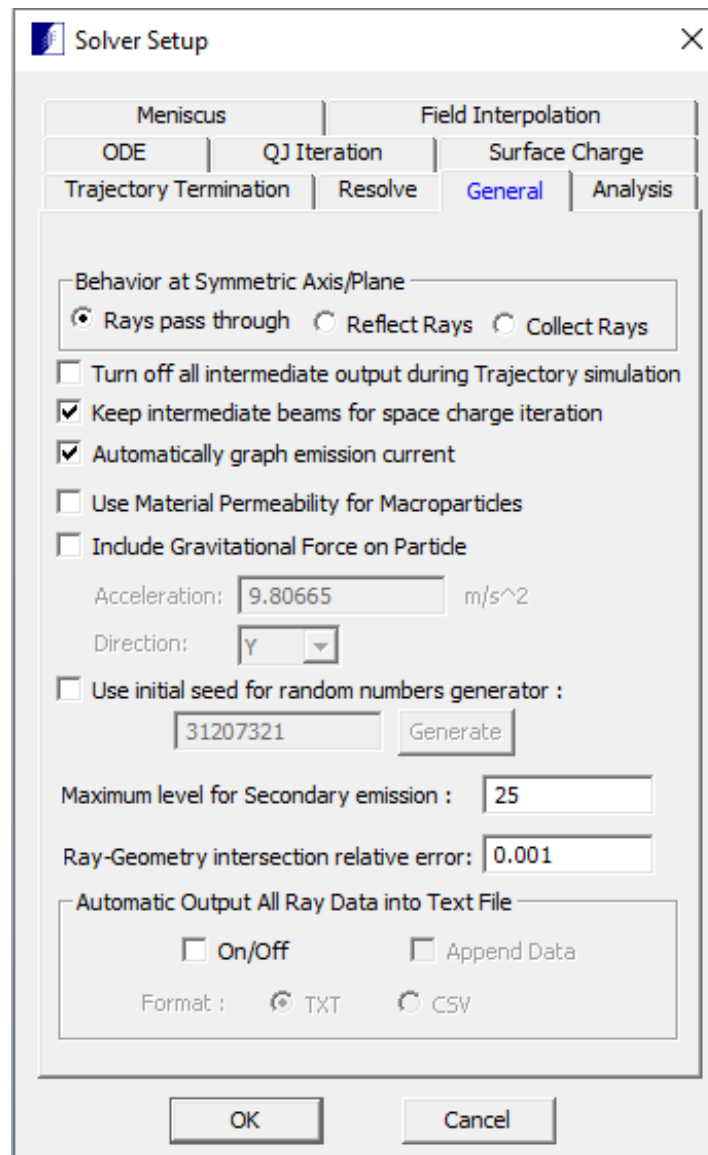


Figure 4.5: Lorentz-2E → Trajectory Mode → Solver Setup → General tab. Here the rays are set to allow crossing of the axis of symmetry. Each intermediate iteration of rays are set to be saved to show the history of the space charge effects from initial to final iterations.

program saves a copy of the entire workbook each time a simulation is run, thus allowing the user to view which modifications were present in a given simulation.

One final setting found in most of these tables is the “Local Y” origin value. It has it’s own “Base [mm],” “Add [mm],” and “Dimensions [mm]” column but does not include a scale factor. The local y-origins, specified on most drawings by a green square, are referenced relative to the global y-origin, which is denoted as a black star highlighted in green on the ionizer drawing. This ensures the correct spacing of components along the axis of symmetry while also allowing this separation to be

	A	B	C	D	E	F	G
9	loni:						
10		Scale Factor 1					
11	Index	Base [mm]	Add [mm]	Dimensions [mm]			
12	R		0	=B12*C\$10+C12			
13	H		0	=B13*C\$10+C13			
14	W		0	=B14*C\$10+C14			
15	D		0	=B15*C\$10+C15			
16	T		0	=B16*C\$10+C16			
17							

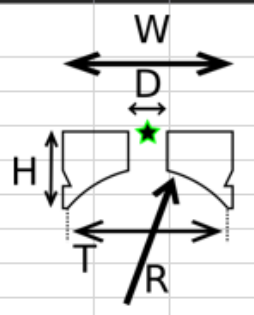


Figure 4.6: An example of the geometry sheet layout for the ionizer. Base dimensions have been redacted to protect intellectual property. Note, detail segments that do not contribute to the electric field distribution in relevant spaces are excluded. The cells under the Dimensions are used by the geometry modules to build the ion source. Their calculation from the Base dimensions is shown and described in the text. Each component of the ion source will have a similar block of dimensions. The star represents the global y-origin. Other components will have a similar point designated as the local-y origin from which to build that piece.

modified. The ionizer drawing contains the global y-origin since this is where the cesium ions will originate and begin the entire sputtering process in the ion source.

Each geometry module begins by acquiring the dimensions and issues a series of commands to build each segment individually. All radial distances are specified with respect to the central axis while all axial dimensions are referenced relative to the local y-origin. The geometry is drawn using accessor functions that specify the start and end points of a straight segment. A simple function was written to determine the centre of curvature of an arc segment using the start and end points as well as the radius of curvature which are more typically known.

Once each component is drawn, it forms a closed two-dimensional shape called a “region.” This region, including all segments that make it up, is assigned as an “object” and given an object name. A region can be assigned to multiple objects. For example, while the segments forming the region specifying the ionizer are assigned to an object labelled “Ionizer,” they are also assigned - along with the segments from the regions specifying the shroud and ionizer base plate - to an object called “IonizerPotential.” Later, that object is assigned a boundary electric potential which will be distributed to all regions, and subsequently all segments that make it up.

An object does not necessarily have to be composed of regions. The single-segment surfaces from which the cesium and negative ions are emitted are assigned

to their own distinct objects as well. Since the object details are stored in memory allocated by Lorentz-2E, they are not limited by the scope of the submodule in which they are defined and can be manipulated by other submodules of Rijke simply by calling the object by name.

At the end of each geometry module, some segment endpoints are assigned to an array of global variables called `Interaction_Segments` which are used to draw the Interaction Region. Their purpose is to contain the finite element mesh which is detailed in Section 4.3.5. For each of the three ion sources, the last geometry module builds the extraction electrode. The identifying number of the last physical segment is assigned to a global variable and the y-position of the exit of this electrode is logged to be assigned as a collector for the negative ion beam. It is at this segment that the negative ion beam profile will be analyzed on its way out of the ion source. By keeping track of the last segment, a for-loop can be used to cycle through them all when assigning segments to be collectors. This will be explained in more detail in Section 4.3.7. This action must be handled using the segment IDs because an accessor function to assign objects to be collectors does not exist at the time of writing.

4.3.5 Extended geometry - the interaction region

Once each component is drawn, the space in between them is closed and divided into three regions (See Figure 4.7):

1. Cesium Region: where cesium ions travel
2. Interaction Region: where cesium and negative ions both travel and interact
3. Extraction Region: where the negative ions travel as they are extracted into the accelerator

Most of the segments drawn in this submodule are not assigned as collectors since they represent fictitious geometries meant only to segregate the space into these three regions. The space is divided this way for the sake of the 2D element mesh to be described in Section 4.3.6. It ensures that a finer density of elements are allocated in the region where cesium and negative ions cross paths to better resolve the space charge interaction. In regions where only a single beam propagates, the

mesh density is relaxed. The density of these elements was adjusted to ensure simulation reproducibility while keeping simulation times manageable. Further details are found in Section 4.5.

The negative ion collector segment mentioned previously is also drawn and

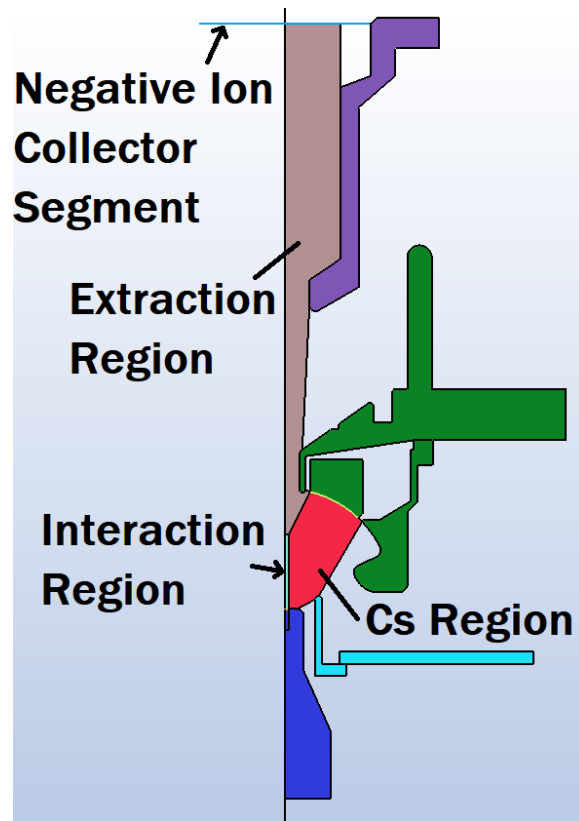


Figure 4.7: The open space in the ion source is broken up into three main regions: the cesium region, the interaction region, and the extraction region. These fictitious boundaries are used later to generate a localized 2D element mesh necessary for space charge simulation.

assigned as a collector in this submodule. The negative ion beam terminates at this segment and its emittance is analyzed. Following this point, the acceleration of the ions is complete and the emittance of the negative ion beam will be maintained as it passes through the conservative ion optics of the low-energy mass spectrometer.

The three regions are assigned as objects and Lorentz-2E is returned to “Electric” mode in preparation for the electric potentials to be set.

4.3.6 Electric Potentials

With the geometry complete, the MainBrain calls the Assign_Electric_Potentials module. This module begins by deleting all existing fields and trajectory solutions

in case any are present. It tells Lorentz-2E to use rotational symmetry about the y-axis for electric field interpretation. The geometry is assumed to be rotated a full 360° about that axis to represent a 3-dimensional model. By taking advantage of this symmetry, a three dimensional problem can be simplified to two dimensions. Depending on the source, the electric field is assigned to the various geometry components as set by the user in the ELECTRIC sheet.

Once electric fields are set, a critical step is to assign boundary elements and finite elements to the appropriate regions of the ion source. These are necessary for ODE solver. Figure 4.8 shows the mesh containing a user-defined number of triangular “finite elements” (also called 2D-elements), which are distributed to various regions. The “boundary elements” (also called 1D-elements) are distributed on surfaces at a user-defined density. This step must occur after the setting of potentials or Lorentz-2E will terminate with errors.

The boundary element method is the faster method for calculating electric

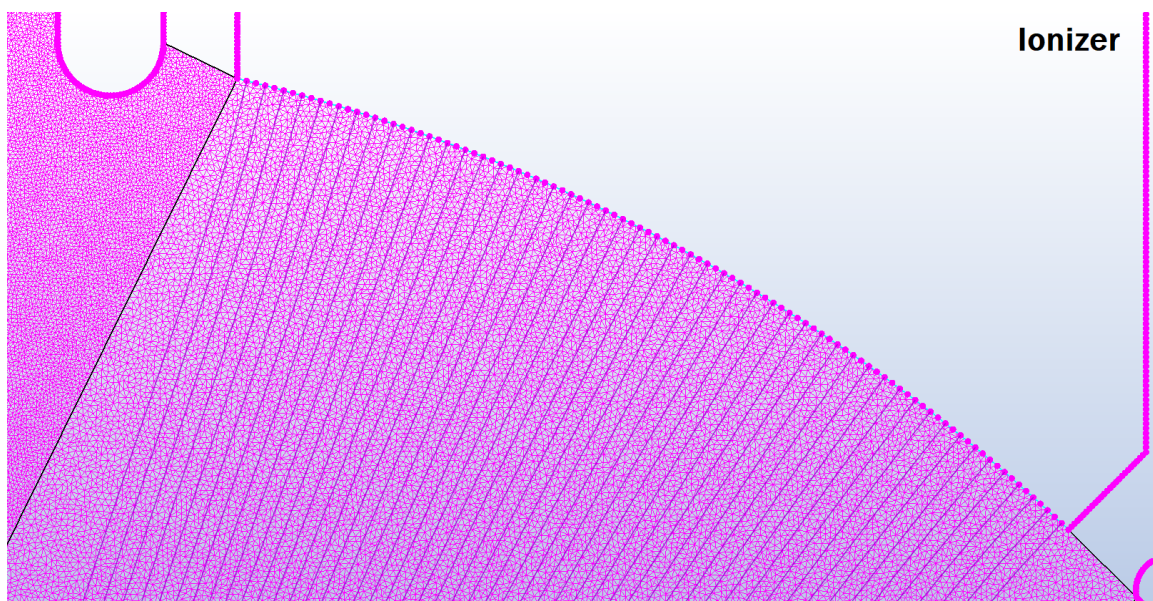


Figure 4.8: A mesh of triangular 2D-elements along with surface 1D-elements are used for the ODE solver. These are shown near the curved surface of the ionizer. The violet lines traversing downward to the left are simulated Cs rays. Ideally, the size of the elements should be smaller than the ray separation for better precision.

potentials generated by surface charge distributions. However, the finite element method is necessary to simulate the space charge deposition. After an iteration where rays of ions are simulated, the charge associated with each ray is represented by adding an appropriate charge to each of the elements that the ray traverses. This

space charge is then included in the electric potential calculation which affects the trajectories of ions in next iteration. This allows the study of space charge effects acting from each beam on the other.

Per recommendation from IES (Dr. D. Craigen, private communication), the size of elements - especially near emitting surfaces - should be smaller than the ray separation of the emitted ions. This allows for more precise calculations of space charge effects on each ray of a beam of ions. This does pose a challenge, however, because the number of finite elements necessary to achieve this is on the order of 10^6 and simulation time scales approximately linearly with the number of 2D elements. This is the second most dominant contributor to simulation time. A detailed discussion of the element density selection is discussed in Section 4.5.

4.3.7 Emitters

With the electric field solution in place, the `AssignEmitters` module is called. This module begins by switching Lorentz-2E to Trajectory mode and writing the details of particles of interest (mass, charge, etc...) into Lorentz-2E. All segments belonging to physical components (ionizer, shroud, etc...) are assigned as collectors. This means that if a simulated ion ray intersects with any of these segments, it will terminate at that intersection and that ray's current will be considered lost. Without this, the rays would pass through those segments as if they were not there. The layout of emitters is standardized on the EMITTERS sheet so that a single function can be used to generate all of the necessary parameters. The module looks on the MAIN sheet to see which ions will be emitted and then passes the location of that ion's parameter information on the EMITTERS sheet to the `GenerateEmitters` function.

The `GenerateEmitters` function behaves as follows:

1. If the ion is positive, emit it from the ionizer surface; else, emit it from the target sample surface
2. Acquire the emitter name at the cell position passed to the function
3. Increment a global variable to indicate how many emitters are generated. This will be used later in Section 4.3.9

4. Generate the emitter on the designated surface and choose a direction. (The user must ensure the ray does not fire backwards)
5. Specify the number of rays to be emitted from this surface. The rays are spaced evenly and are set by default to emit normal to the surface. A real beam would be more complex but this served as an initial approximation.
6. Set the emission regime to either assigned current (each ray carries a fraction of the total assigned current) or Child's Law (each ray emits the maximum amount of current approximated by Child's Law using the local electric field density).
7. If in Child's Law mode, set a small offset distance from the emitted surface for the particle to be emitted - otherwise the calculated current will be infinite and the simulation will crash
8. Set the colour of the ray to distinguish it visually from the others
9. Set what kind of ion the ray will represent (i.e. Cs^+ , $^{12}\text{C}^-$, etc..)
10. Set the initial energy of the ion and the initial temperature of the surface from which it is emitted
11. Finally, assign the rays to deposit their charge so that the mutual space charge interaction between rays will be simulated. There was originally no accessor function for this and no way to address it in the template file. Without this function, one would have to stop the program here, and manually check the box in the emitter's settings before proceeding with the simulation. Thus, for the simulations to be completely autonomous, correspondence with IES was critical in developing this function. This author is grateful for their support in this endeavour.

4.3.8 Trajectory solver

Once everything is set up, the trajectory solver is invoked and control is given fully to Lorentz-2E to conduct the simulation. Lorentz-2E begins by drawing the geometry and assigning all parameters as described above. It then solves the electric

field followed by launching the rays. As it is set up, cesium is launched first and then the negative ion beams are next. The rays in a given iteration do not interact with each other. They only interact with the electric field that is present. Thus, the first iteration is an image of how each beam would behave in the absence of space charge. Once all rays have terminated at a collector or travelled the maximum number of time-steps without collision (this should not happen), Lorentz-2E re-solves the electric field but this time takes into account the charge that is deposited in the finite elements. The rays are re-emitted into a new landscape of fields and forces, informed by previous iterations.

Template File Revisited

First introduced in Section 4.3.3, the template file set a number of parameters that are important for the solver in both Electric and Trajectory modes (these are two separate solvers that run consecutively). These parameters do not have accessor functions and must be set in a template file that was opened before any geometry was drawn.

The Electric solver setup is adjusted as seen in Figure 4.9. The method

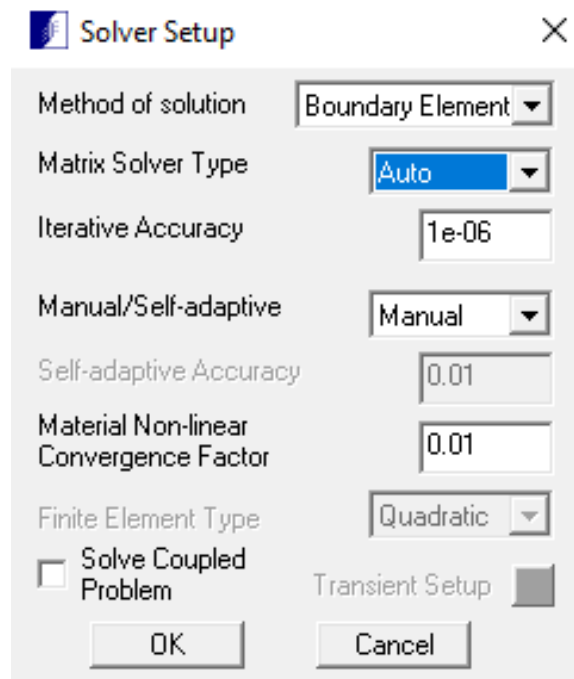


Figure 4.9: Electric Mode → Solution → Solver Setup. Here the method of solution is chosen and the self-adaptive mesh assignment is disabled.

of solution is set to Boundary Element Method. It is important that Manual/Self-adaptive is set to Manual. If set to self-adaptive, the 2D element mesh assigned earlier will be deleted after the first iteration and the program will set its own mesh as part of the Runge-Kutta algorithm. User control over the mesh density was preferred in the setup of these simulations. Manual coerces the program to maintain the user-defined mesh density across all iterations, ensuring all simulations are performed under the same conditions.

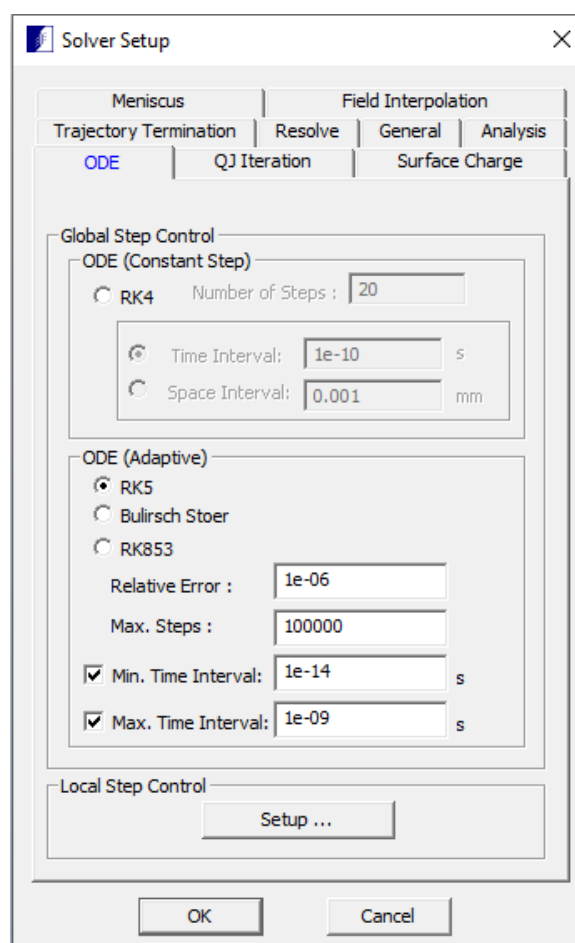


Figure 4.10: Trajectory Mode → Solution → Solver Setup → ODE Tab. Here the Ordinary Differential Equation (ODE) method can be chosen as well as the conditions for terminating the solution.

The Trajectory mode solver setup has many important parameters. In the ODE tab seen in Figure 4.10, the user can set the desired solver algorithm. Lorentz-2E numerically solves the ODEs that describe the motion. Of the solvers listed in the figure, the 4th order Runge-Kutta (RK4) and time-adaptive 5th order Runge-Kutta (RK5) algorithms were used during this work. The maximum time interval

is a critical component as it limits the maximum time - and therefore distance (proportional to its velocity) that a ray is allowed to traverse before recalculating its kinematics from the field at its new position. The process repeats from emission until either the ray terminates on a collector segment or the maximum number of time steps is reached. If the time step is too long, the rays could pass over multiple 2D elements before recalculating their trajectory, effectively missing space charge information in those elements. This parameter is by far the dominant contributor to simulation time. Using roughly 10^6 2D elements distributed between the three ion flight regions and a maximum time interval of 10^{-9} s in RK5 while running cesium and two negative ion species will take roughly 24 hours to complete. Because the RK5 method was producing near-constant time step simulations at this setting (at which point its advantage over RK4 is diminished [64]), the RK4 method was used instead for later studies. This removed at least 6 hours from each simulation while yielding similar results.

As a brief note, simulation work began on an Alienware Aurora-R4™ with an Intel® Core™ i7-4960X CPU at 3.60GHz, 32.0 GB of RAM, running Windows 10 Enterprise. Simulation work later moved to a Dell Precision 3630 Tower with an Intel® Core™ i7-9700X CPU at 3.60GHz, 32.0 GB of RAM, also running Windows 10 Enterprise. A formal comparison of performance between the two computers was not conducted.

The QJ iteration tab of the Trajectory solver setup, seen in Figure 4.11 determines convergence criteria and stability conditions for all beams. After each iteration, the program checks if the relative change in emitted current and space charge deposition (in all 2D elements) is below a certain threshold. The default thresholds are 0.1 % for each and have not been adjusted. This process is repeated until convergence of both charge and current is achieved or the pre-set maximum number of iterations have been completed. The cesium beam current typically converges well before 10 iterations; however, due to the high density of 2D elements, the space charge rarely converges even after 20 iterations. An element may have a ray pass through it in one iteration but even a slight deviation in the ray's trajectory can have it miss that element in the next iteration. Thus an element can go from full charge deposition to no deposition between iterations. It is unlikely for all 10^6

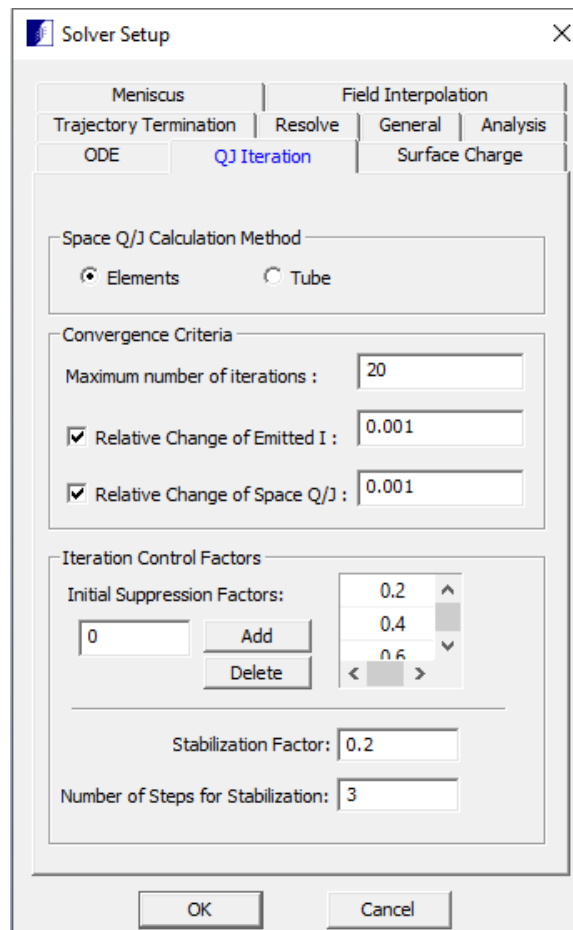


Figure 4.11: Trajectory Mode → Solution → Solver Setup → QJ Iteration Tab: Here the convergence criteria are set. The initial suppression and stabilization factors are critical parameters to ensuring Lorentz-2E converges to a steady-state solution.

elements to reach complete convergence in a reasonable amount of time (iterations) even if the rays themselves approach a steady state. Thus 20 iterations was initially chosen as a reasonable number of iterations.

Below the convergence criteria are the iteration control factors, without which the program would produce nonsensical results. The initial suppression factors suppress the amount of space charge deposited in the mesh in the first few iterations. They have been set to deposit a factor of 0.2, 0.4, 0.6, and 0.8 times the total space charge in the first four respective iterations. In iterations following this, the full space charge of all beams is implemented. This prevents the cesium beam, which is typically allowed to emit the maximum possible current allowed by Child's Law, from overproducing current in the first few iterations and skewing both beam trajectories in the process. In some cases, an over-deposition of charge in front of an emitter from the previous iteration can cause the next iteration of rays to be re-

pelled back into the emitter producing unstable results. Assigning more current to an emitter above the physical limit can also yield unstable simulations. It is important the user recognize which is the case when troubleshooting failed simulations.

The stabilization factor and number of steps used for stabilization are equally

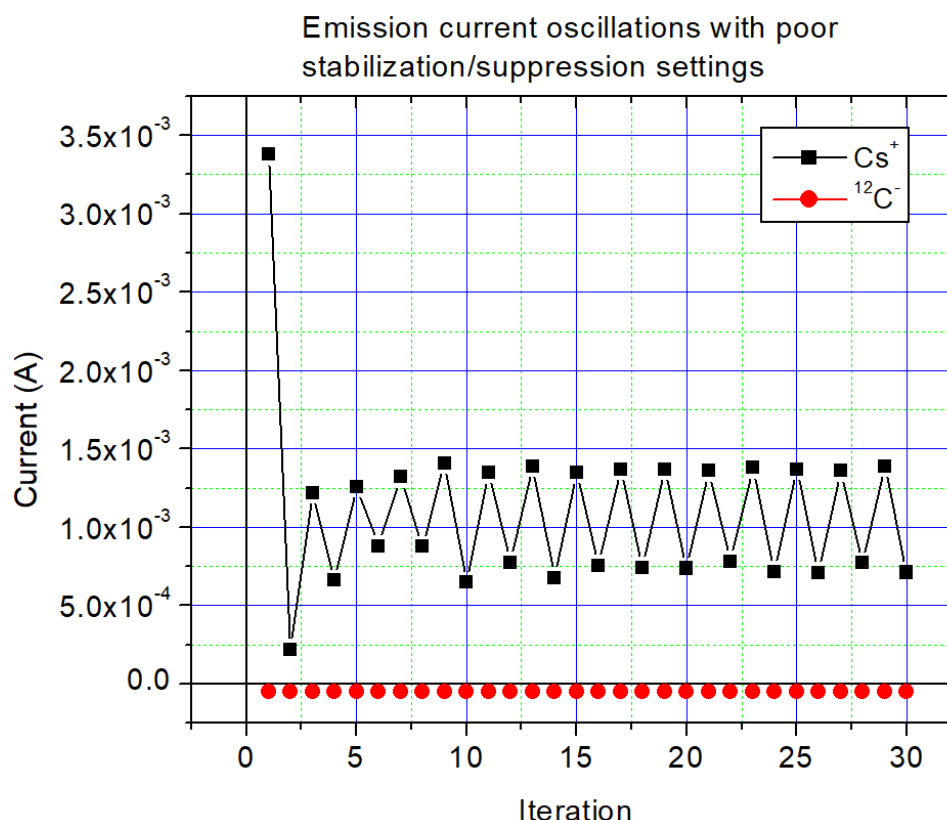


Figure 4.12: Poor stabilization and initial suppression of charge deposition can cause oscillatory behaviour in the emitted Cs. This must be addressed in the template file QJ iteration settings. The negative ion beam ($-50 \mu\text{A}$ of ^{12}C in this example) is run in assigned current mode where the current is fixed. Thus, this oscillation only affects the current Child's Law limited emission of Cs^+ ions. The trajectories of both ions, however, are affected.

important to ensuring a simulation runs smoothly. At the end of an iteration, Lorentz-2E calculates the space charge deposition in the mesh based on the rays emitted in the present iteration as well as the previous iterations (in this case the previous 3 iterations since the number of steps for stabilization is set to 3). The stabilization factor is a value from 0 to 1 that adjusts the weighting of the space charge deposition towards or away from the present iteration (i.e. a stabilization factor of 1 would have the space charge density be dependent entirely on the rays in the present iteration). This effectively creates a weighted average of space charge deposition that suppresses oscillatory behaviour. If only the present ray's charge

deposition was taken into account, the ray in the next iteration would be repelled by the deposited charge and end up elsewhere. Then, deposited charge of that ray would repel the next to a new trajectory, and so on. By keeping the average over multiple iterations - provided by the stabilization factor - a steady state ray trajectory is achieved. As shown in Figure 4.12, poorly chosen suppression factors and stabilization parameters lead to non-convergent oscillation of the current emission of the Child's Law limited cesium ions (the effects on the trajectory are worse). This oscillatory behaviour was also reported by Brown et al. [39] who employed a similar mitigation technique in their simulations.

4.3.9 Analysis

Rijke-Based Analysis

Once a simulation is completed, a multi-staged analysis begins. The `Analyze-Cs_at_Target` module is run, followed by the `Analyze_Carbon_at_Exit` module. To understand this process, some Lorentz-2E nomenclature must be defined. Because the template file has the program keep each iteration of space charge deposition and beam emissions, there will be as many “beams” as there were iterations. Each beam is composed of as many emissions as was set in the `Build_Emitters` module and they are indexed in the order they were built into Lorentz-2E (for example, cesium is typically emitter 1 because it is the first emitter to be defined). Each emitter has a user defined number of rays. These rays are broken up into markers and their number may vary from ray to ray as seen in Figure 4.13. When a ray is emitted, it propagates for a set time-step (or distance) before recalculating the kinematics based on its new position and the forces acting on it at that position. This calculation node is referred to as a “marker.” The ray will continue to step and increment markers until it either intersects with a collector segment or the maximum allowed number of time-steps have been executed.

The first module analyzes the Cs beam as it impacts with the target. It obtains the last marker of each ray of the first emitter (Cs^+) of the last beam (last iteration). The radial position, y-position relative to the global origin, the time after emission, distance travelled, radial and axial velocities, and ray area (each ray cor-

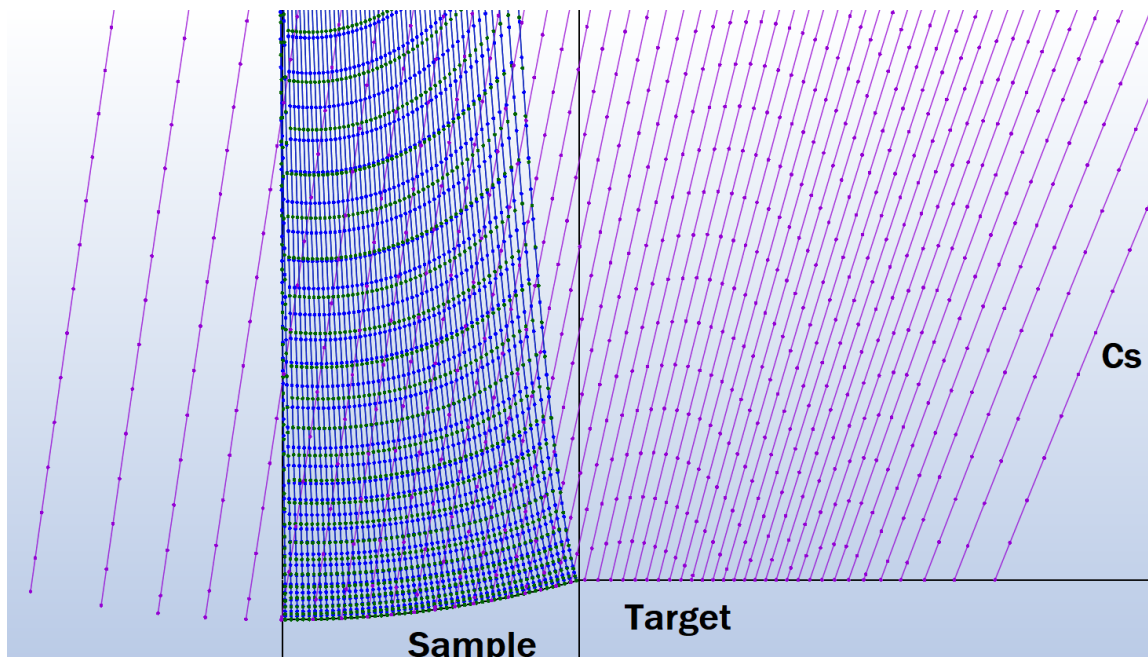


Figure 4.13: A depiction of markers on the rays of a simulation near the target. The violet rays are Cs^+ ions while the green and blue are $^{12}\text{C}^-$ and $^{12}\text{C}_2^-$ respectively. A ray propagates for a set time-step before recalculating its dynamics. The point of recalculation is called a marker.

responds to an areal ring of surface charge due to rotational symmetry) are obtained and the module calculates the current density. These values are then output to the CsANALYSIS sheet in a plot-ready format.

The program checks whether each ray hits the sample and keeps a running tally of the amount of current that does. At the end, the total current emitted is reported along with the percentage of the current that impinged on the sample. This gives a quantitative metric for how accurately the cesium is focused on the sample.

The negative ion beams are analyzed in the same manner and the results are output to the CExitANALYSIS sheet. If the axial position of the terminal marker of a negative ion ray is not coincident with the globally defined “negative ion collector segment” (as seen in Figure 4.7), then the ray must have been lost elsewhere in the source (typically the ionizer base plate bore hole) and is counted as a lost current in a running tally. As one of the most typical plots of merit, the radial displacement and the angular deviation (from coaxial in mrad) of each ray are tabulated together for ease of plotting of the phase space distribution. This is typically referred to as an $x-x'$ plot. Finally, the RMS emittance according to Equation 3.4, as well as the three Twiss parameters are calculated.

Lorentz-2E-Based Analysis

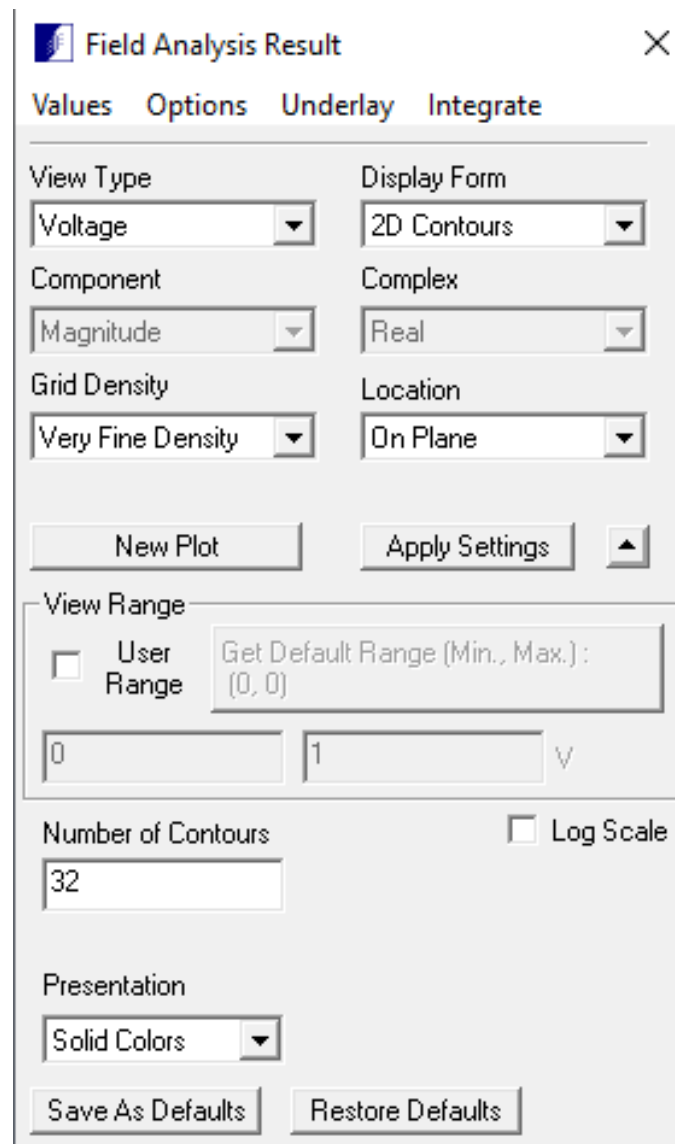


Figure 4.14: Electric Mode → Analysis → Field Results: This tool allows the plotting of the electric field, potential, and volume charge deposition in various visual formats overlaid on the source geometry.

As a brief aside, Lorentz-2E offers a number of other analysis tools that cannot be accessed by Rijke but are useful to ion source simulations. The ones relevant to this work are:

1. Electric Mode → Analysis → Field Results: This tool, seen in Figure 4.14, overlays a mapping of (among others) the electric potential, electric field strength, or volume charge deposition on the model of the ion source. One

can also plot the strength of each of these tracing along a user defined line segment.

2. Trajectory Mode → Analysis → Emittance: This analysis tool, seen in Figure 4.15, allows the user to specify a plane orthogonal to the axis of symmetry and obtain the RMS and normalized RMS emittance results of the beam at that plane. The user can also output x-x' and emittance ellipse plots. This tool was discovered after the x-x' plotting function was written into Rijke. The two are confirmed to produce identical results. The advantage of the Rijke-based x-x' plot is that it is automatically generated in more convenient units and saved in a plot-ready format. The disadvantage is that it is limited to the negative ion beam collector segment (since it takes the last marker of each ray) while the Lorentz-2E based tool can analyze the emittance at any point of the emitter's trajectory.

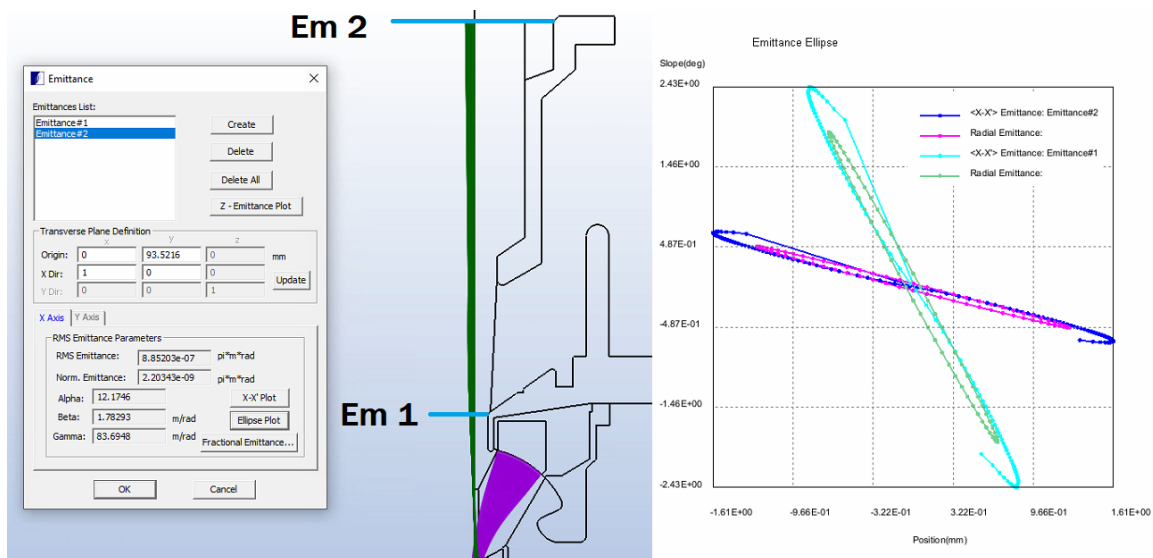


Figure 4.15: Trajectory Mode → Analysis → Emittance: This tool allows the user to analyze the emittance, as well as plot the x-x' and emittance ellipse graphs at any user-specified plane (as seen right).

Once a simulation is completed and saved, the user must employ these tools manually.

4.3.10 Log and results

With the analysis complete, the Logger module is run to compile important results and starting parameters before the program saves itself. This module also manages the batch sheets for plotting convenience. Information is compiled and split between two separate sheets: LOG and RESULTS.

Log

On the LOG sheet, the timestamp, source model, description, simulation time, as well as a number of important setup parameters are recorded. One row in the LOG sheet represents an entire simulation. The Lorentz-2E version and the template file used to generate the necessary settings are also logged. There is an additional space for the user to input any comments they may have about that particular simulation. Such comments are added and saved manually and are not part of the code. If the user ran a simulation where not all parts were used (for example they built geometry and set electric potentials but did not build emitters), the parts that do not run will be greyed out. To make it conspicuous when a different source model is used (SO-110A instead of SO-110C for example), the description cells are colour coded to each ion source.

Results

The RESULTS sheet displays the timestamp and simulation description again but outputs information on how the various ions behaved. For cesium, the emission mode, the total emitted current, and the accuracy (percentage of the current that hit the sample) is logged. The result is colour coded based on how high the accuracy is. Then the emitted current and, percent lost, RMS emittance of the negative ions exiting the ion source as well as the Twiss parameters are presented for each negative ion species that ran. Each row encompasses data from a single simulation. This compilation makes for easy comparison by inspection, serves as a history of source development, while also being in a plot-ready format.

4.3.11 Batch Sheets

The final part of this module is to update the batch sheets. The radial displacement vs current density of the Cs beam are copied from the CsANALYSIS sheet and appended to the CsBATCH sheet. Additionally, for each negative ion species, the radial displacement and angular deviation (x-x' plot information) at the negative ion collector segment are copied from the CExitANALYSIS sheet and appended to the CExitBATCH sheet. They are each labelled with the timestamp and simulation description of the present simulation. This sheet records all previously run simulation results. This convenient format allows a user to analyze a whole batch of cesium current density and negative ion x-x' plots simply by opening the batch sheets of the last simulation to run in a batch. It also allows simple inter-comparisons of data between batches without having to open each Excel workbook individually.

4.3.12 Save

Once everything is finished, the timestamp is recorded and logged on the MAIN sheet where there is an automatic calculation of the start-to-finish duration of the simulation. The last few lines of code save everything. First, the Lorentz-2E file is saved. Then the Master workbook itself is saved. And finally, a copy of the workbook is saved with the unique, timestamped file-path generated at the beginning of the code. This saving convention was chosen to maintain one single Excel workbook for running batches and making developments. All completed simulations and the parameters used to generate them are available for future viewing in a separate folder. This way, if any Lorentz-2E simulation files are lost, they can be regenerated using the corresponding Excel workbook that generated them.

4.4 Batch module Example

Since the MainBrain module compiles an entire simulation from start to save, by calling it between code that adjusts setup parameters, one can construct a batch of consecutive simulations to run autonomously. Figure 4.16 shows a sample of this code as it was used for Batch 35. In this batch, the ionizer potential was fixed at

```

Sub Batch()
Dim i As Long

'Target Potential 11 kV
Worksheets("ELECTRIC").Range("D7").Value = -24000

'Cs Current 0.175 mA
Worksheets("MAIN").Range("F18").Value = 0.175
Worksheets("MAIN").Range("E2").Value = "B35-TP11kV-TR1mm-Cs175uA"
MainBrain

'Cs Current 0.250 mA
Worksheets("MAIN").Range("F18").Value = 0.25
Worksheets("MAIN").Range("E2").Value = "B35-TP11kV-TR1mm-Cs250uA"
MainBrain

'Cs Current 0.325 mA
Worksheets("MAIN").Range("F18").Value = 0.325
Worksheets("MAIN").Range("E2").Value = "B35-TP11kV-TR1mm-Cs325uA"
MainBrain

```

Figure 4.16: A sample of the batch processing code from Batch 35. The code shown would run three separate iterations of the MainBrain module using three different cesium current settings.

-24 kV relative to ground (therefore a -11 kV target potential with 35 keV total energy). In this batch, the cesium current was ramped from 0.175 mA to 0.325 mA in steps of 0.075 mA. The actual batch had more (irregular) steps but only the three above are shown in this example. Each block of code changed the cesium current, updated the description to reflect the change, and then called the MainBrain module to run the simulation to completion. When compiling changes of a parameter with equal change intervals, one can use a “for-loop” for a more elegant batch execution.

There is no one batch code that fits all purposes. It is re-written according to the user’s needs. As such, this module has no corresponding, “front-end” Excel sheet and can only be adjusted directly in the Excel VBA compiler. It is generally recommended that the user include a batch number in the description, both to distinguish simulations as part of a batch and to keep track of all simulations that were part of that batch.

4.5 Convergence tests

A number of tests were run to examine the reproducibility of the simulated trajectory results as a function of various simulation parameters. For example, the 2D element density for space charge deposition needed to be sufficient such that the elements fit between rays and facilitated the mutual space charge interaction. The

density was increased until the simulated result did not change appreciably. The 1D and 2D element density, maximum time step, and number of iterations were ramped until the change in results was minimal while still keeping the simulation times manageable.

4.5.1 Step Size Convergence

The maximum step size (time interval) for the RK5 algorithm was tested early in development. As seen in Figure 4.17, the extraction region had yet to be implemented. Later, it became apparent that this upper bound was forcing a near-constant step size; thus, it became the fixed step size for the RK4 algorithm to save time.

The phase space of the carbon beam at the collector segment at the exit of the

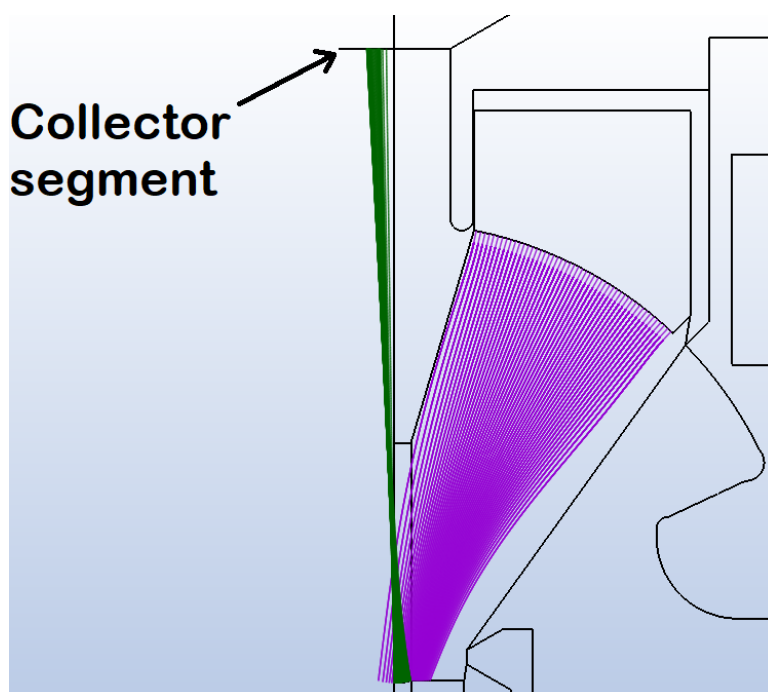


Figure 4.17: The step size test was run using an early version of Rijke, before the source dimensions were refined and extraction region was included. Carbon rays were collected at the end of the ionizer base plate bore hole.

interaction region was acquired and plotted. Using modified template files, simulations were first run for time intervals of 10^{-8} s and 10^{-9} s. There was a significant difference between these results so the time interval was further reduced from 10^{-9} s to 10^{-10} s in a number of steps. The results of this are shown in Figure 4.18.

Figure 4.18a shows the zoomed out view of the carbon phase space. The points

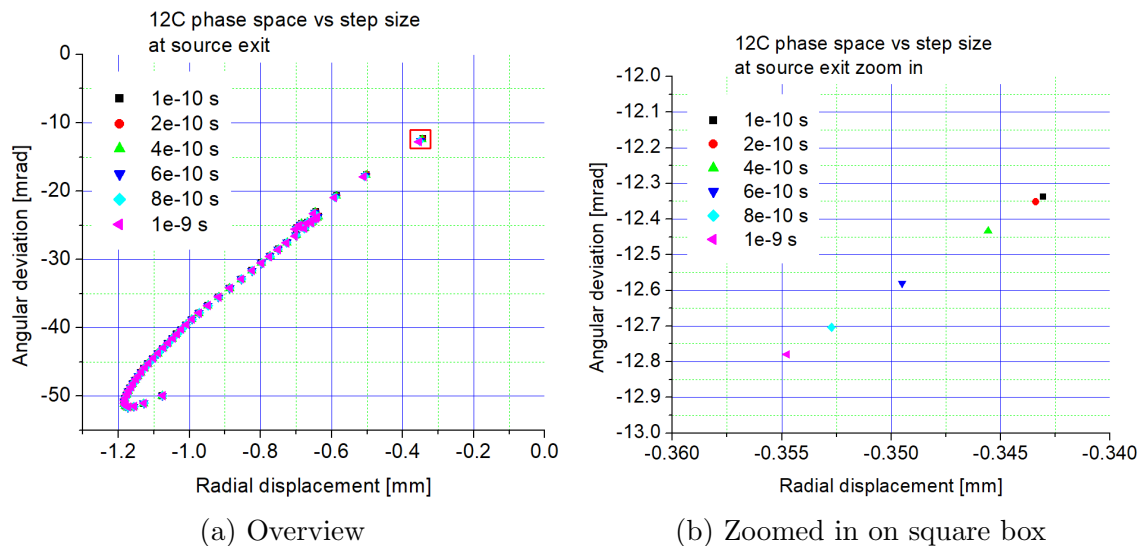


Figure 4.18: The phase space parameters of the outgoing carbon beam were plotted as a function of the time interval. Note the origin is at the top right corner of the left graph.

are almost indistinguishable. When zoomed in, it becomes clear that the individual displacements and angular deviations vary by less than a few percent.

Figure 4.19 gives the elapsed time for each simulation at the various step

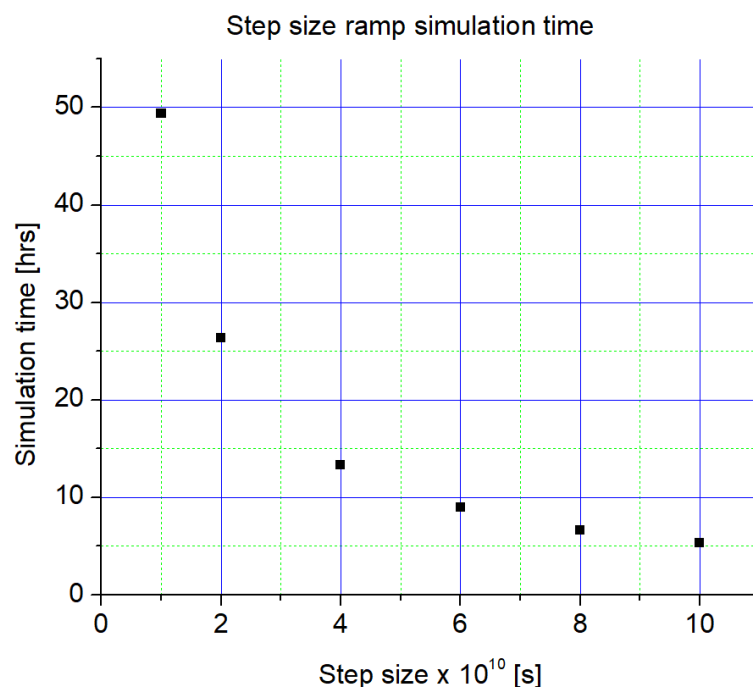


Figure 4.19: The simulation time has an approximate reciprocal relationship with the step size.

sizes. The simulation time increases approximately linearly with the reciprocal of the step size. Given the minimal relative change from 10^{-9} s to 10^{-10} s, and that a

longer path length would be implemented when the extraction region was included, the time step was fixed at 10^{-9} s.

4.5.2 2D Element Convergence

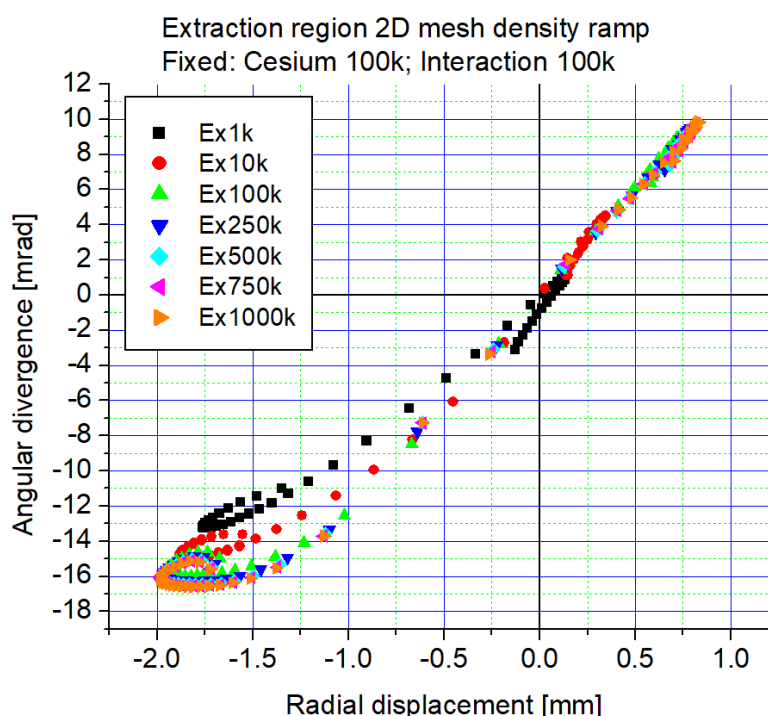


Figure 4.20: The first of three phase space diagrams. The cesium and interaction region had a fixed number of 2D elements assigned while the number was ramped in the extraction region.

Once the extraction region was implemented and the simulation algorithm was switched to RK4, a similar study was conducted to ensure reproducibility at various densities of 2D elements. The space inside the source was divided into three major regions as shown in Figure 4.7. In sequence, the extraction, interaction, and cesium regions had their 2D mesh densities ramped to find and fix a number of 2D elements that would provide adequate stability. The phase spaces of the carbon rays were collected at the negative ion collector segment and plotted in Figures 4.20, 4.21a, and 4.21b. Additionally, the simulation times and RMS emittances were plotted in Figure 4.22.

The difference in emittance from 500 to 750 thousand elements in the extraction region was 0.4%; from 100 to 250 thousand elements in the interaction region

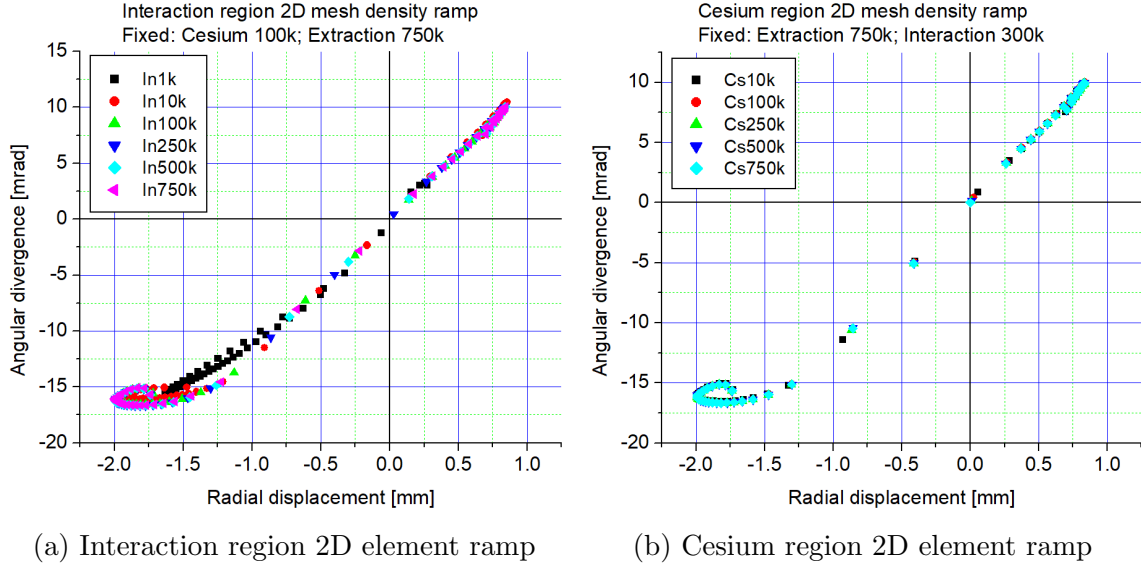


Figure 4.21: The second and third of three phase space diagrams. The cesium and interaction region had a fixed number of 2D elements assigned while the number was ramped in the extraction region.

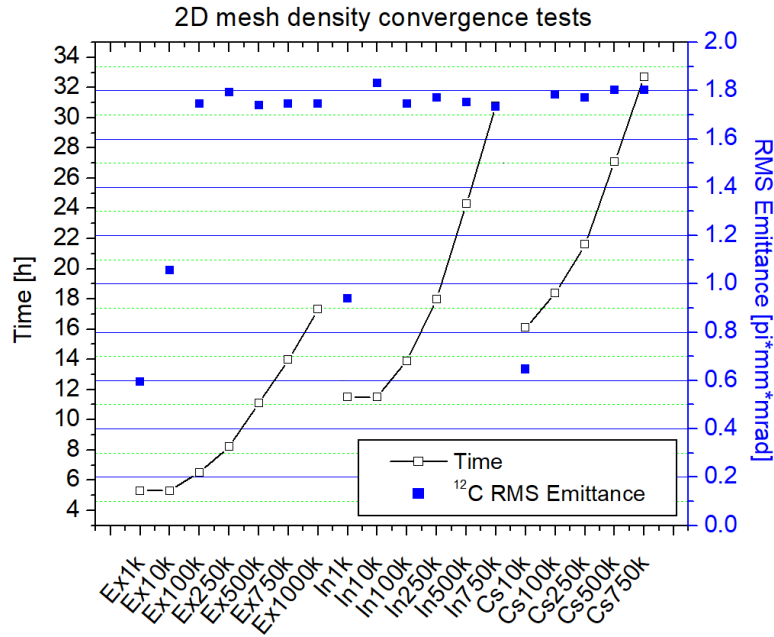


Figure 4.22: The simulation time (black) and RMS emittance of the ^{12}C beam at the collector segment (Figure 4.20a) are plotted together for all three sets of 2D element ramp tests.

was 1.4%; and from 100 to 250 thousand elements in the cesium region was 0.8%. The change in their phase space distributions at each of these steps was also minimal. In all cases, the cesium beam phase space changed by even less. Thus, 500, 100, and 100 thousand elements were chosen for the extraction, interaction, and cesium regions respectively.

4.5.3 Other parameters

Other parameters were chosen in a similar fashion. 10,000 1D elements were spread uniformly across all non-emitting surface segments. Emitting segments were coded to guarantee multiple 1D elements between each emitted ray, as per IES's recommendation. Additionally, the number of iterations of space charge deposition and re-emitting rays was set to 20 by inspecting the intermediate outputs.

Chapter 5

Results and Discussion

Preamble

This section details noteworthy simulation batches in the order that they were conducted. Due to the complexity of the shroud and ionizer mounting, making changes to them is difficult and expensive. Thus, early simulations avoided changes to these objects. In terms of geometry, the simplest and most cost effective components to alter in the ion source are the extraction electrode, the target aperture, and the target. Physical parameters such as the electrode potentials and the cesium oven temperature (which affects the flux of cesium) are also readily adjustable.

Each simulation batch has its own motivation, setup, and foci of analysis depending on the behaviour of the emitted ions. Each are described in their own self-contained section.

5.1 Important foreword about target apertures and cesium currents

5.1.1 Target apertures

Throughout this chapter, there are mentioned three separate target aperture versions. The AEL-Bmod aperture is a modified version of the original SO-110B version aperture. The HVEE-C aperture is as per the original manufacturer design. The AEL-Cmod aperture is a modified version of the HVEE-C aperture designed

at Lalonde AMS. All three can be seen in Figure 5.1

The AEL-Bmod model was used erroneously during early, exploratory simula-



Figure 5.1: A comparison of the three target apertures discussed in this chapter

tions. While these early studies are unreliable for quantitative discourse, qualitative information obtained in these studies were academically interesting. Following the notice of the error, the HVEE-C model replaced this model in the simulations that followed.

Due to some electric discharging complications with the HVEE-C model, the AEL-Cmod model was used instead. Once the schematics were made available, simulations were adjusted to reflect this change in geometry and allow for comparison with experiment.

5.1.2 Cesium currents

Following numerous simulations and experiments, it was noticed that the results of simulations using Child's Law to limit the cesium emission at target potentials of 6 kV and above were not reproducing reality well. Measuring the exact cesium current in the ion source is technically challenging and has not been accomplished to date. However, it is likely that the actual current of cesium used in routine analysis at Lalonde AMS is in the neighbourhood of $250 \mu\text{A}$ at target potentials around 6-7 kV. Thus, for the early exploratory studies where Child's Law was used, quantitative discussions are minimal.

5.2 Exploratory Simulation: Extraction tip removal test

5.2.1 Motivation

This exploratory batch examined the role of the extraction electrode on the behaviour of the outgoing negative ion beam. Ions entering the extraction region are initially focused by the Pierce geometry - the combination of the conical surface back of the ionizer base plate and conical tip of the extraction electrode. The ions then enter the extraction electrode through a small opening at the tip of the cone. This cone is held at ground potential. Simulations during development had shown that this small entrance to the cone compressed the field to a strong radial divergence at its entrance. It was hypothesized that, by widening the opening, the radially divergent component of the field would be reduced at the electrode entrance and perhaps result in a narrower beam.

This batch was set up to include the four major species of carbon to examine if the difference in mass had any significant bearing on the negative ion output. If not, some of the species could be removed in later batches to save simulation time.

5.2.2 Setup

Rijke Version	Lorentz-2E Version	Source Model	Batch #
η_2	10.1	SO-110C	NA
Cs Mode	Current	Negative Ions	Current
Child's Law	$\approx 560 \mu\text{A}$	$^{12}\text{C}^-$	$16.5 \mu\text{A}$
		$^{13}\text{C}^-$	$0.2 \mu\text{A}$
		$^{14}\text{X}^-$	$6\text{e-}5 \mu\text{A}$
		$^{12}\text{C}_2^-$	$13.3 \mu\text{A}$
Target Assembly Potential		Ionizer Assembly Potential	
-35 kV (w.r.t ground)		-28 kV (w.r.t ground)	
Aperture Version		Geometry Variation	
AEL-Bmod		Extraction electrode	

Table 5.1: Setup parameters: $^{14}\text{X}^-$ represents the contributions from ^{14}C and its more dominant molecular isobars.

Table 5.1 shows the setup for this batch. In each of the simulation sections in this chapter, this standardized table will appear. The setup parameters that are varied in each study will be coloured green with further details given in the text.

The tip of the extraction electrode was removed such that the electrode resembled a hollow cylinder. The negative ion current distribution was set according to the relative emissions detailed in Table 2.1. The maximum allowed current of cesium, as governed by Child’s Law, was allowed to be emitted from the ionizer. The typical target potential difference used in routine experiments on carbon at this point was about 7 kV with an extraction potential difference of 28 kV. This gives the ions an overall energy of 35 keV.

5.2.3 Results

Figure 5.2 shows the differences in the two geometries. The differences in trajectory of the negative ion beam are not obvious on this scale. A collector segment at the top of this image collects the carbon rays as they leave the ion source. It is at this position that the r - r' graph seen in Figure 5.3a is acquired and plotted. This graph plots the radial displacement and angular deviation (off from parallel with the axis) of the outgoing rays for all isotopes present. From this graph, it is clear that the hollow cylinder geometry gives a larger radial displacement and angular divergence. Thus, removing the cone does not improve the outgoing beam quality.

Figure 5.3b zooms in on a single ray point of the simulation with the extraction tip intact. The difference in the radial displacement and angular deviation between the four isotopes of carbon is negligibly small. Later simulations justified their omission to reduce simulation time.

The reason for the lack of improvement in 5.3a is made more apparent in Figure 5.4 when the equipotential lines are overlaid on the extraction region. One can see that the Pierce geometry of the ionizer base plate ensures an initially focusing field. However, the field penetrated deeper into the more open cylinder design than the cone-tipped design resulting in more of the equipotential lines spanning -28 kV to 0 kV to be of a radially diverging nature. Thus increasing the inner diameter of the extraction cone appears to be counterproductive to maintaining a focused beam.

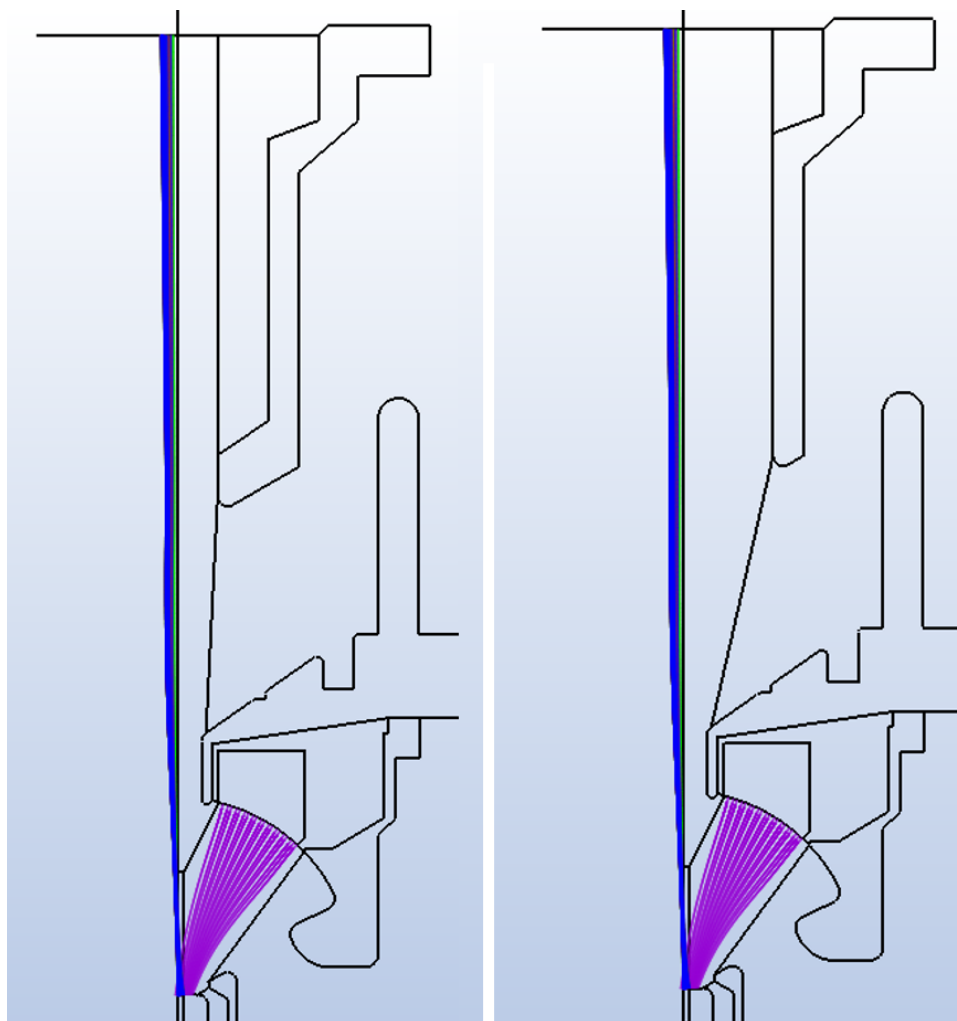


Figure 5.2: The original SO-110C geometry is seen left. The violet rays are Cs^+ ions while the overlapping green and blue are $^{12}\text{C}^-$ and $^{12}\text{C}_2^-$ respectively. These are axially symmetric half-cross-section views. On the right, the extraction cone has been hollowed out to more closely resemble a hollow cylinder.

5.2.4 Summary

This batch suggested that opening the tip of the extraction electrode does more harm to the outgoing negative ion beam focusing. A more open geometry increases the path length along which the negative ions experience a defocusing field. While the constricting of the field by the more closed geometry does increase the defocusing field intensity at the entrance, it does so across fewer equipotential lines, a smaller path length, and at a point where the ions already have a higher momentum.

This batch also demonstrated that the variation in trajectory of the four species of carbon is not significant. The next batch will examine if the ^{13}C and ^{14}X (^{14}C and its more dominant molecular isobars) beams can be omitted entirely because

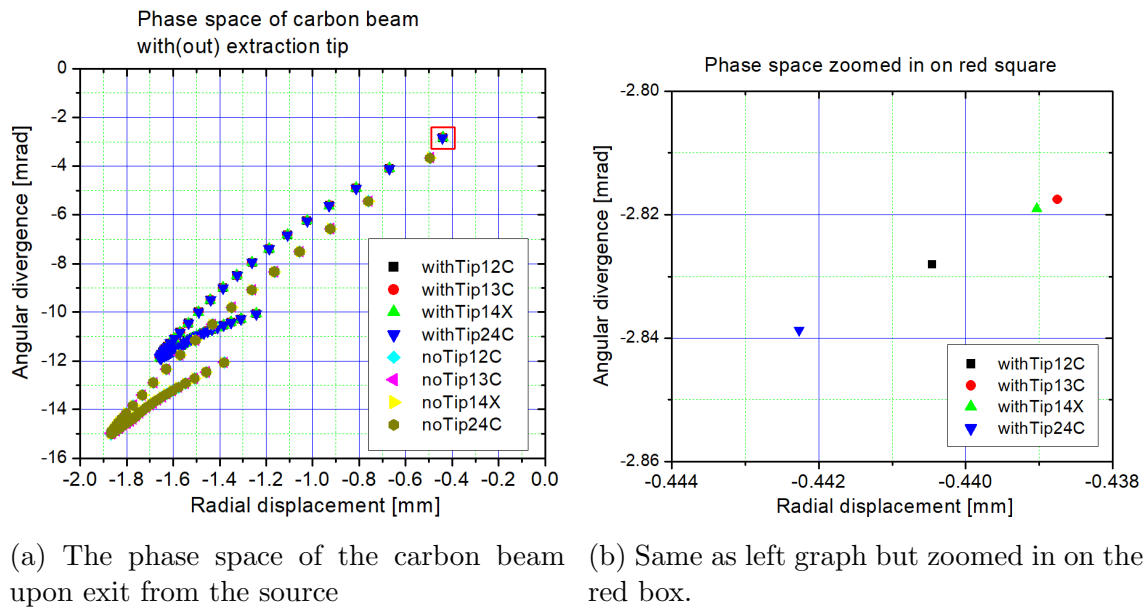


Figure 5.3: An r - r' graph detailing the phase space of the negative carbon ions as they exit the ion source. Notice the origin - which represents the axis of symmetry - is in the top right corner of the left graph. All the phase data of the various carbon species are stacked tightly such that they cannot be individually distinguished in either geometry. In the right graph, one can see the microscopic differences in the ray trajectories between the four species of carbon emitted.

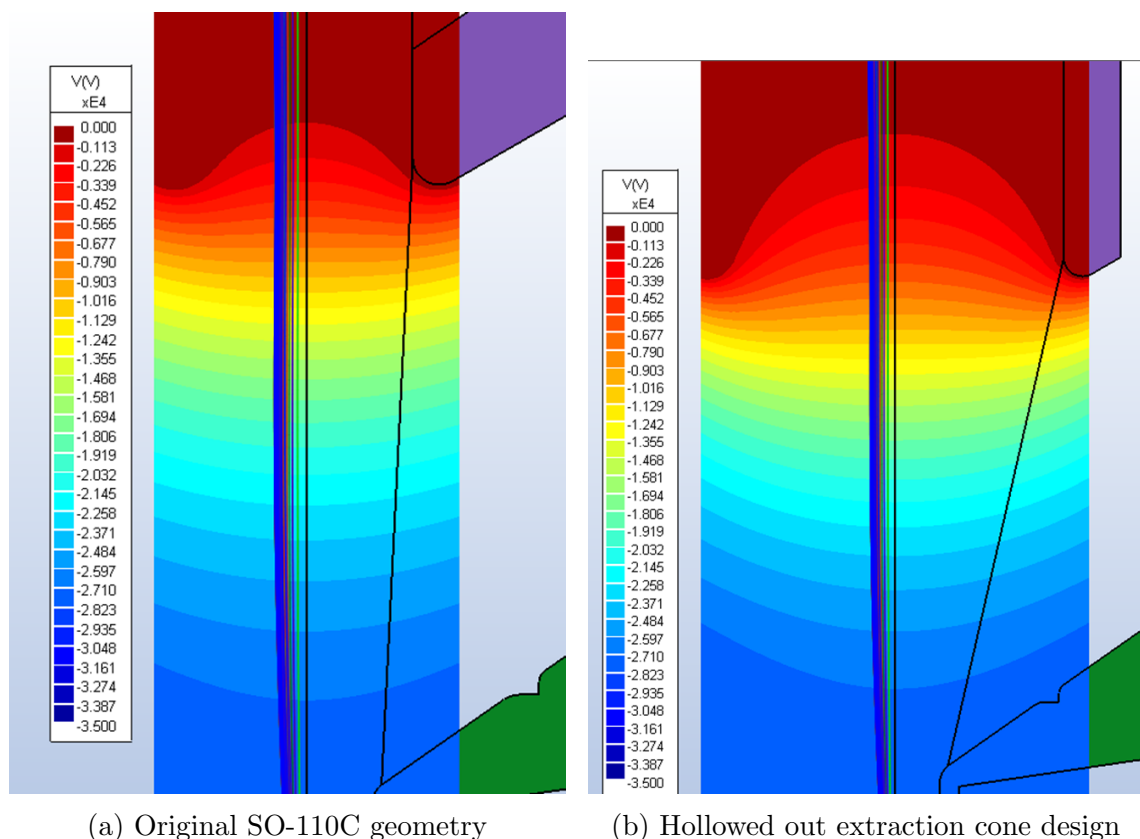


Figure 5.4: Overlaid on the extraction region are the equipotential lines as displayed by Lorentz-2E.

they contribute less than 1 % of the total current.

5.3 Exploratory Simulation: Cesium negative-ion interaction verification & emission reduction

5.3.1 Motivation

Having shown in the last batch that the four species of carbon did not differ from each other in their trajectories, this batch sought to examine whether removing ^{14}X and ^{13}C would cause significant changes. If not, the simulation times could be cut down by nearly half. Simultaneously, this batch would examine the effects of the cesium space charge on the negative ion beam and the purely hypothetical situation without cesium present. This would confirm Lorentz-2E's ability to account for the interaction of the two beams and inform on the importance of this interaction over the ambient field distribution (produced only by the electrodes).

5.3.2 Setup

Rijke Version	Lorentz-2E Version	Source Model	Batch #
$\eta 2$	10.1	SO-110C	NA
Cs Mode	Current	Negative Ions	Current
Child's Law	$\approx 560, 0 \mu\text{A}$	$^{12}\text{C}^-$	$16.6 \mu\text{A}$
		$^{12}\text{C}_2^-$	$13.4 \mu\text{A}$
Target Assembly Potential		Ionizer Assembly Potential	
-35 kV (w.r.t ground)		-28 kV (w.r.t ground)	
Aperture Version		Geometry Variation	
AEL-Bmod		None	

Table 5.2: Setup Parameters: Simulations ran with and without cesium to verify the space-charge interaction.

Table 5.2 shows the setup for this batch. The geometry was reverted to use the original extraction electrode design but this time emitting only $^{12}\text{C}^-$ and $^{12}\text{C}_2^-$ ions. Their relative currents were again set according to Table 2.1. Following this, a simulation was run omitting the Cs^+ ions entirely.

5.3.3 Results

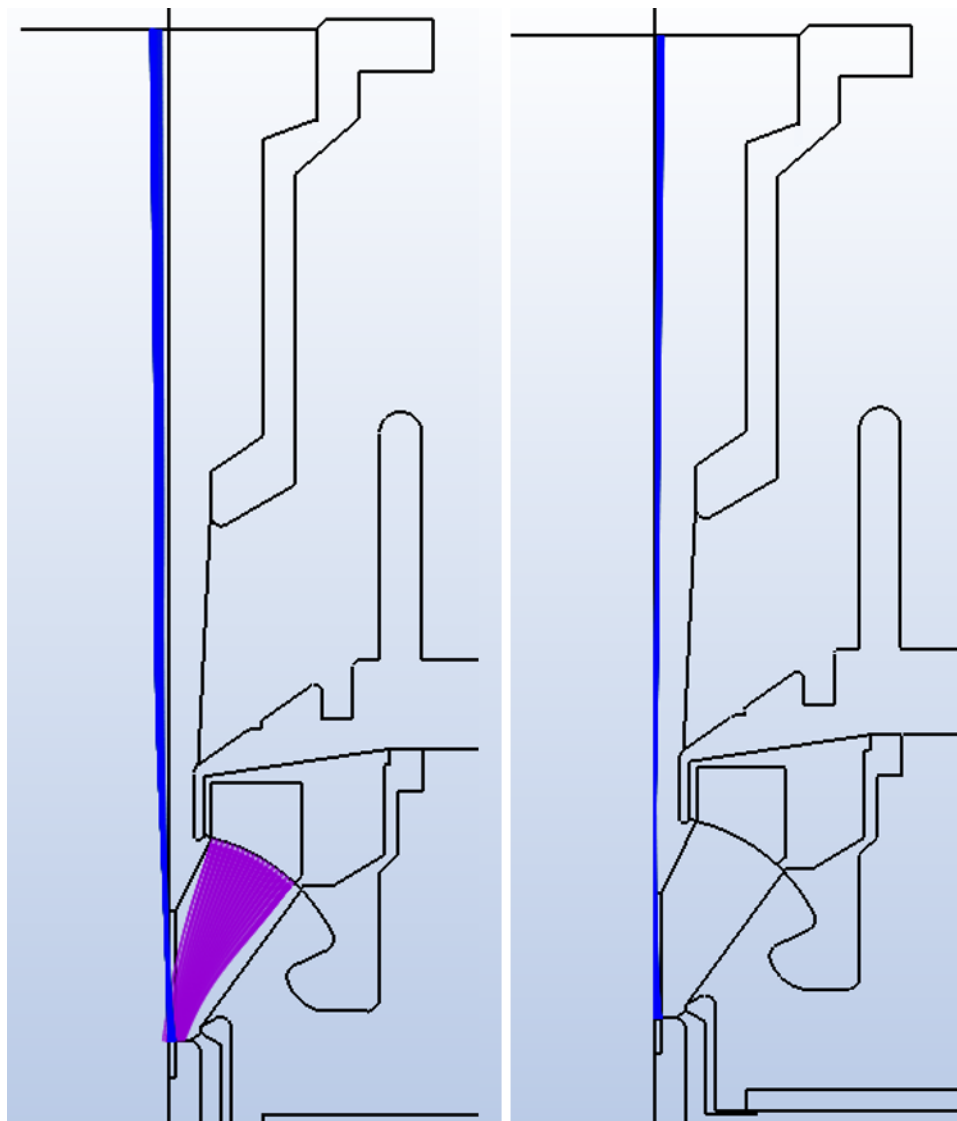


Figure 5.5: A comparison of the two simulations in Lorentz-2E. On the left, both negative ion species and cesium are present. On the right, cesium has been omitted.

Figure 5.5 shows the differences in the two simulations. With cesium present, the negative ion beam is attracted across the axis of symmetry. The ambient field alone would have it remain on the positive side of the axis. This is likely due to a strong buildup of positive space charge on the central axis where the full cesium beam converges.

Figure 5.6 shows the phase space of the carbon beams at the exit of the ion source. The ^{13}C and ^{14}X beams do very little to affect the trajectory of the whole beam. Thus, they will be omitted in future simulations to save time. The

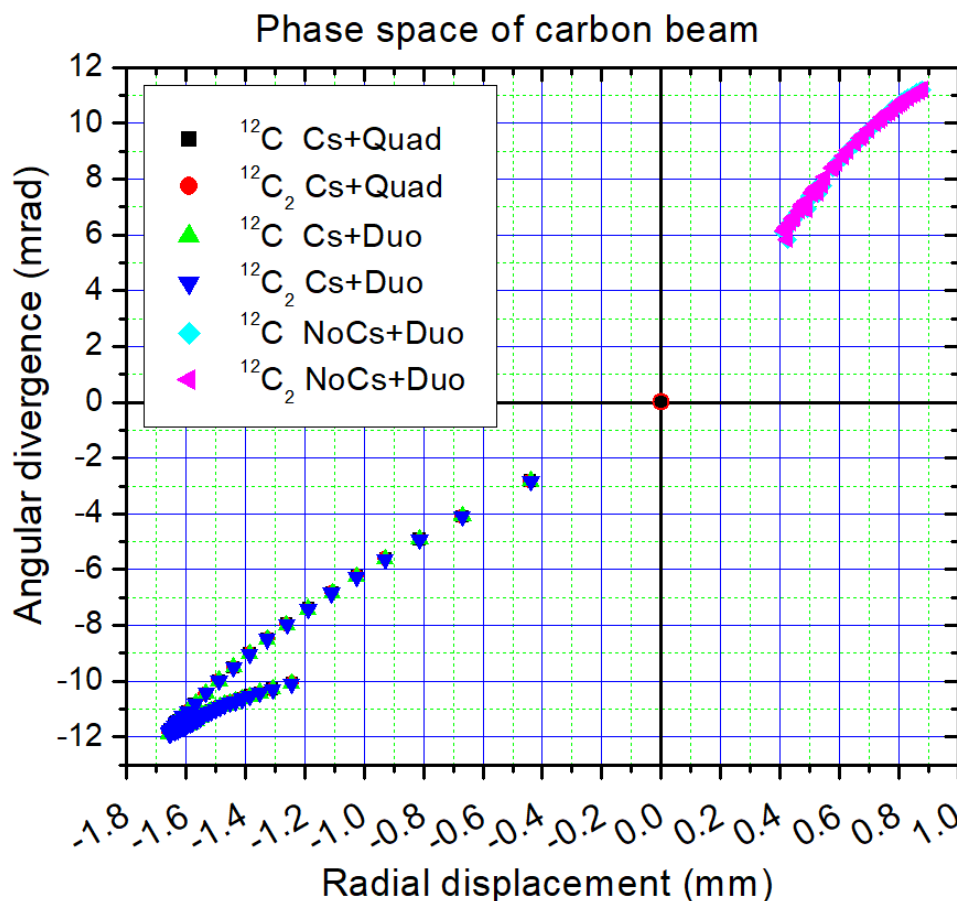


Figure 5.6: The difference between the monomer and dimer of ^{12}C with (Quad) and without (Duo) ^{13}C and ^{14}X is negligible. This makes them difficult to discern on the graph because they overlap entirely.

assumption is that they will continue to follow a similar path to the monomer and dimer beams.

The presence of Cs clearly provides an effect on the negative ion beam. This phenomenon will be further explored in Chapter 5.6.

5.3.4 Summary

This batch confirmed that the cesium space charge effects are significant and accounted for by Lorentz-2E. It also confirmed that ^{14}X and ^{13}C could be neglected in simulations to save time.

5.4 Exploratory Simulation: Cratering Test

5.4.1 Motivation

Among the first exploratory studies was the examination of the emission of carbon from a cratered sample. As the cesium sputters a sample, it slowly bores through the material until it reaches the copper pin at the back. Thus, the sample shape is continuously changing during a measurement. This is accounted for in practice using reference materials (standards) and running all samples in a batch using the same procedure. This batch would approximate a sample crater emission of carbon to examine the electrodynamics of the system.

5.4.2 Setup

Rijke Version $\eta 3$	Lorentz-2E Version 10.1	Source Model SO-110C	Batch # NA
Cs Mode Child's Law	Current $\approx 560 \mu\text{A}$	Negative Ions $^{12}\text{C}^-$ $^{12}\text{C}_2^-$	Current $40 \mu\text{A}$ $20 \mu\text{A}$
Target Assembly Potential -35 kV (w.r.t ground)		Ionizer Assembly Potential -28 kV (w.r.t ground)	
Aperture Version AEL-Bmod		Geometry Variation Cratered Sample	

Table 5.3: The sample crater shape was approximated and a simplified implementation was coded into Rijke to be built in Lorentz-2E.

Table 5.3 shows the setup for this batch. The relative emission of ^{12}C to $^{12}\text{C}_2$ was changed from as it was in Table 2.1 to a 2:1 ratio. The output in that table was performed using the SO-110B version of the ion source and has not since been repeated with the SO-110C. The 2:1 ratio was chosen arbitrarily to be in the neighbourhood of routine emission while also making for simpler numbers.

The geometry of a sample crater was approximated based on a sputtered sample that had been cut in half, as seen in Figure 5.7. Based on that image, the geometry of the crater drawn in Lorentz-2E was simplified by specifying a point at a radial half-width (off-axis) of 0.175 mm and a vertical depth of 0.8 mm referenced

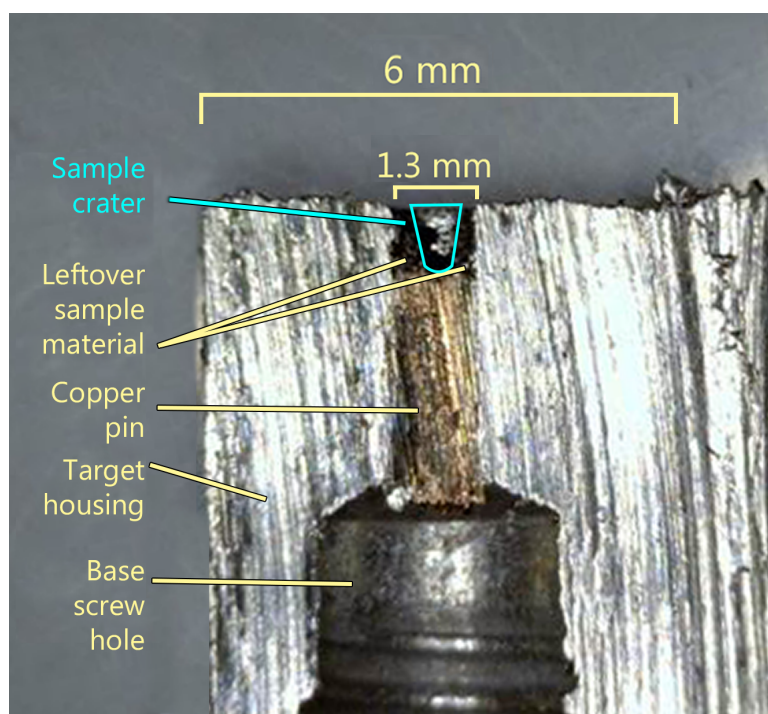


Figure 5.7: The cross section view of a sputtered sample cut in half. The approximate shape of the crater is drawn out in cyan. While some small chunks of the leftover graphite sample material (dark black) may have been dislodged when machining the target, the overall shape of the crater appeared intact. Negative ions were extracted vertically upwards from this orientation. The top of the target housing, into which the graphite is pressed is called the target face.

from the target face. A straight line segment was drawn from this specified point to the inner edge of the target housing at the target face. To draw the curved line representing the deepest surface in the crater, a script was written to calculate the necessary radius and centre position to ensure the curve joined smoothly (matching y derivatives) with the linear segment and terminated with a zero y -derivative (where y is the component parallel to the axis of symmetry) at a radial position of zero. The negative ion current was distributed with a constant current density across the entire surface of the sample - both the linear and curved segments.

Admittedly, machining a target in half is a crude method of ascertaining the crater shape and risks pieces of the crater wall being dislodged. Shanks and Freeman [67] demonstrated casting the sample crater in latex was effective for determining the crater shape. If future studies focus on the crater, such a method is recommended for better precision. Machining the target was sufficient in this case for providing a quick estimate of the geometry.

5.4.3 Results

Figure 5.8 shows the full simulation in Lorentz-2E. The carbon beam diverges widely enough to hit the inner surface of the ionizer base plate. All of the rays that make it into the extraction region are focused into the extraction cone and out the exit of the ion source without further loss.

In the first iteration of a simulation, both carbon and Cs travel as dictated by the ambient field without accounting for space charge. By the last iteration, the space charge is fully incorporated. Both the first and last iterations are compared in Figure 5.9. A strong buildup of negative charge is present at the point where all the rays from the spherical crater bottom converge. This is likely an artifact of how the crater was drawn. A less circular base would result in fewer rays converging on the same position which would likely reduce the strong repulsion of this deposition.

Because all the rays converge on a single point, they deposit large amounts of negative charge there. By the 20th iteration, it is apparent that this locus of negative charge repels the bottom-most carbon rays back into the crater. Said another way, the current density assigned to the circular segment at the bottom of the crater exceeds the local Child's Law limit of emission and is therefore not physically possible. This demonstrates the sensitivity of the simulation to geometry in regions where space charge is important. The current density emitted in reality is very likely not homogeneously distributed along the surface of the sample like has been assigned here in Lorentz-2E. Furthermore, a cratered geometry reduces the strength of the ambient field that penetrates to the base of the crater which has to be offset by the positive cesium space charge to adequately extract negative ions from the surface.

5.4.4 Summary

From this batch, it is clear that the trajectory of the negative ion beam is dependent on the crater geometry. Simulating the crater shape effectively remains a challenge. The importance of cesium space charge to assist the ambient field with negative ion extraction is evident. The way that the cesium beam bores into the

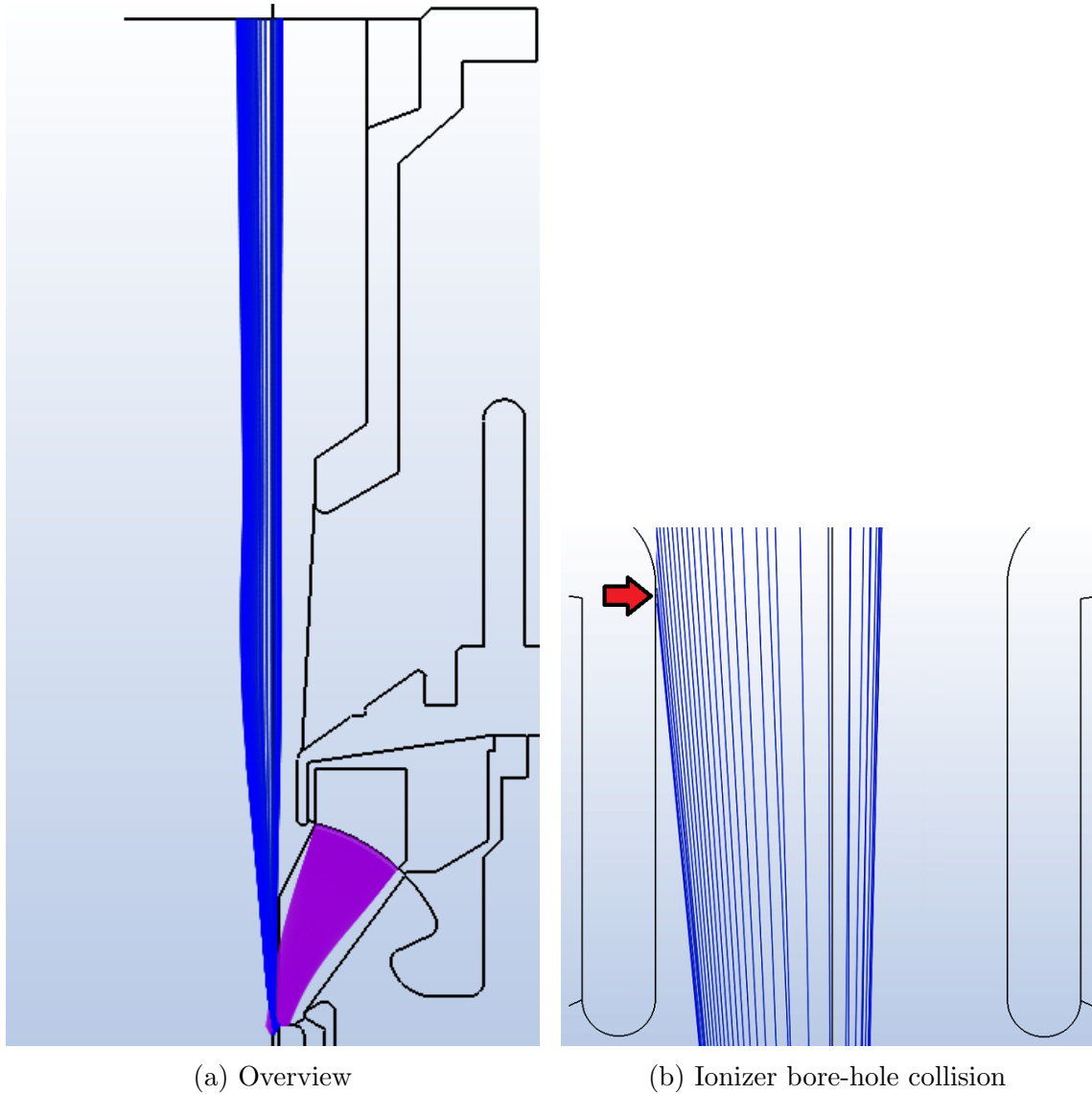


Figure 5.8: An overview of the complete simulation in Lorentz-2E is shown on the left. Cs is in violet, while the carbon beams are in blue. The right image shows three rays, carrying about 10% of the total beam current, collide with the inner bore-hole of the ionizer base plate (See Figure 2.4 for labelled source components) and are lost.

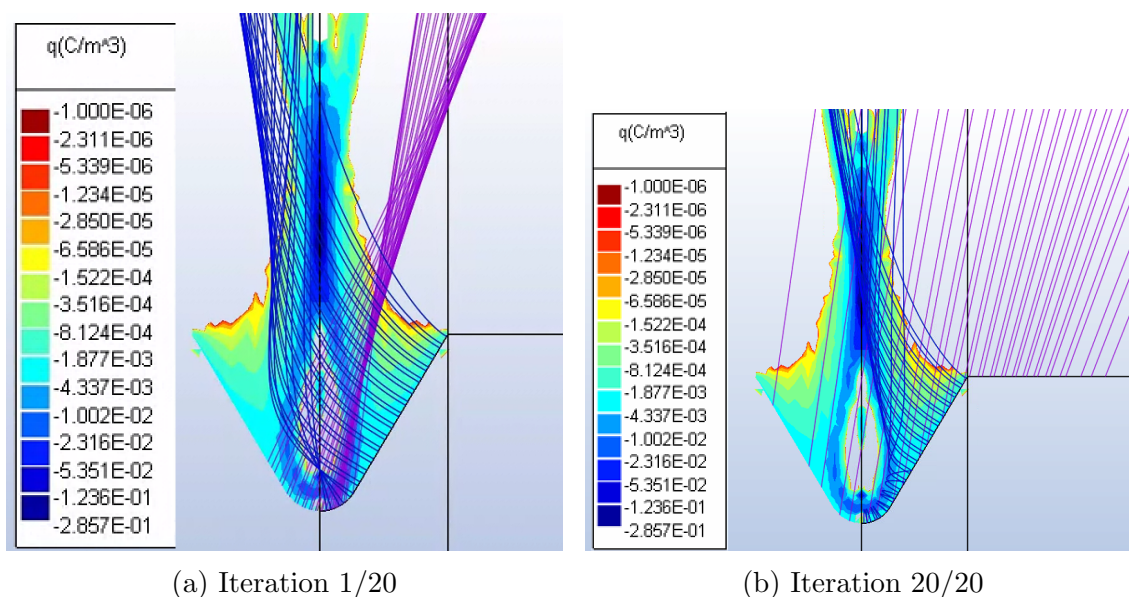


Figure 5.9: Zoomed in on the target crater, the first and last iterations are compared. The negative space charge density of the completed simulation is also displayed under the rays.

sample is not easily controlled; therefore, exploring other parameters would provide more manageable improvements.

5.5 Exploratory Simulation: Target aperture protrusion and constriction

5.5.1 Motivation

The target aperture is the cheapest and simplest component of the ion source to modify. The mindset of this batch, which was still using Child's Law of limited emission (See Section 5.1.2), was to examine the increase in the maximum achievable cesium emission by reducing the distance between the ionizer at ionizer potential and the nearest point at target potential - the target aperture. This would take advantage of the $1/d^2$ dependence of Child's Law. The behaviour of the cesium beam would be monitored for possible improvements.

Rijke Version $\eta 3$	Lorentz-2E Version 10.1	Source Model SO-110C	Batch # 22
Cs Mode Child's Law	Current $\approx 560 \mu\text{A}$	Negative Ions $^{12}\text{C}^-$ $^{12}\text{C}_2^-$	Current 40 μA 20 μA
Target Assembly Potential -35 kV (w.r.t ground)		Ionizer Assembly Potential -28 kV (w.r.t ground)	
Aperture Version AEL-Bmod		Geometry Variation Target aperture	

Table 5.4: The target aperture was protruded and also the diameter reduced. Both were done in incremental steps.

5.5.2 Setup

Table 5.4 shows the setup for this batch. All the typical settings about the ions and potentials were kept the same as the previous batch. The target aperture was protruded by 1, 2, and 3 mm. Then, the aperture inner diameter was reduced by 1 mm and run with protrusions of 1 and 2 mm. For this batch, Rijke was updated to check whether each cesium ray impinged on both the target face and the sample face. This was due to the observation that all simulations up to this point (which were all running using Child's Law for cesium) had a significant portion of the beam missing the sample. If a ray missed, the program would keep track of the current that was lost and create a running count of the cesium accuracy (percent of the total emitted cesium current that hits the sample/target).

5.5.3 Results

The total Child's Law limited currents emitted from the ionizer at each geometric modification as well as the percentage of that current that impinges on the target and sample are presented in Table 5.5. The sample is contained within the target area. The cases where part of the cesium missed the target were due to the rays hitting the aperture instead.

The first thing to notice is that the limited cesium emission is greatly increased by a change of mere millimetres. However, protruding the aperture worsened the

Description	Cesium current [μA]	% hit Target	% hit sample
Original	560	100	29
Prot1mm	723	100	25
Prot2mm	951	100	21
Prot3mm	1268	79	17
ID-1mmProt1mm	677	100	31
ID-1mmProt2mm	883	88	26

Table 5.5: Prot 1-3 mm represent the geometries where only the aperture was protruded. ID-1mm means that the inner diameters of all features of the aperture was reduced by 1 mm. This reduced aperture was then protruded 1 to 2 mm. The cesium currents represent the Child’s Law limit of cesium emission under those geometric conditions. The two right most columns represent the percentage of the total emitted cesium current that impinged on the target/sample.

distribution and accuracy of the cesium beam. The rays that travel near the aperture are drawn further away from the axis by the defocusing field and some even hit the aperture itself. This gets worse with increased protrusion. Reducing the diameter of the aperture made some improvement but also made it easier for the rays to hit the aperture, thus limiting the amount that could be protruded without loss.

Figure 5.10 shows the cesium current densities for the various simulations. The reduction in the inner diameter of the aperture appears to mainly affect the outer most rays as they are the ones that come the closest to the aperture (or in some cases hit it).

Figure 5.11 shows the original SO-110C geometry (barring the AEL-Bmod aperture being used - see Section 5.1.1 for details) in comparison to the current and current density of cesium emitted. The target aperture is the closest object at target potential to the spherical ionizer. The outer-most edge (furthest from the axis) of the ionizer is closer to the aperture than the inner-most edge, which results in rays from that region having a higher current density. Even if the current density was constant across the whole ionizer (as it is in assigned current mode), the outer most rays have a larger area which increases the amount of current held in each of those rays. When both Child’s Law limited current density and the geometric artifacts are considered, the outer-most ray currents increase further. As a result of those processes, even though roughly half of the rays do impinge on the sample, they carry much less than 50% of the total cesium current.

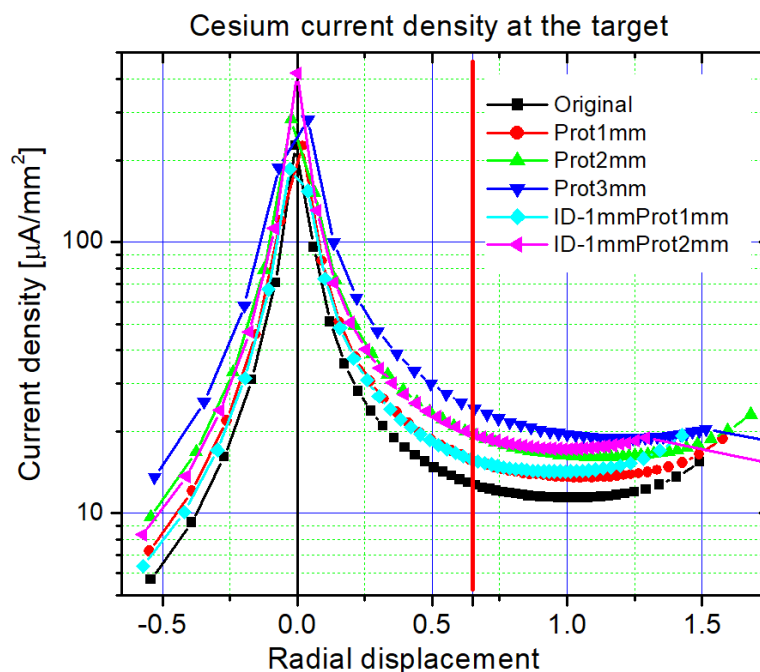
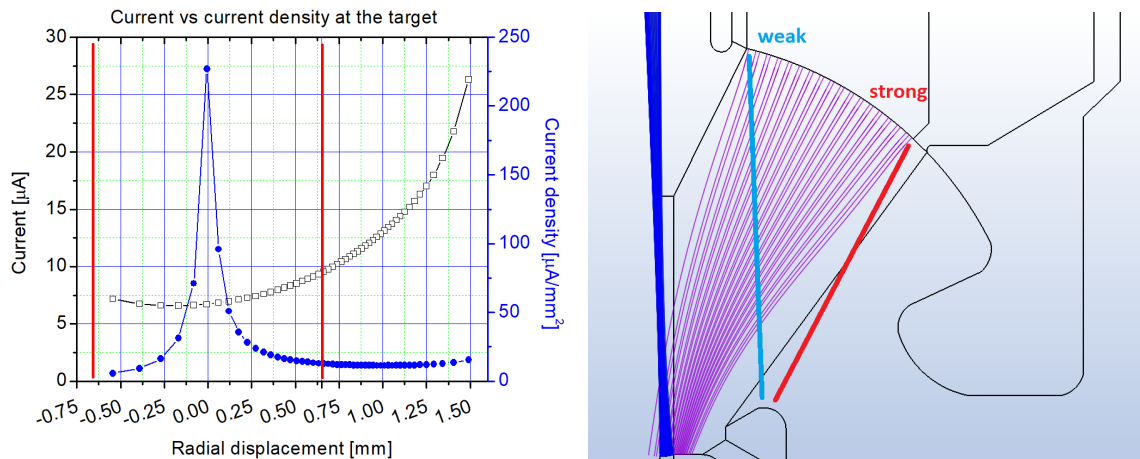


Figure 5.10: The current densities of the cesium rays for each geometry setting are seen above. Each point represents a ray. The vertical scale is logarithmic to better separate the trends. The Prot3mm and ID-1mmProt2mm simulations both had rays hit the aperture outside the extents of this plot. The height of the near axis points is an artifact of the ray's proximity to the central axis. The overall increase in current is seen in the bulk of the rays. The vertical red line denotes the extent of the sample on the positive side of the axis.

Figure 5.12 shows the 3 mm protruded aperture field distribution. A common misconception in discussions at the time of this simulation was that by the time the cesium ions came near the aperture, they would be moving too fast to be significantly affected by the aperture. This was shown to be incorrect as the field is the strongest near to the aperture. About half of the energy of the cesium beam is obtained close to the aperture. This is due likely in part to the shielding effect the shroud has on the surface of the ionizer, compressing the field closer to the aperture. This compression of field line density is increased the further the aperture is protruded into the ion source.

This study focused mainly on improving the cesium behaviour. The negative ion beam output was not considered. At this point, there was a healthy amount of skepticism that the cesium accuracy could be as poor as these simulations seemed to suggest. One would expect to see a sort of etching or strong cesium deposit on routinely measured targets. This was not the case and would motivate further inquiry in the upcoming batches.



(a) Current and current density plotted together for the same rays using the original non-protruded aperture geometry.

(b) A pictorial comparison of distances from the target aperture to the two edges of the ionizer.

Figure 5.11: The geometry of the ionizer and its relative distances from the aperture plays a strong role in the behaviour of the cesium beam. Note, the current density is taken at the terminal point of each ray where they impinge on the target face. The vertical red lines in the left graph represent the extents of the sample.

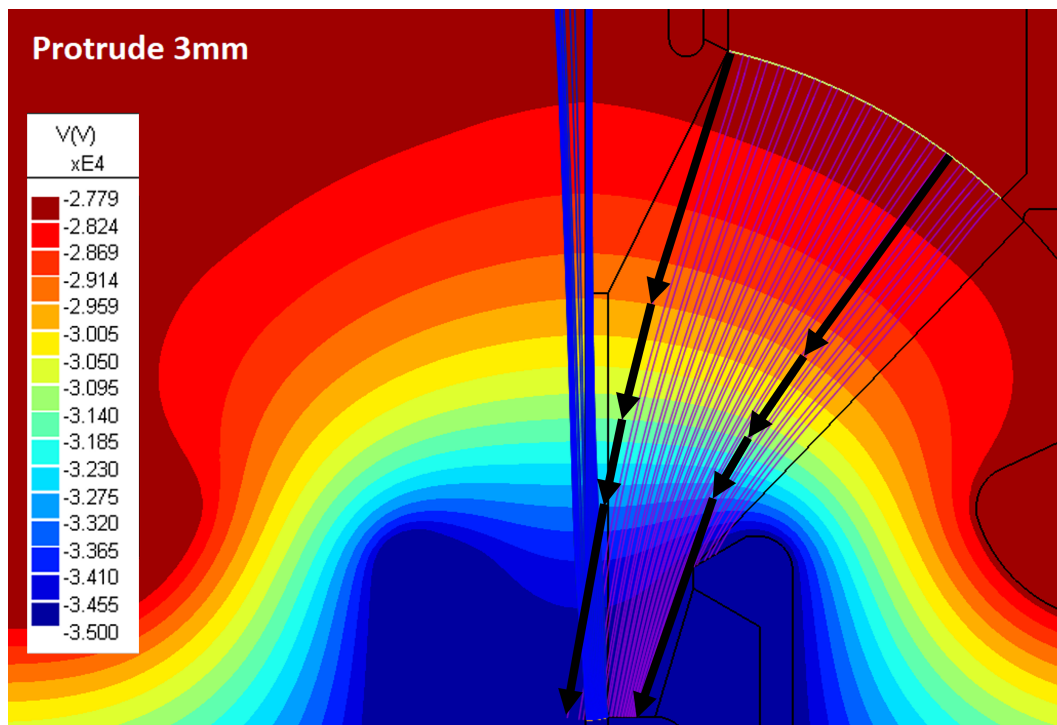


Figure 5.12: Sixteen equipotential lines from -28 to -35 kV are overlaid onto the 3 mm protrusion simulation as seen in Lorentz-2E. Each of the black arrows spans four equipotential lines to better illustrate the density.

5.5.4 Summary

As expected, moving the target aperture closer to the ionizer greatly increases the Child's Law limit for maximum possible cesium emission. The improvements

stop there because more cesium rays miss the sample as the aperture is protruded. Decreasing the diameter of the aperture slightly improves the accuracy of the cesium by reducing the defocusing field length but the aperture is more prone to being hit by the cesium rays. The degree of detriment to the cesium accuracy in these simulations, even in the original geometry, seemed unrealistic and would be examined more closely in upcoming batches.

5.6 Exploratory Simulation: Space charge effects of ramping cesium ion current

5.6.1 Motivation

Protruding the aperture had shown little promise and the degree to which the cesium was missing the sample seemed anomalously high. Before running the target recess experiment, detailed in Section 5.7, a short batch was run to examine the distribution of cesium on the sample at lower cesium currents. All simulations up until this point had been using the Child's Law limit of about $560 \mu\text{A}$ at 7 kV target potential difference. This batch would quickly check if the poor accuracy was present at lower - but still within an order of magnitude of Child's Law - currents.

5.6.2 Setup

Rijke Version	Lorentz-2E Version	Source Model	Batch #
$\eta 3$	10.1	SO-110C	23
Cs Mode	Current	Negative Ions	Current
Assigned I	50, 250, & 500 μA	$^{12}\text{C}^-$	40 μA
		$^{12}\text{C}_2^-$	20 μA
Target Assembly Potential		Ionizer Assembly Potential	
-35 kV (w.r.t ground)		-28 kV (w.r.t ground)	
Aperture Version		Geometry Variation	
AEL-Bmod		None	

Table 5.6: The cesium current was assigned at 50, 250, to 500 μA

Table 5.6 shows the setup for this batch. It was a simple set of three simulations at three different assigned cesium currents. The carbon monomer and dimer

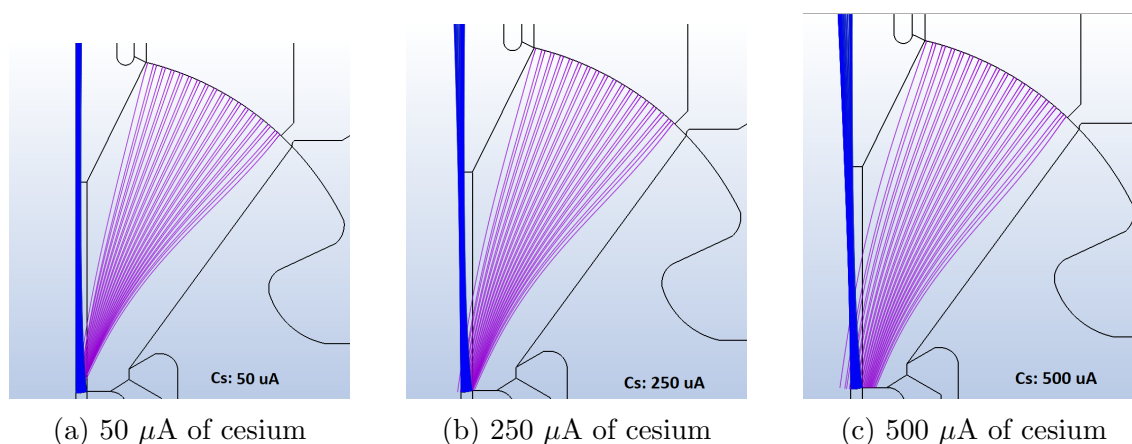


Figure 5.13: The self-repulsion with increasing current of cesium is already evident looking at the simulations. Though not explored in this batch, the negative ions appear to also be affected.

beams were kept as they were for previous batches. Apart from the target aperture, all of the geometry was per the original SO-110C design.

5.6.3 Results

As seen pictorally in Figure 5.13 and graphically in Figure 5.14, lower current beams of cesium have a better accuracy due to a reduced self-repulsion by their own space charge. From 50, through 250, to 500 μA , the percentage of the cesium current that hits the sample drops from 100%, through 94%, to 32% respectively. If this is indeed the case, that means that achieving a high cesium flux with sufficient accuracy would require a redesign of the geometry to compensate for the space charge repulsion. One proposed offset would be to recess the target away from the ionizer to allow more time/space for a high current cesium beam to come to a focus.

Figure 5.15 shows the current and current densities of the rays of cesium. The vertical scale is identical to that of Figure 5.11a for ease of comparison. Both graphs were generated using the same geometry. The only difference is one emitted approximately 560 μA of cesium governed by Child's Law of limited emission while the other emitted exactly 500 μA , distributed across the surface of the ionizer with a uniform current density. From this, one can intuit the contribution of Child's Law based setting of current emission added onto the existing geometric artifact. Child's Law adds extra current to the parts of the ionizer furthest from the axis. Both are approximations of emission because the true emission may also be partially governed

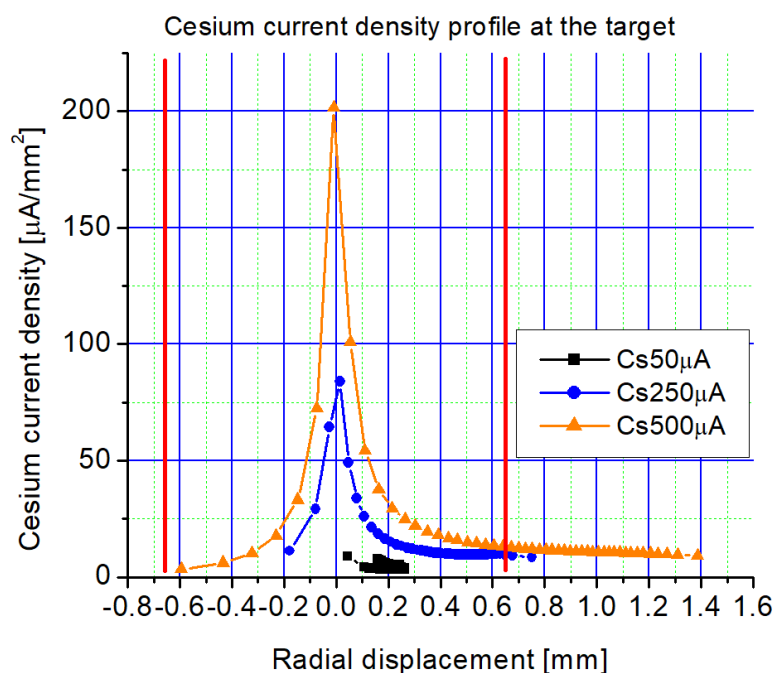


Figure 5.14: The difference in coverage on the target changes dramatically over the course of ramping the cesium current from 50 to 500 μA .

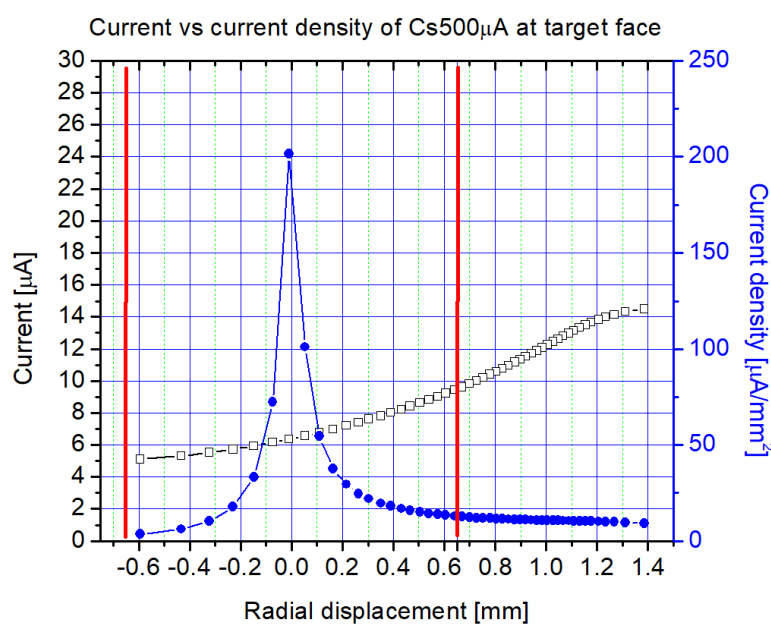


Figure 5.15: Current and current density plotted together for the same rays using the original non-protruded aperture geometry. Note, the current density is taken at the terminal point of each ray where they impinge on the target face. The red lines represent the extents of the sample.

by the rate of arrival and spatial density of cesium atoms effused from the six holes in the shroud onto the ionizer.

When considering these results and contemplating whether Child's Law emissions in the neighbourhood of 560 μA was realistic - with no simple way to measure

the cesium current directly - some simple estimates were calculated (C. Tiessen, W. Kieser, & X. Zhao group discussion). A single ampule, containing 5 g of ^{133}Cs , typically lasted an entire year of analysis. At an average usage rate of $250\ \mu\text{A}$ or $500\ \mu\text{A}$, the ampule would be completely used up in about 170 or 80 days respectively. Given that the accelerator at Lalonde AMS runs often for 24 hours a day and 7 days a week during routine analysis with periodic (un)planned maintenance, sample switching, and other forms of down-time, the 170 day estimate given by $250\ \mu\text{A}$ made more sense than 80 days. The next batch of target recess tests was designed to better confirm this hypothesis.

5.6.4 Summary

This batch demonstrated the importance of the cesium space charge effects on its own (de)focusing. The next batch of simulations would build on this knowledge to test some estimates while also targeting an improved design for carbon emission.

5.7 Simulation: Target recession tests on carbon - preliminary simulation

5.7.1 Motivation

The previous batch demonstrated that there is a substantial difference in the distribution and accuracy of the cesium beam at $250\ \mu\text{A}$ as compared to near the Child's Law limit (at 7 kV) of about $560\ \mu\text{A}$. At the higher current, the positive charge self-repulsion causes as much as 70% of the cesium current to miss the sample. It seemed unlikely that this is what occurs in reality. A rough calculation of the cesium ampule depletion rate over a year of routine analysis suggested that the real current may be much lower than this limit. However, even at $250\ \mu\text{A}$, there is still some cesium current that is repelled to miss the sample. The hypothesis: recessing the target (translating it along the axis of symmetry away from the ionizer) while holding all other geometry fixed would give the cesium ample space/time to come to a better focus on the sample. Better cesium accuracy and focusing would ideally increase the negative ion flux as well.

To verify whether routine operations had a high (about 560 μA) or low (about 250 μA) current, both would be simulated and an experiment would be run testing various target recesses to determine the appropriate settings.

5.7.2 Setup

Rijke Version $\eta 3$	Lorentz-2E Version 10.1	Source Model SO-110C	Batch # 24
Cs Mode Assigned I Child's Law	Current 250 μA $\approx 560 \mu\text{A}$	Negative Ions $^{12}\text{C}^-$ $^{12}\text{C}_2^-$	Current 40 μA 20 μA
Target Assembly Potential -35 kV (w.r.t ground)		Ionizer Assembly Potential -28 kV (w.r.t ground)	
Aperture Version AEL-Bmod		Geometry Variation Target Recess	

Table 5.7: For both Child's Law limited and an assigned cesium current of 250 μA , simulations were run examining target recessions of 0, 1, 2, 3, and 5 mm

Table 5.7 shows the setup for this batch. The target was recessed in steps of 1 mm from 0 to 5 mm, skipping 4 mm for time purposes. The simulation was run for cesium in Child's Law limited emission mode and then repeated in assigned current (of 250 μA) mode.

5.7.3 Results - AEL-Bmod Aperture

Table 5.8 gives the accuracy of the cesium beam as a proportion of the total current and Figure 5.16 shows the distribution of the rays on the sample surface. The assigned current mode achieves the best coverage of the sample somewhere between 0 and 1 mm target recess while the same of the Child's Law emission occurs between 2 and 3 mm. This clear difference is ideal for distinguishing performance by experiment.

5.7.4 Summary - Transition to AEL-Cmod results

While these were the results with which to compare at the time, they were done using a different target aperture and electrode potentials than those used in the

Description	Cesium current [μA]	% hit sample
Child0mm	560	29
Child1mm	560	48
Child2mm	558	85
Child3mm	559	96
Child5mm	556	89
Assign0mm	250	94
Assign1mm	250	100
Assign2mm	250	100
Assign3mm	250	100
Assign5mm	250	0

Table 5.8: All cesium rays hit the target in each simulation. The percentage of the total current that hits the sample is presented above for both sets. Recessing the target makes for very small changes in the Child’s Law limit.

later experiment. They were also run with a version of Rijke that predated negative ion emittance results. They showed that the target recess tests held promise for determining which mode of cesium was realistic while potentially also improving the output in a meaningful way. The simulations would later be re-run with parameters that better reflected the experiment setup for a more meaningful interpretation found in Section 5.9.

5.8 Experiment: Target recession tests on carbon

5.8.1 Motivation

See Section 5.7.1 for more details. This experiment was run in parallel to those simulations to ascertain what mode of cesium was used in actuality.

5.8.2 Setup

Custom target bases allowing target recesses of 1, 2, 3, 4, and 5 mm were designed and created in the University of Ottawa machine shop. The targets could remain the same size so that the samples could be pressed into the target without modifying the pressing apparatus. The targets would then screw into the custom bases. One unrecessed sample and the five recessed samples were pressed with Alfa-

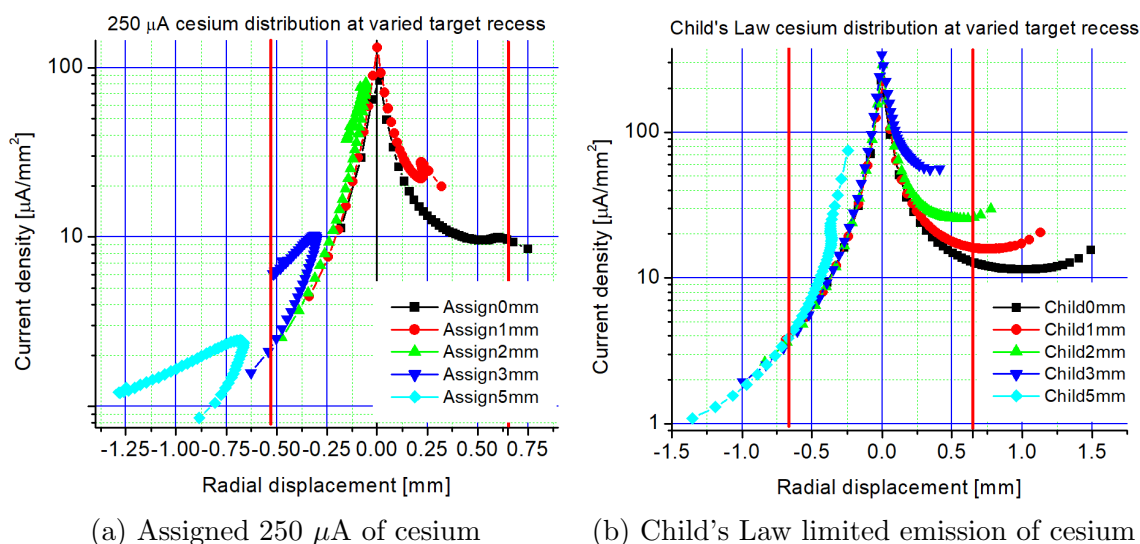


Figure 5.16: The cesium current density distribution on the face of the target is shown with the sample limits specified by the vertical red lines. Data from both high and low cesium current modes are present for each target recess simulated.

Aesar graphite blank material. These samples were analyzed as part of a larger routine batch of carbon samples unrelated to this experiment. Thus, the tuning of the accelerator components was optimized for unrecessed targets and not adjusted between batch measurements.

The T-I P was 6 kV and the extraction potential difference was 29 kV, yielding a total source energy of 35 keV. The samples ran for 11 turns of 15 blocks, each lasting 20 seconds.

Note: the AEL-Cmod aperture was used in this experiment.

5.8.3 Results

Figure 5.17 shows that the average currents of ^{12}C and ^{13}C behaved similarly at the six different recess settings. The output of carbon peaks at the 1 mm recess but then falls off exponentially with increased target recess.

If one examines the performance over time, shown in Figure 5.18, one can see that the output of the unrecessed target peaks early and then decays rapidly. The 1 mm recessed target peaks at a slightly lower current but is sustained for more blocks resulting in a higher average current. It is the most stable of the two. Following this, the 2 through 5 mm recessed targets produce constantly weaker

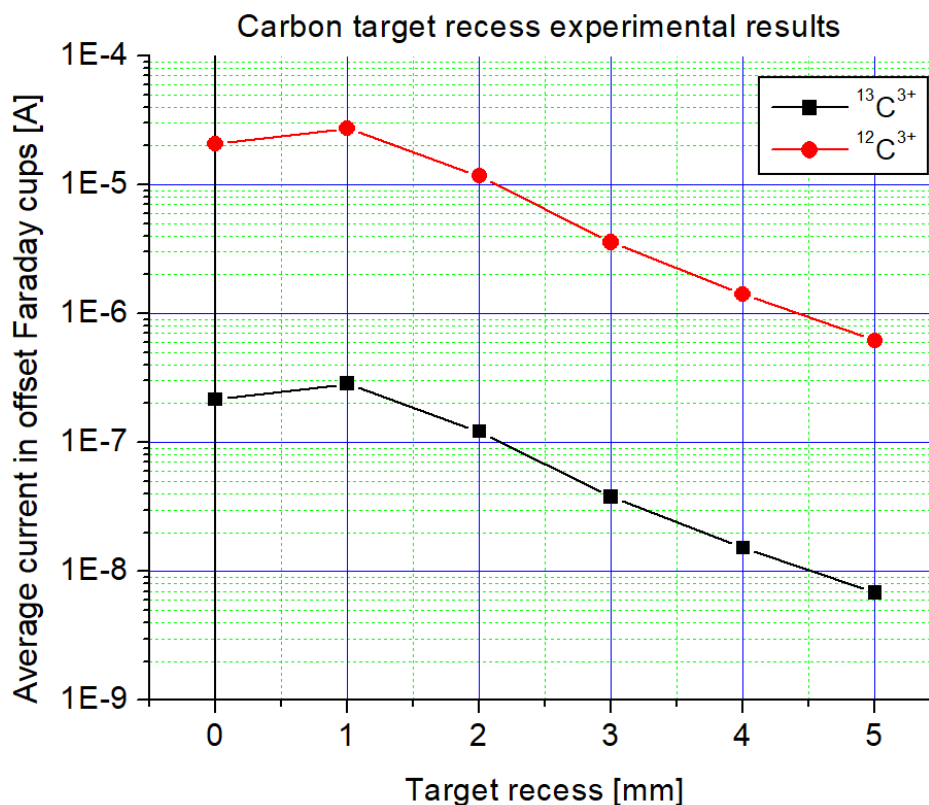


Figure 5.17: The average currents (uncorrected for charge state) of ^{12}C and ^{13}C in the high-energy offset Faraday cups are presented in red and black respectively for each of the six different target recess settings. They are plotted on a logarithmic scale to fit both ^{12}C and ^{13}C on the same plot despite the two orders of magnitude difference in abundance.

currents.

Close-up images of the faces of each of the six targets can be seen in Figure 5.19. The 0, 1, 2, and, surprisingly, 4 mm recessed target samples sputtered to the pin while the 3 and 5 mm ones did not. It is clear that the 1 mm recessed target has the highest coverage/usage of the sample material due to it having the widest hole. This is more in line with the low ($\approx 250 \mu\text{A}$) cesium current simulation result as will be more accurately portrayed in Section 5.9

Also of note is the “halo” of deposition on the target face outside of the sample. Because of the manner in which the craters peak in usage at the 1 mm recess, it is suspected that this halo is not resulting from the primary cesium beam originating from the ionizer. Rather, this deposition may be from cesium that has ionized on other hot surfaces near the ionizer like the shroud. The approximate diameter of this halo is 3.0, 3.8, 4.7, and 5.3 mm for the 0, 1, 2, and 3 mm recessed targets respectively. At 4 mm recess, the entire surface of the 6 mm diameter target is

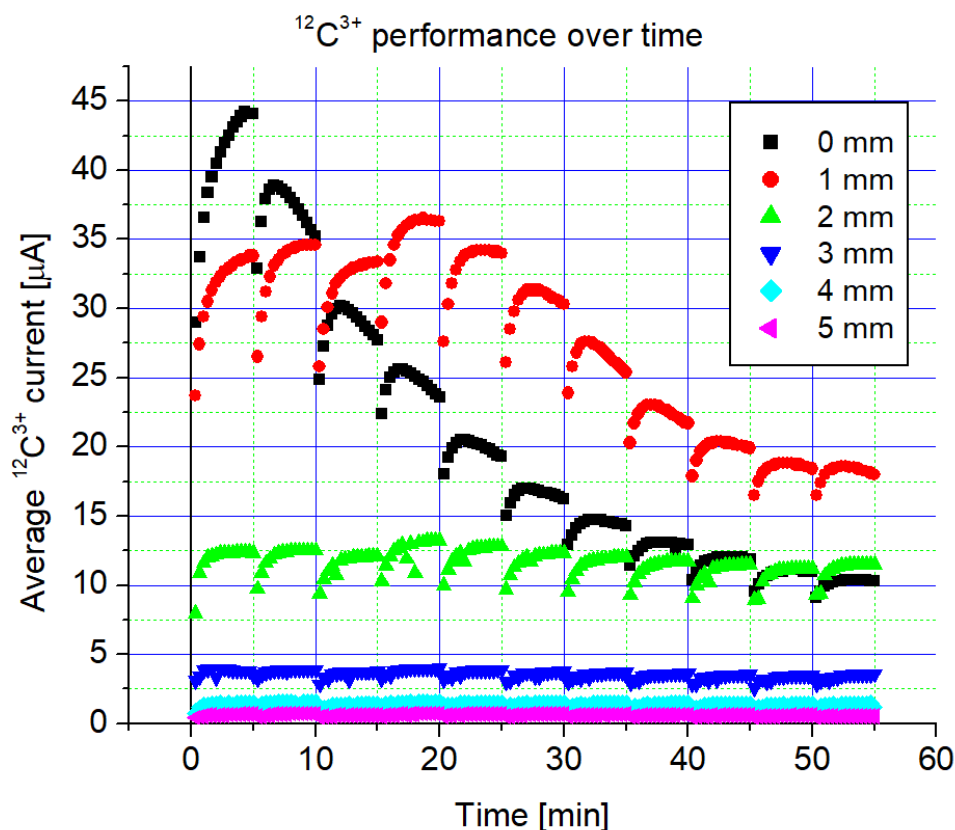


Figure 5.18: For each target recess setting, the raw (uncorrected for charge state) current of $^{12}\text{C}^{3+}$ collected in the offset Faraday cup is presented above. Each target was sputtered for all eleven turns of fifteen blocks of measurement, lasting 20 seconds each.

covered. This is also true for the 5 mm recessed target; however, the deposition appears more sparsely spread out, resulting in a less reflective appearance. The cesium trajectory causing the halo is overfocused at the unrecessed geometry and widens further at increased target recess.

The settings in this experiment are similar to the routine settings used on the SO-110B version prior to the source upgrade. Cesium oven temperatures at Lalonde AMS are nominally around 110 to 120 °C. However, the SO-110C is capable of running at higher ion energies, electrode potentials, and cesium fluxes. In the paper by Klein and Mous [30] from HVEE detailing the SO-110C, a similar study was performed using a T-I P between 9 and 10 kV and a cesium oven temperature of 135 °C. At these settings, they performed a similar target recess experiment and found the optimum recess at 2 mm, yielding a $^{12}\text{C}^-$ current of 350 μA from graphite samples. The ion source energy was not explicitly stated in this paper but it is likely the source was also operated at higher energies than the 35 keV setting used in this

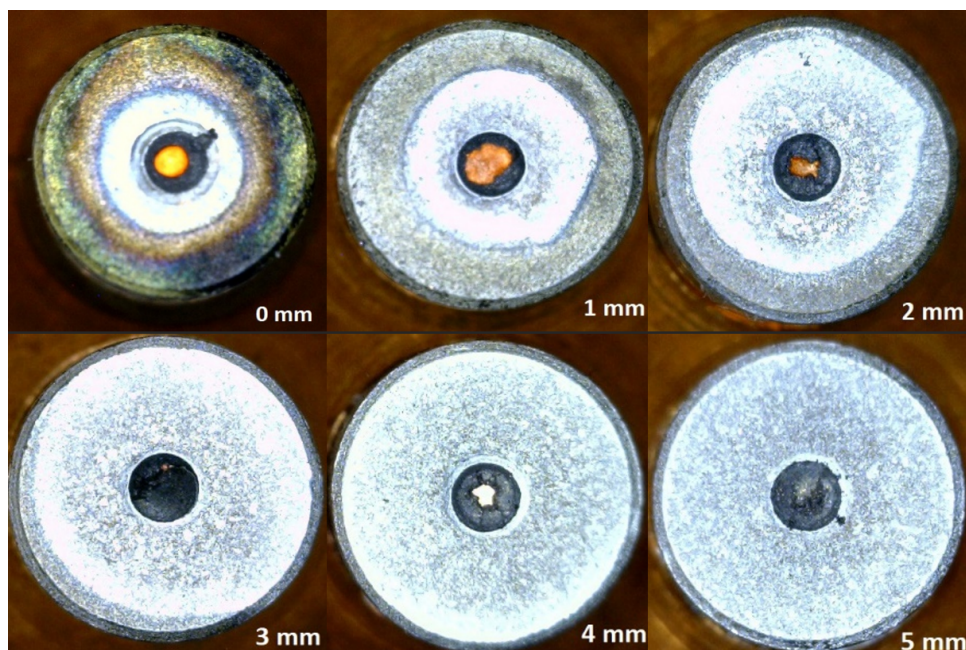


Figure 5.19: High resolution photographs of the target faces post-sputtering. Target recesses 0, 1, 2, and 4 mm are cratered to the copper pin behind the sample. The crater of the 1 mm recess was the widest and had the best usage of the sample material. A halo of cesium deposition on the target face - seen as the bright ‘silvered’ region external to the sample - thought to originate elsewhere from the ionizer is overfocused and expands with increased target recession.

experiment. Nevertheless, even at the lower output settings in this chapter, the simulation software has demonstrated its value for informing improved operation.

5.8.4 Summary

At the settings used in this experiment, the 1 mm recessed target was found to have the most sustained high output and best usage of the sample material. This is in agreement with the lower ($\approx 250 \mu\text{A}$) cesium current mode. Thus, it is likely that the amount of cesium emitted is not near the Child’s Law limit predicted by Lorentz-2E. Also noticed in this experiment is a “halo” of cesium deposition that is overfocused in the original SO-110C geometry and broadens as the target is recessed further.

5.9 Simulation: Target recession tests on carbon - post-experiment simulation

5.9.1 Motivation

Section 5.7.1 covered the initial motivation for this study and presented preliminary guideline predictions for what to expect. However, the settings in those simulations were not the same as those used in the experiment, as detailed in Section 5.8. This batch re-examined the simulations while setting geometric and electrostatic potentials to what they were in the experiment for a better comparison with the results.

5.9.2 Setup

Rijke Version $\theta 3$	Lorentz-2E Version 11.0	Source Model SO-110C	Batch # 36
Cs Mode Assigned I Child's Law	Current 250 μA $\approx 430 \mu\text{A}$	Negative Ions $^{12}\text{C}^-$ $^{12}\text{C}_2^-$	Current 40 μA 20 μA
Target Assembly Potential -35 kV (w.r.t ground)		Ionizer Assembly Potential -29 kV (w.r.t ground)	
Aperture Version AEL-Cmod		Geometry Variation Target Recess	

Table 5.9: For both Child's Law limited and an assigned cesium current of 250 μA , simulations were run examining target recesses of 0, 1, 2, 3, 4 and 5 mm. Routine operations of the SO-110C had shifted from 7 kV target potential difference to 6 kV. The AEL-Cmod aperture was modelled and implemented in Rijke for this simulation.

Table 5.9 shows the setup for this batch. The target was recessed in steps of 1 mm from 0 to 5 mm. The simulation was run for cesium in Child's Law limited emission mode and then repeated in assigned current (of 250 μA) mode. As it turned out, the 7 kV target potential difference was the norm for routine analysis of carbon using the SO-110B and initially the SO-110C; however, over time Lalonde AMS adopted 6 kV as a better setting for the SO-110C. This simulation was run later to

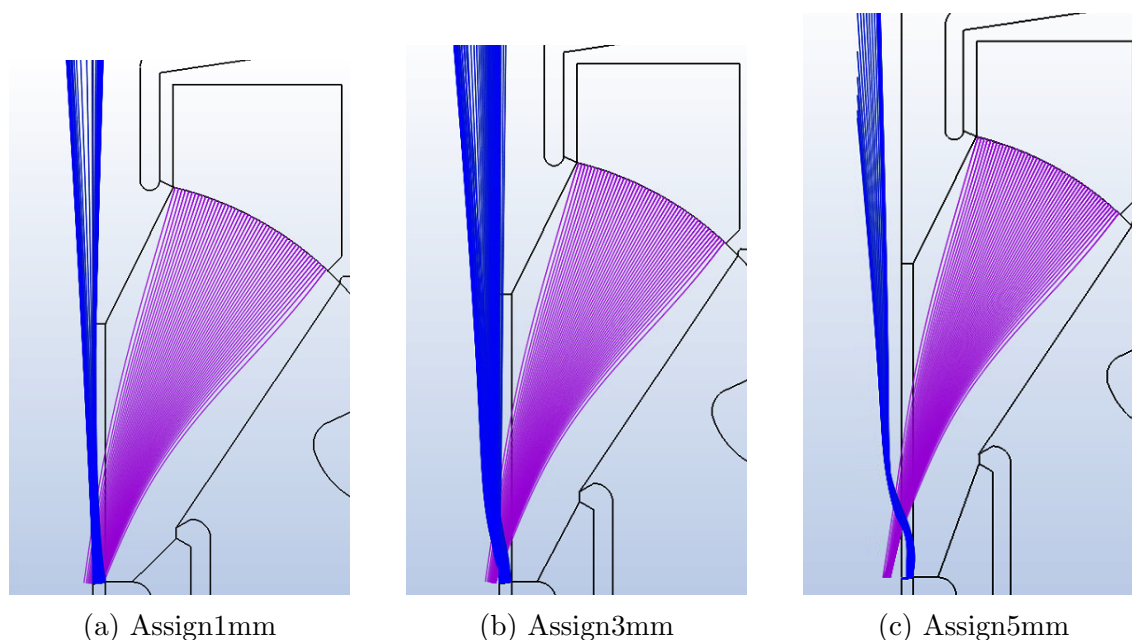


Figure 5.20: Images of the interaction region in Lorentz-2E for the assigned cesium current ($250 \mu\text{A}$) simulations of 1, 3, and 5 mm target recess are shown. Each image shows iteration 20/20 of the simulation. The current assigned to the negative ion beams in Assign5mm were too much to be extracted by the ambient field and the distant positive space charge. Thus, the negative ion emission in this case was a failure. Violet rays are Cs^+ and blue are $^{12}\text{C}^-$.

be more consistent with the experiment that was conducted. Of particular note is that the AEL-Cmod target aperture was used in the experiment and therefore also in this batch of simulations.

5.9.3 Results - AEL-Cmod Aperture

Figures 5.20 and 5.21 show the half beams of the two current modes for the 1, 3, and 5 mm target recesses for comparison. These provide visual context for the following analysis and discussion.

In Rijke version $\theta 3$, the code was updated to split the scoring of cesium accuracy into two components:

1. Cesium accuracy: the percentage of the total emitted current that impinges on the sample
2. Cesium coverage: the percentage of the sample surface that was covered by the cesium rays.

Multiplying the two percentages together gives the “cesium product” which acts

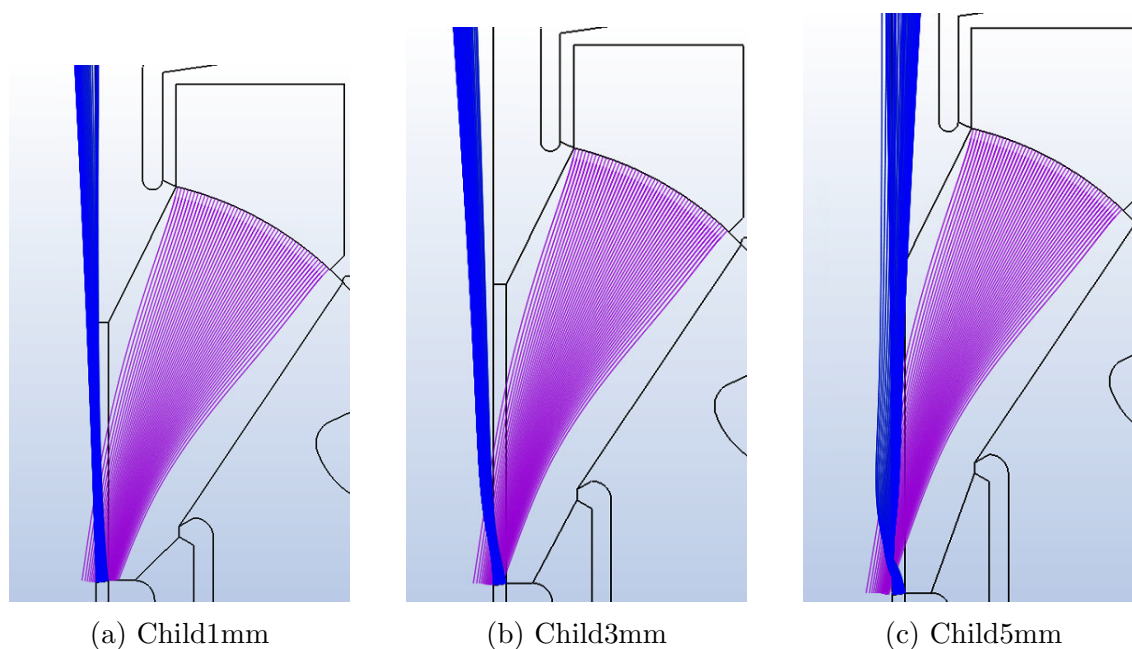
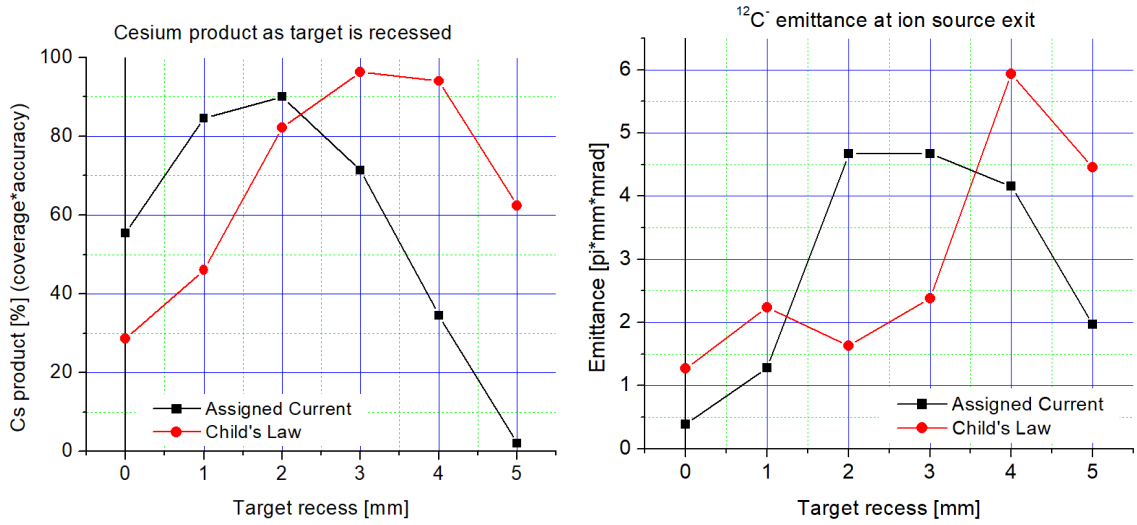


Figure 5.21: Images of the interaction region in Lorentz-2E for the Child's Law cesium current ($\approx 430 \mu\text{A}$) simulations of 1, 3, and 5 mm target recess are shown. Each image shows iteration 20/20 of the simulation. Violet rays are Cs^+ and blue are $^{12}\text{C}^-$.

as a quality factor for cesium distribution on the sample surface to be optimized. While increasing the accuracy of the cesium rays is an obvious improvement, it is also important for the sample to be covered well by its flux. Due to the cylindrical geometry, the majority of the sample volume is found at higher radii from the axis of symmetry. Thus, it is critical the cesium beam access the highest radial extents of the sample material.

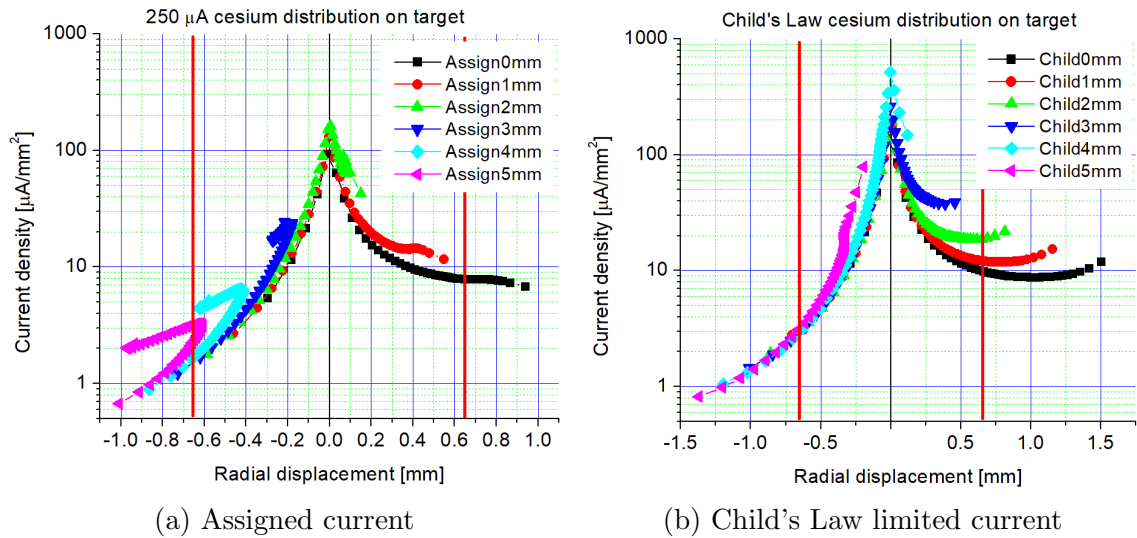
Figure 5.22 show plots of the cesium product as well as the emittance of the outgoing negative ion beams for each of the target recesses and current modes. It is evident that the earlier peak of the assigned current mode more closely resembles the output of the experiment. Thus, the Child's Law simulations will be neglected for the remainder of this discussion. While the value and shape in phase space of the accelerator acceptance is not known, minimizing the emittance to increase the likelihood of it matching the acceptance is a goal. The emittance was low for the 0 and 1 mm assigned current run but then rose sharply at target recesses above 1 mm.

If one compares the simulated cesium products in Figure 5.22 with the experimental results in Figure 5.17, one will notice that the 1 mm target recess had the highest output of carbon experimentally while the simulated best coverage is at a



(a) Cesium product (% of sample face covered by cesium rays $\times$ % of cesium current hitting the sample) (b) Emittance at the exit (collector segment at the end of the extraction electrode) of the ion source

Figure 5.22: When compared, the cesium accuracy-coverage product peaks earlier for the low assigned cesium current mode over the Child's Law mode. The emittance of the negative ion beam rises sharply in the low current mode after a 1 mm target recess.



(a) Assigned current

(b) Child's Law limited current

Figure 5.23: The cesium current densities for each of the recesses are presented above for the two different cesium emission modes. Red vertical lines indicate the limits of the 1.3 mm diameter sample. Note that the distribution of current density from rays impingent on either side of the axis seen above, due to the rotational symmetry also applies equally at the same radial position on the opposite side of the axis.

2 mm recess. Three probable reasons for this discrepancy are as follows:

1. First, Figure 5.23a shows the distribution of Cs on the target face. Both the 1 and 2 mm recess have excellent cesium coverage on the sample. However, in the case of the 2 mm recess, most of the rays are on the negative side of the axis with radial momenta away from the axis. Due to this momentum, as the cesium beam bores into the sample, the rays close to the edge may hit the walls of the sample instead of boring through more sample. Since most of the rays in the 1 mm case impinge on the positive side of the axis with a radial momentum towards the axis of symmetry, they will continue to bore into more sample as it is cratered.
2. The rays originating from the outer-most part of the ionizer, carrying the most current, are strongly focused on the centre of the sample for the 2 mm recess but impinge on the outer portion of the 1 mm recessed target. A high current density on the central axis is an inevitable result of the cylindrical symmetry, but having the higher current rays hit the outer portion of the sample could be why the 1 mm recess had a more stable and sustained emission with better usage of the material. In the region from 0.2 mm from the axis of symmetry to the edge of the sample at 0.65 mm, the 1 mm target recess simulation has the highest sustained current density. This is likely why it gave the most stable output and highest use of the sample material as seen in Figures 5.18 and 5.19.
3. As will be further expounded below, the recession of the target relative to the aperture weakens the penetrating field acting on the surface of the sample and makes the output more unstable. It may also be a detriment to the sputtering and negative ion efficiencies. The role of space charge then becomes more important. This may be at least partly responsible for the increase in emittance seen in Figure 5.22b. It is unknown to what degree this increased emittance could contribute to the reduced output of targets recessed beyond

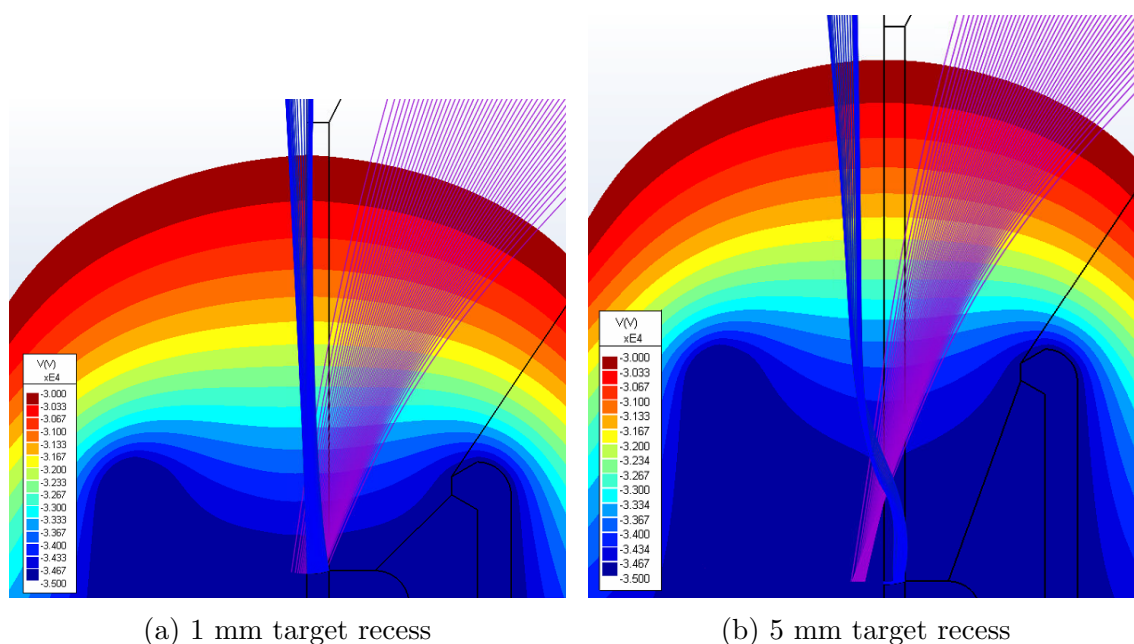


Figure 5.24: The equipotential lines from -35 kV to -30 kV are presented for the 1 and 5 mm target recesses in assigned current mode.

1 mm but it remains a concern nonetheless.

Figure 5.24 shows the equipotential lines near two selected targets in assigned current mode. As mentioned above, the strength of the field at the target surface is shielded by the aperture as the target is recessed. This weakens the extracting field, which culminated in the failure of 5 mm target recess simulation.

Recalling Figure 5.19 where the targets were examined post-sputtering, there was a reflective deposition on the target face presumed to be due to cesium that increased in diameter with increasing target recess. It was suggested that this is not likely from the primary cesium beam because the sample cratering behaved similarly to what was predicted by the primary beam simulation. This “halo” of cesium deposition was suggested to have originated from cesium ionizing on surfaces other than the ionizer. Due to its close proximity to the ionizer, the shroud is the most likely source of this cesium.

As a proof of concept, the 2 and 4 mm target recess simulations above were modified to emit an assigned cesium current of $200\ \mu\text{A}$ from the ionizer and $50\ \mu\text{A}$ from the inner lip of the shroud closest to the ionizer - maintaining a total of $250\ \mu\text{A}$. Figure 5.25 shows the results of these simulations. This halo beam is overfocused and impinges on the target face further from the axis of symmetry as the target is re-

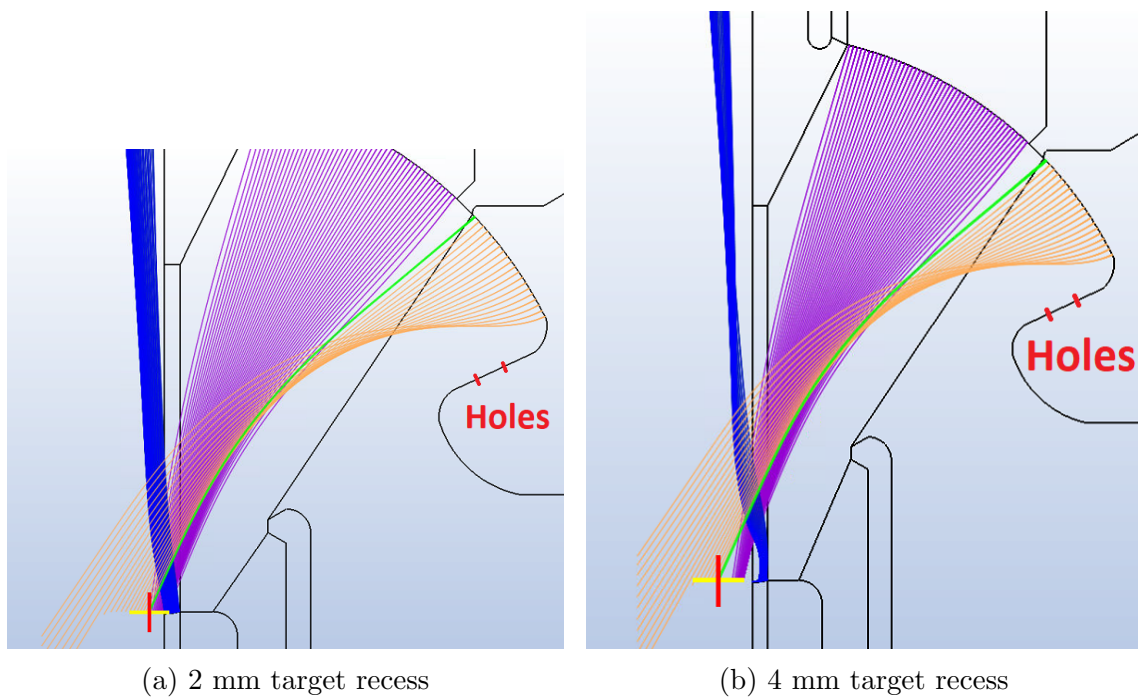


Figure 5.25: In this manual simulation, the assigned current of the primary cesium beam from the ionizer (violet) was reduced to $200\ \mu\text{A}$. $50\ \mu\text{A}$ was assigned to a small section of the shroud (orange) and simulated with identical conditions to others in this batch. Using Lorentz-2E's Trace Along Ray function on the inner-most ray (outlined in green) showed the rays closest to the ionizer are bent to hit closest to the axis of symmetry. Where it impinges on the target face is represented by the yellow and red cross-hair.

cessed further. This was seen in the deposition on the targets. While this simplified simulation assigned current to the entirety of this single segment of the shroud, due to its position relative to the holes that spray the cesium onto the ionizer, the rays further from the ionizer are increasingly unlikely to encounter this spray of cesium. Thus, only the rays closest to the ionizer are likely contributing to the halo. This appears to match well with the deposition profile in Figure 5.19.

5.9.4 Summary

By comparing this simulation batch with the experimental data, it is apparent that the amount of cesium emitted in the ion source is likely in the neighbourhood of $250\ \mu\text{A}$ and not the Child's Law limit ($\approx 430\ \mu\text{A}$ at 6 kV target potential difference). The results suggest that having the highest current rays impinge on the sample on the positive side of the axis and further from the axis is useful in producing and maintaining a stable output. Recessing the target weakens the extracting field at the surface of the target. This puts an electrodynamic limit on the amount of current that could be extracted regardless of sputtering kinetics. It also increases the dependence of the output on the cesium space charge, which detracts the outgoing carbon emittance.

5.10 Experiment: Target recession and target potential ramp with beryllium

5.10.1 Motivation

In much the same way as carbon, a preliminary simulation of cesium accuracy as a function of target recess was performed for beryllium (BeO^-). This time, the focus was on approaching the Child's Law limit of cesium emission by raising the cesium oven temperature to try and coax more BeO^- from the sample. ^{14}C is already measured at satisfactory currents for precise and timely analysis, so the focus shifted to ^{26}Al and ^{10}Be . Both suffer from much lower sputtering efficiencies resulting in lower output currents than carbon. Beryllium was chosen because it was the nearest

(in time) isotope to be measured in the Lalonde AMS measurement schedule and there was a perceived need to increase the BeO^- current.

The settings of the preliminary simulations preceding the experiment used the AEL-Bmod aperture. The results of those simulations are of little academic value compared with the post-experiment simulations (Section 5.11) using the correct aperture matching that of the experiment. Therefore, they will not be detailed here. Similar to the carbon case in Figure 5.16, the preliminary simulation suggested that a target recess between 2 to 3 mm would optimize the cesium product (see Section 5.9.3 for a description of this product) at cesium currents approaching the Child's Law limit. This experiment would attempt to raise the cesium current from the typical routine settings by increasing the cesium oven temperature. The self-repulsion would be mitigated by a combination of recessing the target and adjusting the T-I P. The goal was to achieve a higher output by scanning broadly with these parameters.

5.10.2 Setup

For each of the target recesses of 2.0, 2.5, and 3.0 mm, five bases (fifteen total) were made. The sample material was loaded into copper targets and pressed from behind with a copper pin at a pressure of about 3.2 bar. The samples contained Nishiizumi ^{10}Be reference material mixed with a Nb:BeO ratio of 4:1 by weight. The $^{10}\text{Be}/^9\text{Be}$ ratio of this reference material was 2.85×10^{-12} [68]. An unrecessed base and the 2 and 3 mm recessed bases from the previous carbon study (Section 5.8) were also included for a total of eighteen samples.

After the first day of exploratory measurements on these bases, it was clear that all three recessed settings gave inferior outputs to the typical unrecessed geometry. To salvage the study, the unsputtered targets were switched to the bases with recesses of 1, 2, 3, and 4 mm that were created for the carbon target recess study to better examine the trend across a wider recess range. In addition, a set of ten targets were screwed onto unrecessed bases in case an improved measurement setting was found during the experiment.

5.10.3 Results

Exploratory settings

On the first day of measurements, the accelerator was tuned first to optimize the transmission of the unrecessed target per routine settings. The cesium oven temperature was raised from 110 °C to 130 °C and allowed to stabilize. Cycling through all the target recesses and quickly (a few seconds) noting their output current at target potential differences of 4-10 kV showed that the unrecessed target gave the highest output. The $^9\text{Be}^{2+}$ current measured at the offset Faraday cup decreased with increased target recess. The ^{10}Be counts were measured in the GIC. A sample plot of the energy spectrum in the GIC from this experiment was described in Figure 2.11.

To confirm that the lower output of the recessed targets was not caused by tuning, which was optimized for the unrecessed target, the 2 mm recessed target was inserted and all electrostatic components other than the magnets and ESAs were tuned. None of the components gave any significant improvement. The tuning was reverted to the unrecessed-optimized settings.

One thought was that at 130 °C on the cesium oven, the cesium current was still well below a level where space charge broadening was important. At increased currents, the recessed target performance was expected to improve. The temperature was raised to 140 °C and then again to 150 °C and allowed to settle. At each temperature, a similar study was performed on each of the recessed targets, ramping the target potential difference. Only the relative currents between recesses were compared during this short study. This is because these tests were performed on the same samples each time and the absolute current sputtered from the samples changes depending on how long the sample has been sputtered (e.g. Figure 5.18). Raising the cesium oven temperature did appear to improve the recessed targets relative to the unrecessed one as expected; however, they were still emitting significantly less current than the unrecessed target. The targets were changed as mentioned in the setup for a more systematic set of measurements on the next day.

5.10.4 Systematic Results

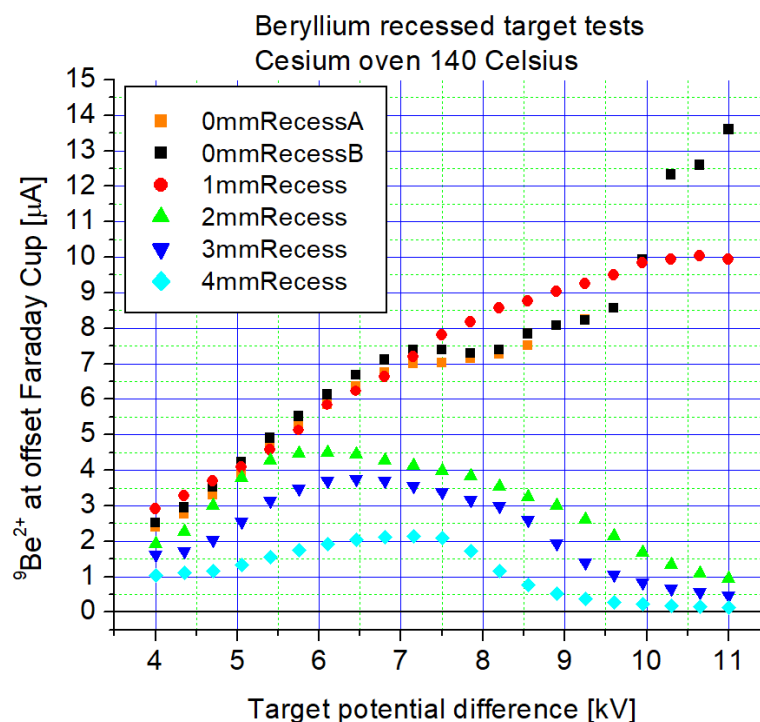


Figure 5.26: All five recessed geometries were tested first at 140 °C. The beryllium current was measured as a function of the target-ionizer potential difference. The 0mmRecessA was cut short when the extraction current was rising to dangerous levels. 0mmRecessB re-attempted the full scale of measurements but took extra time to let the source settle between changes. This sample would be revisited at other temperatures.

On the second day of study, the cesium oven was prepared and settled at 140 °C. This time, fresh targets were inserted and measurements began immediately. Using the virtual control function of the accelerator control software, the ion source was set to change the ionizer assembly potential from -31 kV to -24 kV in steps of 5% of the full 7 kV range. Concurrently, the T-I P was ramped from 4 to 11 kV, so that the target assembly and extraction cone were left at -35 kV and 0 kV respectively, giving the outgoing ions a consistent 35 keV of energy. The ${}^9\text{Be}^{2+}$ current at the offset Faraday cup was recorded at each step before quickly moving to the next. By dwelling only long enough to have a stable reading, the entire measurement could be completed on each recessed target before the overall current drifted significantly. The study was repeated at 130 °C and then 135 °C. The results, are shown in Figures 5.26 and 5.27.

The first challenge at 140 °C on an unrecessed target was that the extraction

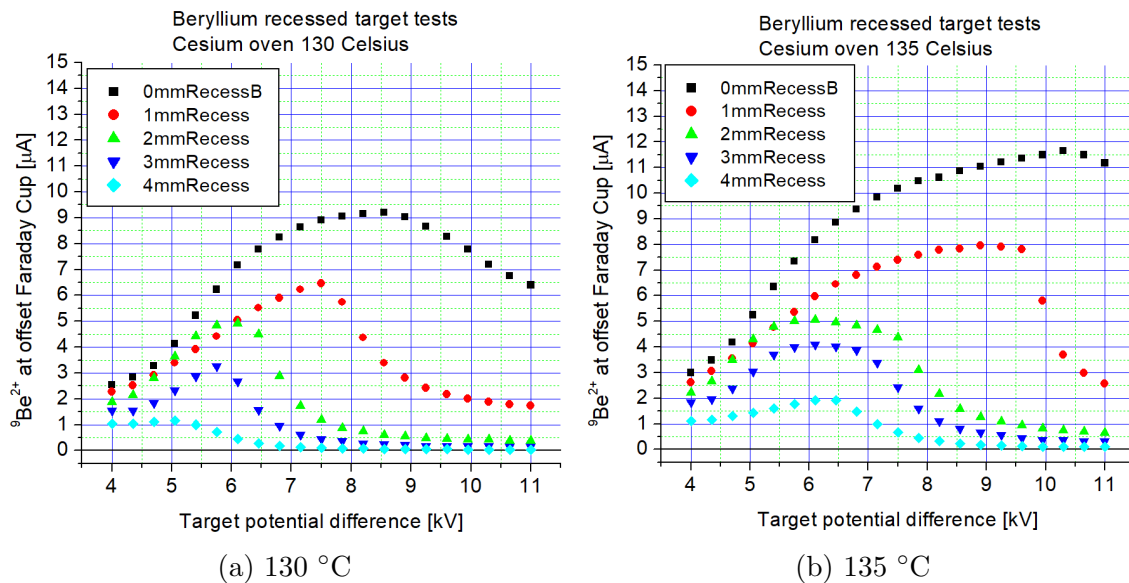


Figure 5.27: The beryllium current is plotted for 130 and 135 °C. Results for all five recessed geometries are plotted.

current, which indicates the total current between the ionizer assembly and the grounded extraction cone, was rising to near the limit of what the power supplies can manage. This worsened as the target-ionizer potential difference was raised and the ionizer-extraction potential difference was decreased suggesting the mechanism for the leakage originated from the interaction region rather than leakage current across the insulators. This effect was also worsened at higher cesium oven temperatures. This is possibly a result of poorly focused negative ions (not necessarily originating from the sample material) colliding with the inner hole of the ionizer base plate causing secondary electrons to spray onto the extraction electrode. Figure 5.28 shows the extraction electrode removed for cleaning following the experiment. The non-symmetrical pattern on the electrode is somewhat unexpected. Regardless, in 0mmRecessA, measurement stopped short to protect the ion source power supplies. However, a new unrecessed target (0mmRecessB) was attempted. It had much the same problem, but a few extra seconds of letting the source settle between changes allowed the source to survive the full 11 kV T-I P.

Examining all of the runs, target recesses in excess of 1 mm emitted much less current. Most of the recessed targets emit similar currents to the unrecessed target at 4 kV, begin to deviate from each other around 5.5 kV, and then experience a sharp fall off at varied potential differences and temperatures. Raising the temperature increases the potential difference at which the falloff occurs. At 140 °C, the current

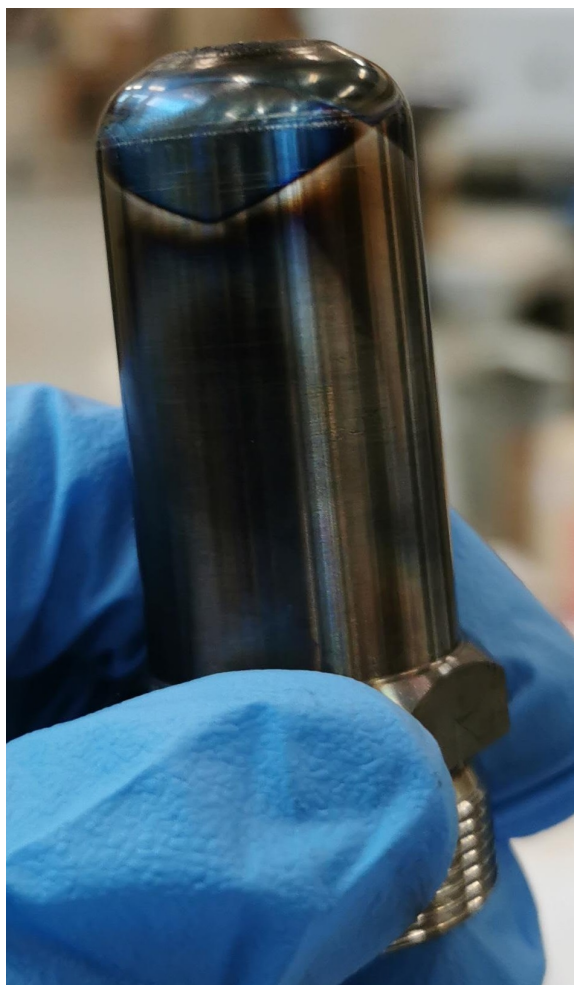


Figure 5.28: A burn pattern, likely from electrons colliding with the extraction cone. This is probably the reason for the elevated extraction current seen in the experiment.

of the 1 mm recessed target exceeded the unrecessed target from 7 kV to 10 kV as the unrecessed target experienced a peculiar depression in output. This depression was present for both the 0mmRecessA and 0mmRecessB targets. However, above 10 kV, the current from the unrecessed target suddenly increased to about $13.5 \mu\text{A}$, the highest level seen in the entire experiment.

Figure 5.29 shows the targets post-sputtering. The halo of cesium deposition, seen before in the carbon run in Figure 5.19, is present again. It appears to have behaved nearly the same as before. The main difference is that the sputter hole was widest on the unrecessed sample and not the 1 mm recessed one.

Despite the strange behaviour, these results were already promising. Measurements of ${}^9\text{Be}^{2+}$ at Lalonde AMS prior to this experiment had not exceeded $10 \mu\text{A}$ even at their peak output. This experiment so far had outdone that limit.

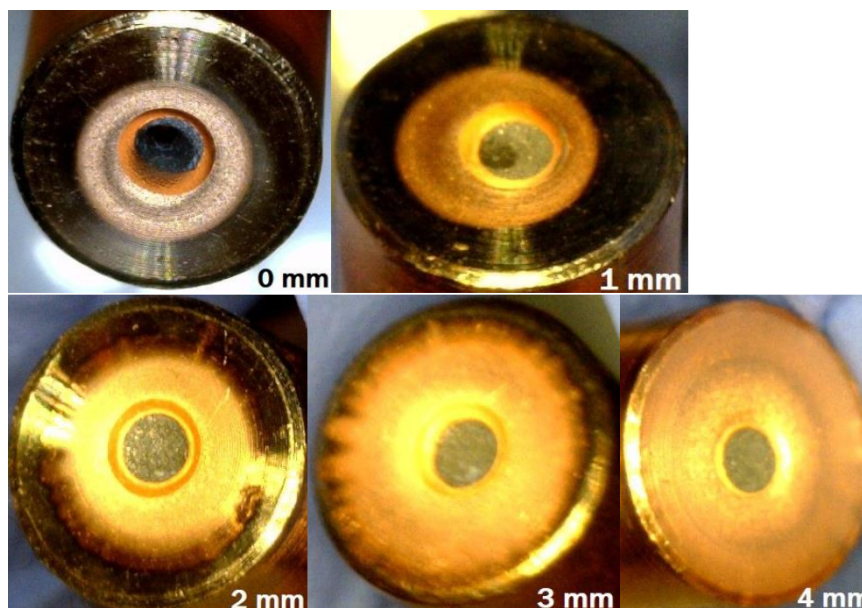


Figure 5.29: The recessed targets post-sputtering show a similar halo of cesium deposition outside the hole as the previous carbon recess experiment.

Stability batch - unrecessed

Based on the results in Figures 5.26 and 5.27 and the extraction current being problematic at higher cesium oven temperatures and potential differences, the ion source was set to 130 °C and a target-ionizer potential difference of 8.5 kV. This was where the unrecessed target peaked at that temperature and had an extraction current low enough to be confidently left running unattended overnight. A batch of ten unrecessed targets was run to examine the long-term stability of the samples under these conditions. The targets ran for 7 turns of 50 blocks, each block lasting 30 seconds. The results of this study are compared with all targets previously run at Lalonde AMS using the same material. Both can be found in Figure 5.30.

The output of this batch exceeded all previous measurements of the same reference material by a significant margin. Most of the samples peaked at 12 μA , which is more than double the average peak of previous measurements. In less than one hour, the targets in this batch achieved an excellent 0.5% precision on the $^{10}\text{Be}/^9\text{Be}$ ratio. In previous measurements, it took many hours of sputtering nearly the entire sample material to reach this precision.

The procedure for producing the lower graphs of Figure 5.30 was as follows:

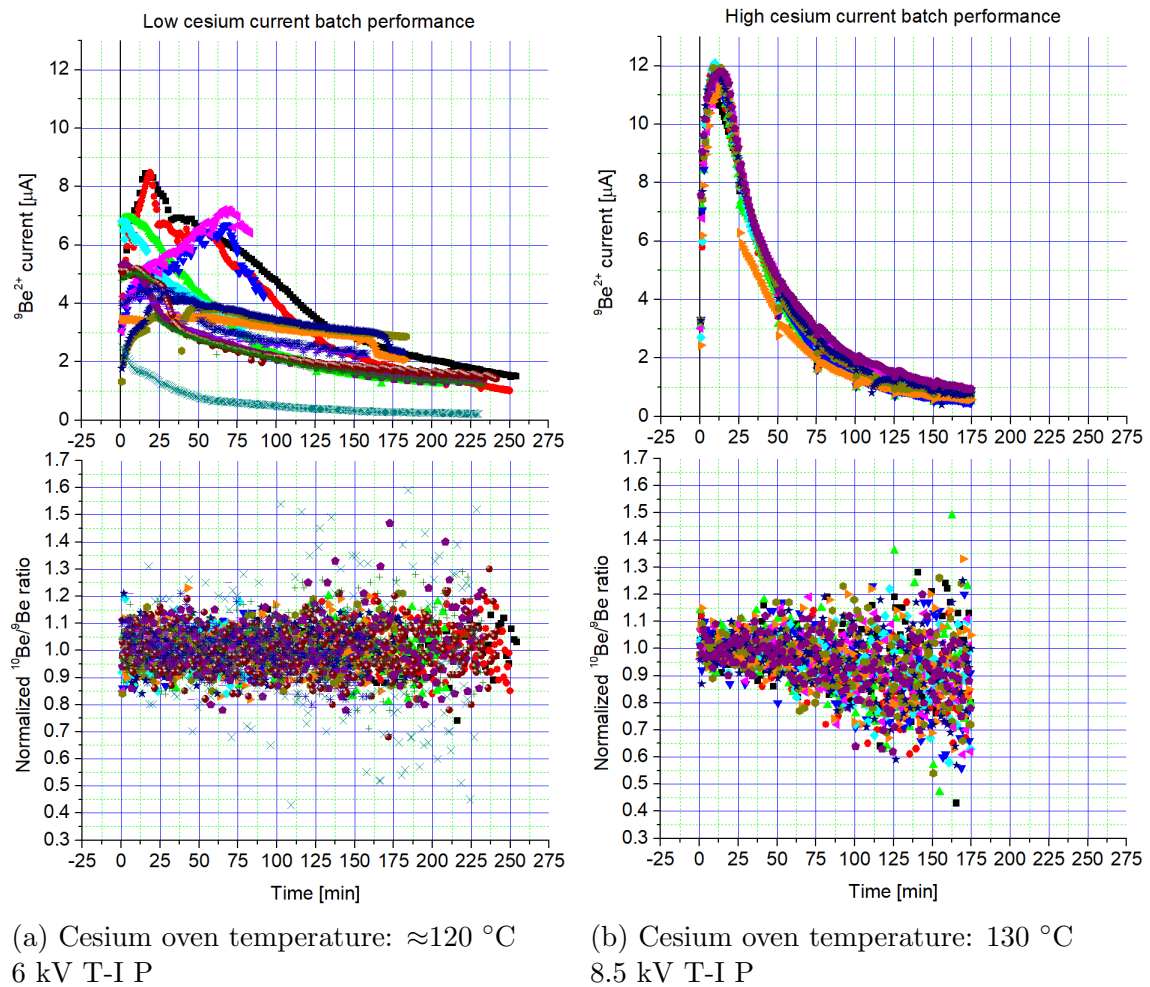


Figure 5.30: A comparison of Nishiizumi standard material samples measured previously (left) at Lalonde AMS and in this experimental batch (right). The top graphs give the raw (uncorrected for charge state) ${}^9\text{Be}^{2+}$ current as a function of time. The lower graph plots the measured ${}^{10}\text{Be}/{}^9\text{Be}$ ratio normalized to its reference value.

1. The raw ratio data points of each sample were used to calculate a current/counts-weighted mean for that sample.
2. For samples processed as part of the same batch and containing the same material, the mean of their individual weighted means was computed. For the purposes of this discussion, this will be called the “batch mean”.
3. The batch mean was then compared to the known $^{10}\text{Be}/^9\text{Be}$ ratio of the Nishizumi standard material to determine a normalization factor for that batch.
4. This normalization factor was then applied to each of the raw ratios to form the data points in the graphs.

Although all of the datasets provided used the same sample material and preparation technique, the accelerator tuning differed slightly between batches and measurement dates. In the case of the right graphs, all samples were measured as part of a single batch and would have the same batch mean and normalization factor. Data in the left graphs originate from multiple batches measured on different days. Each data set was normalized with its own batch mean and associated normalization factor.

In the case of the lower right graph of Figure 5.30, the normalized ratio appears to drift below unity as time progresses. This fractionation becomes the most apparent as the sample nears depletion. Initially, this may seem to be an issue, but must be considered in the context of the upper right graph. The ratio calculated from the weighted mean is dominated by the first 50 to 75 minutes of the measurement where the $^9\text{Be}^{2+}$ current, and associated ^{10}Be count rate, is high. Data points after 75 minutes, where the drift is most apparent, make little difference to this mean. These samples were measured to depletion to examine the effect over the course of sputtering the entire sample. A practical AMS measurement with the currents achieved in this batch would typically halt after 75 minutes as a satisfactory statistical significance has already been achieved. Measuring longer at low currents yields a diminishing return on the precision.

In a similar study of the SO-110C by Klein and Mous at HVEE [30], using a cesium oven temperature of 135 °C, a target recess of 2 mm, and a T-I P of 11 kV, 30 μA of $^9\text{BeO}^-$ was achieved on samples containing BeO mixed 1:1 with Nb pow-

der. Their settings were informed by simulations performed in Tricomp software by Field Precision LLC (techinfo@fieldp.com) which similarly includes space charge interactions. The ion source energy was not explicitly stated in this paper, but it is likely the source was operated at higher energies than the 35 keV setting used in this experiment.

5.11 Simulation: Target recess and target potential ramp with beryllium

5.11.1 Motivation

Following the experiment detailed in Section 5.10, and now including the correct geometry of the AEL-Cmod aperture (see Section 5.1.1), this batch of simulations would examine the behaviour of the ion source at three particular target potentials: 5, 8, and 11 kV. These were chosen due to the difference in behaviour each had from each other as seen in Figures 5.26 and 5.27. At these potentials, there were five main behaviours that were to be explored and explained by the following simulations:

1. At 5 kV T-I P the output of ${}^9\text{Be}^{2+}$ at the offset Faraday cup was low at 5 kV and below for all target potentials and cesium oven temperatures.
2. At 8 kV T-I P, the unrecessed sample begins with a relatively high output at 130 °C, improves at 135 °C, but then is lower at 140 °C.
3. At 8 kV T-I P, the 1 mm recessed sample begins with a low output at 130 °C, but increased output at higher temperatures.
4. At 11 kV T-I P, the output of the unrecessed target begins at a lower current than at 8 kV at 130 °C, but then increases as the temperature is raised to the highest achieved output.
5. At 11 kV T-I P, the 1 mm recessed sample output begins very low at 130 °C, only slightly higher at 135 °C, but then is greatly improved at 140 °C.

Rijke Version 03&4	Lorentz-2E Version 11.0	Source Model SO-110C	Batch # 35
Cs Mode Assigned	Current [μA] 175, 250, 325, 400 500, 600, 689, 985	Negative Ions $^9\text{BeO}^-$ $^{16}\text{O}^-$	Current [μA] 10 100
Target Assembly Potential -35 kV (w.r.t ground)		Ionizer Assembly Potential -30, -27, -24 kV (w.r.t ground)	
Aperture Version AEL-Cmod		Geometry Variation Target recessed 0 and 1 mm	

Table 5.10: At three potentials and two target recesses, the cesium current was ramped as high as allowed by Child’s Law

5.11.2 Setup

Table 5.10 shows the setup for this batch. The numbers 689 and 985 μA come from scaling a cesium current of 350 and 500 μA at 7 kV potential using the $V^{3/2}$ scaling of Child’s Law to what they would be at 11 kV. The Child’s Law limit at 7 kV is slightly above 500 μA , so 985 μA should be slightly below the limit for 11 kV. Lorentz-2E Version 11.0 introduced a corrected calculation for the negative ion emittance and Rijke was modified to acquire both it and the cesium product automatically as part of the post-processing code.

5.11.3 Results

When examined together, the emittances and cesium products at varied target recess, cesium current, and T-I P, as seen in Figure 5.31, provide insight for the behaviour of the five configurations mentioned above. It was estimated from the carbon target recess results and cesium ampule usage that typical operation of the ion source from about 110 to 120 °C cesium oven temperature was likely producing in the neighbourhood of 250 μA .

If one supposes that 130 °C cesium oven temperature produces somewhere between 250 and 325 μA and that the cesium current reached at 140 °C is about 400 μA (possibly even higher at 11 kV T-I P), then a plausible explanation for all five phenomena emerges:

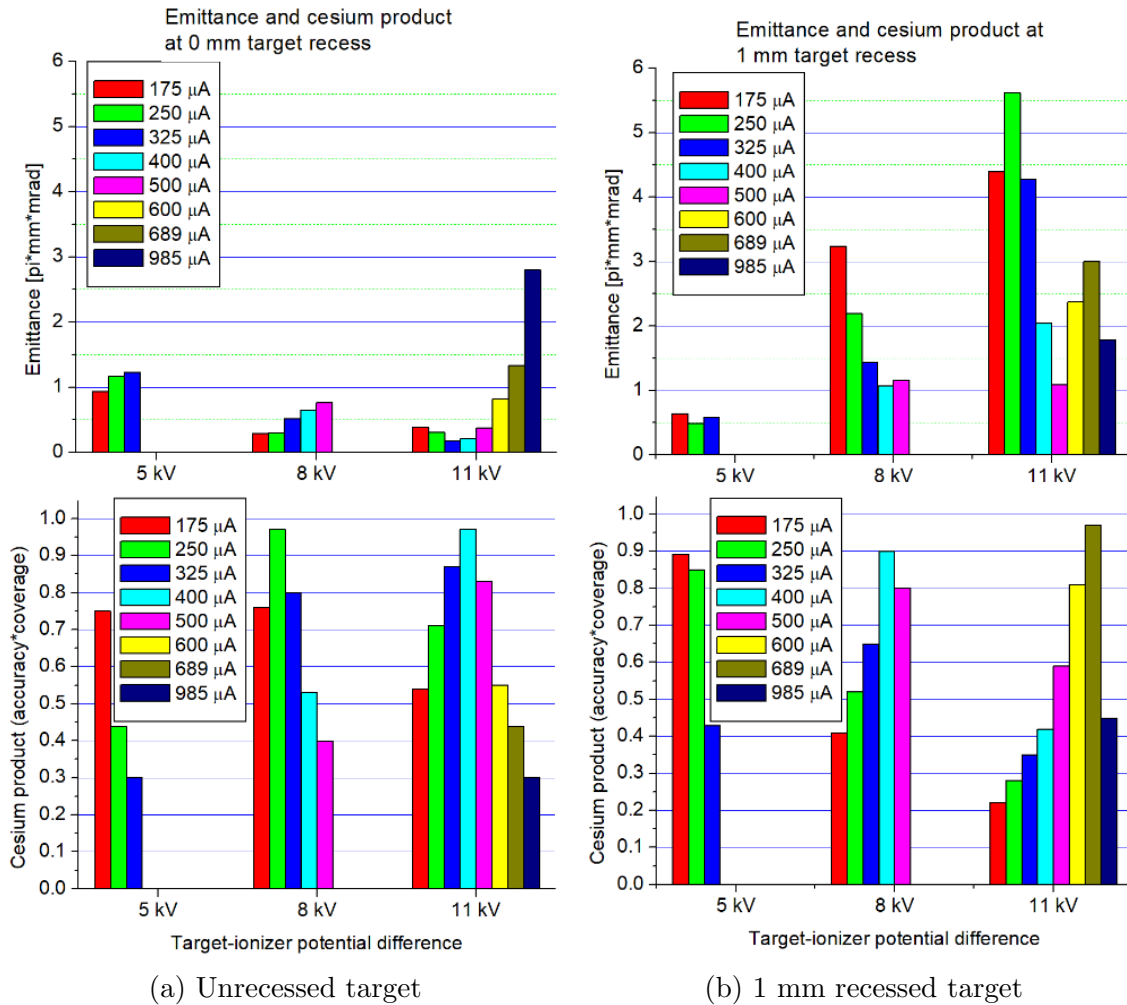


Figure 5.31: Emittance and cesium product results plotted for various cesium beam currents. The number of accessible cesium currents at each target potential is limited by Child's Law. Note: In all cases, the left side of the cesium product peak is reduced due to poor coverage of cesium on the sample while the right side is due to cesium beam self repulsion causing some cesium rays to miss the sample.

1. At 5 kV T-I P, for both the unrecessed and 1 mm recessed samples, at 325 μA , the cesium product is significantly decreased because most of the cesium rays miss the sample entirely. It is also likely that the reduced potential is to the detriment of the negative ion production.
2. At 8 kV T-I P, the unrecessed sample begins with good coverage at 250 μA , but rays begin to miss the sample as the cesium current increases. Roughly 240 of the full 250 μA , 260 of the full 325 μA , and 200 of the full 400 μA beams of cesium impinge on the sample which likely explains why the output rose slightly before decreasing in the experiment. The emittance remains fairly low for the entirety of this range.
3. At 8 kV T-I P, the 1 mm recessed sample begins with an elevated emittance significantly higher than its unrecessed counterpart at 250 μA . The emittance reaches a minimum, and therefore best focusing, at 400 μA . The coverage of cesium on the sample also began quite low at 250 μA , but reached a maximum at 400 μA . This would explain the poor behaviour until a significantly improved output at 140 °C.
4. At 11 kV T-I P, the unrecessed sample has a low emittance across the entire 250 to 400 μA range. However, the coverage on the sample increases to a maximum at 400 μA of cesium current.
5. At 11 kV T-I P, the 1 mm recessed sample begins at 250 μA of cesium with the highest emittance, and therefore worst focusing of all simulated runs. The emittance continues to decrease to a minima near 500 μA . All the while, the coverage of the full cesium on the sample is continuously increasing.

From examining the cesium product behaviour, it is clear the somewhat arbitrary cesium product definition is useful more as an interpretation guide than a quantitative descriptor. The right side of the peak (where cesium rays miss the sample) is of higher detriment to the output than the left side (where the full cesium beam hits the sample but is poorly distributed across its surface). This is likely why the negative ion output of the 1 mm recessed target increased at higher oven temperatures despite sub-optimal coverage.

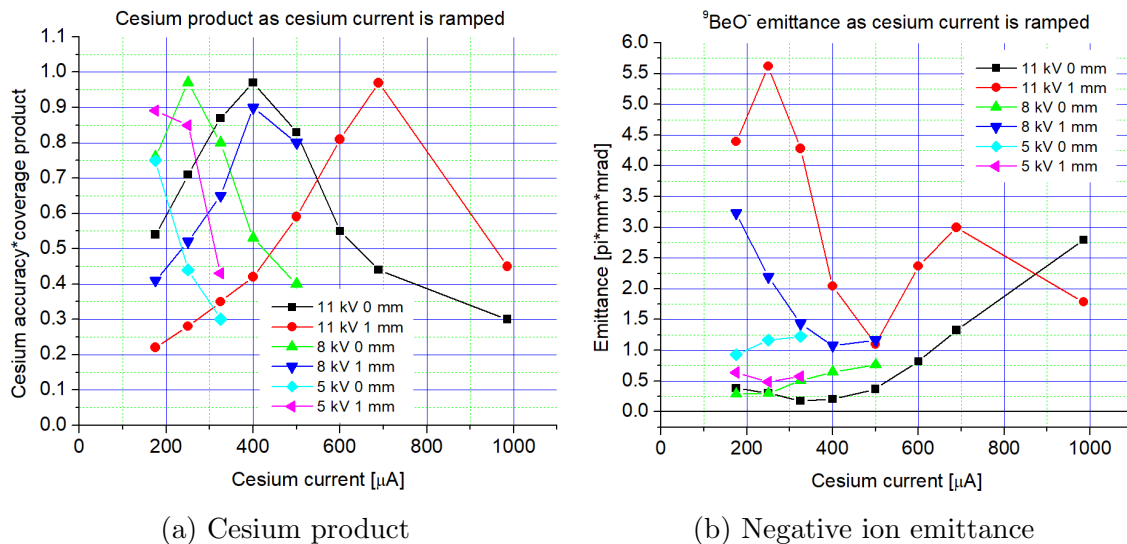


Figure 5.32: The cesium product on the sample and the $^9\text{BeO}^-$ emittance exiting the ion source are plotted separately against the cesium current for both the 1 mm recessed and unrecessed targets at target potentials 5, 8, and 11 kV. The number of accessible cesium currents at each target potential is limited by Child's Law.

Figure 5.32 takes the same data but framed a different way. From the cesium product, it is clear that recessing the target causes the best focusing of the cesium to occur at a higher cesium current than the unrecessed target. However, the recessed target produces higher and more erratic emittance values.

To better understand the underlying physics of this result, the following four sections will examine the charge deposition for the 11 kV T-I P runs that produced extrema on the emittance plots, beginning with the unrecessed targets.

11 kV, 0 mm, 400 μA

Figure 5.33 gives the overview of the negative ion behaviour. Most of the rays remain on the positive (right) side of the axis with a few crossing over.

The positive charge distribution is shown in Figure 5.34. This was the run with the highest cesium coverage-accuracy product. The blank region of space above the sample is where the negative space charge deposition deposited more charge than the cesium beam in the 2D element mesh resulting in that space having a net negative space charge. There is a small "locus" of positive charge on the axis just above the sample which results from the convergence of cesium rays from every azimuthal direction to a small, concentrated region of space. This is a consequence

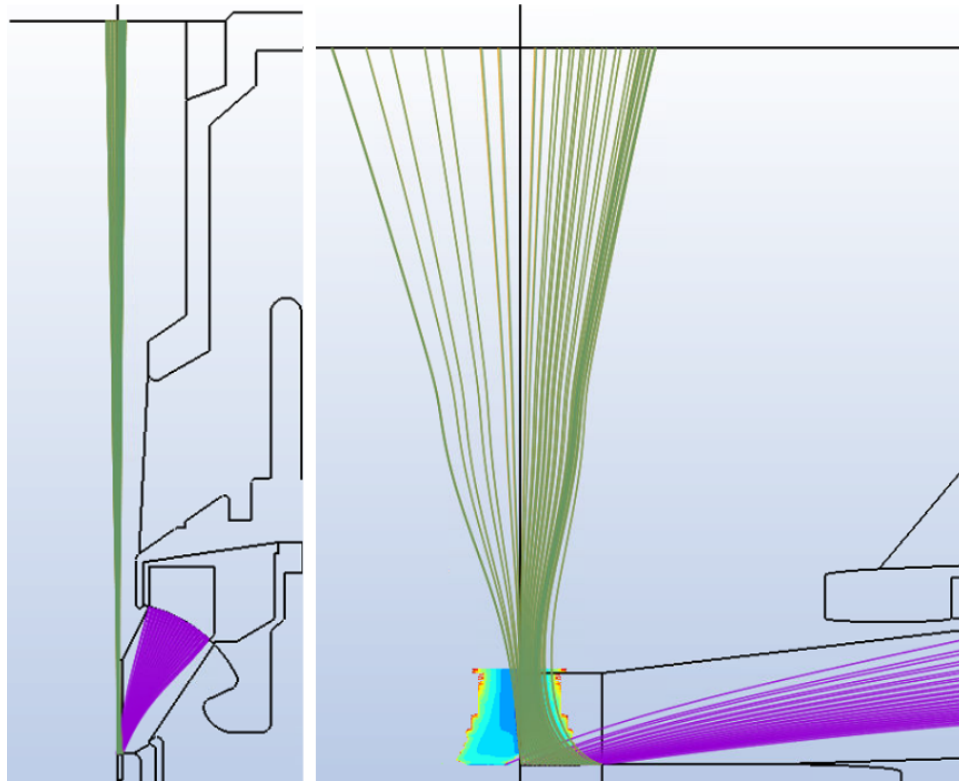


Figure 5.33: 11kV T-I P; 0 mm target recess; 400 μA of cesium; overview: Left is an overview of the simulation while the right shows the same but stretching the radial dimensions to better examine the behaviour of the rays.

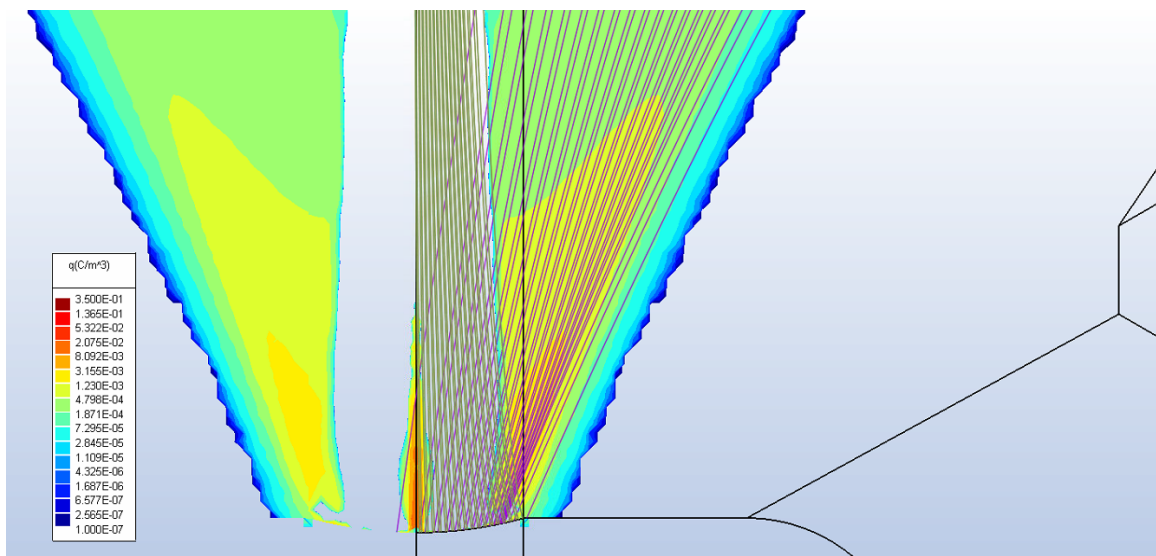


Figure 5.34: 11kV T-I P; 0 mm target recess; 400 μA of cesium; positive charge distribution.

of the cylindrical symmetry and will be shown to have a significant effect on the focusing of the negative ions. It is at this point that the highest density of positive charge is achieved. In this case, it peaks at 0.021 C/m^3 . Of the four selected examples, this is the lowest value for the positive locus. Due to geometry, the bulk

cesium beam external to the negative ion beam produces a reduced charge density that is primarily dependent on the magnitude of the cesium beam current.

Figure 5.35 shows a radially stretched view of the negative charge deposition.

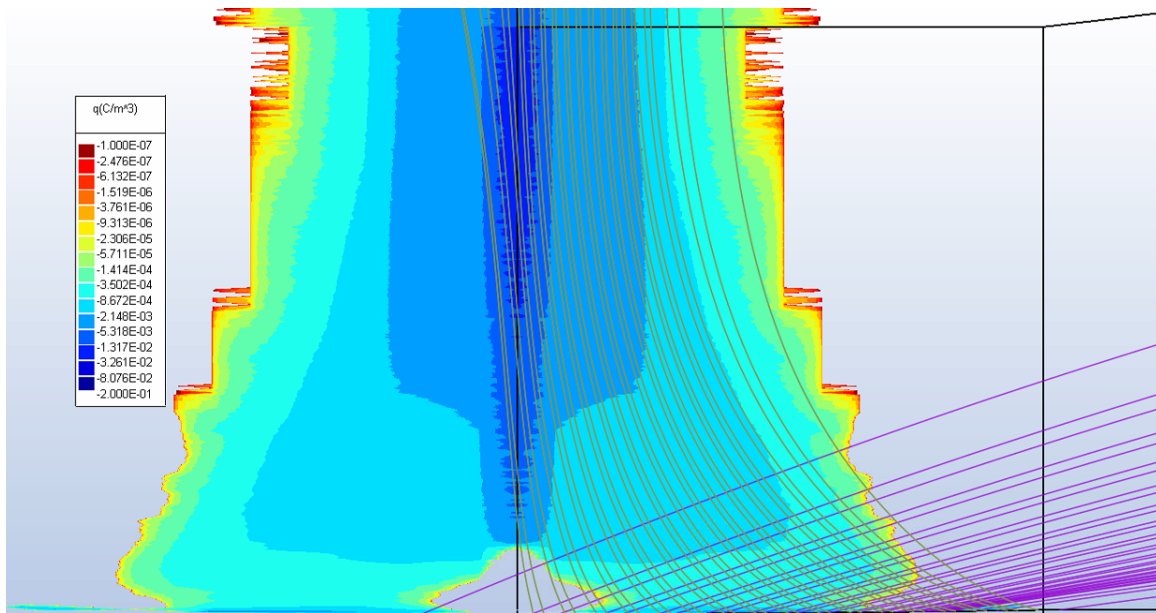


Figure 5.35: 11kV T-I P; 0 mm target recess; 400 μA of cesium; negative charge distribution, radial dimensions stretched. For reference, the black vertical line on the right represents the outer limit of the sample at 0.65 mm from the central axis.

A locus of negative charge is seen downstream peaking at about -0.032 C/m^3 . This locus acts as a potential barrier to any negative ion rays on track to cross the axis, repelling those with insufficient radial momenta. To rays already moving away from the axis, this locus accelerates their defocusing to the detriment of the beam emittance. As will be demonstrated, in general, the further along the axis this locus is, the lower the emittance of the negative ion beam.

Visible in this plot, the inner rays of the negative ion beam are drawn towards the axis by the positive locus of charge while the outer rays of the negative ion beam are drawn away from the axis by the bulk cesium space charge external to the beam.

11 kV, 0 mm, 985 μA

Figure 5.36 shows that most of the rays cross the axis. This simulation had the highest emittance of the unrecessed target simulations.

Figure 5.37 shows the positive volume charge density. Here it is very evident that a large portion of the cesium rays miss the sample entirely. In addition, the

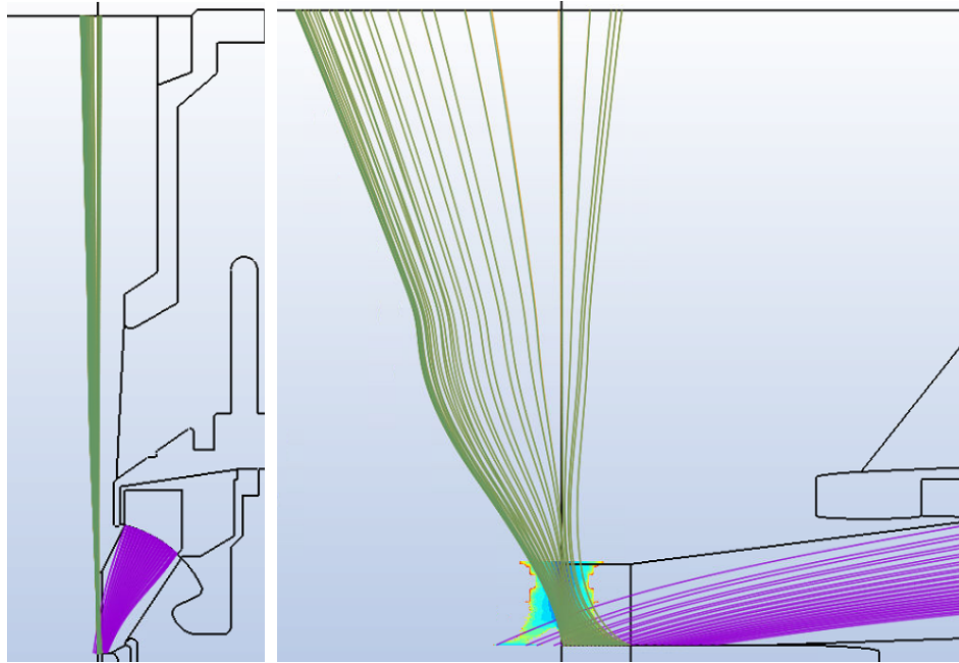


Figure 5.36: 11kV T-I P; 0 mm target recess; 985 μA of cesium; overview: Left is an overview of the simulation while the right shows the same but stretching the radial dimensions to better examine the behaviour of the rays.

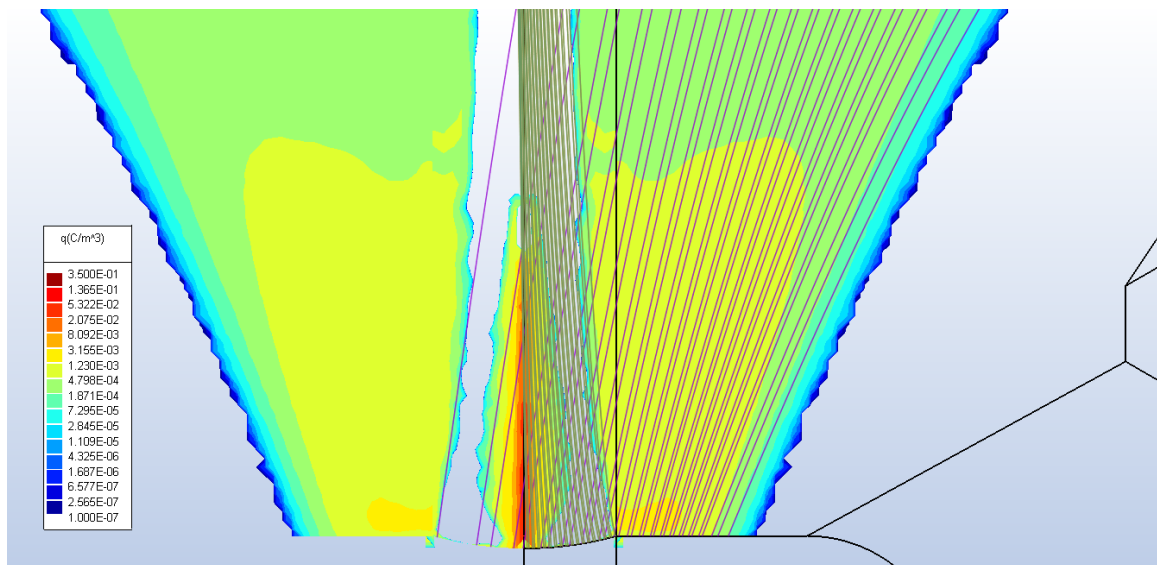


Figure 5.37: 11kV T-I P; 0 mm target recess; 985 μA of cesium; positive charge distribution.

locus of positive charge is higher, peaking at 0.050 C/m^3 , and dominates a larger region of space than in the $400 \mu\text{A}$ case.

Looking at the negative charge deposition in Figure 5.38, the inner negative rays are quickly drawn across the axis. The locus of negative charge occurs almost immediately after the positive locus with a peak density of -0.082 C/m^3 . This forms

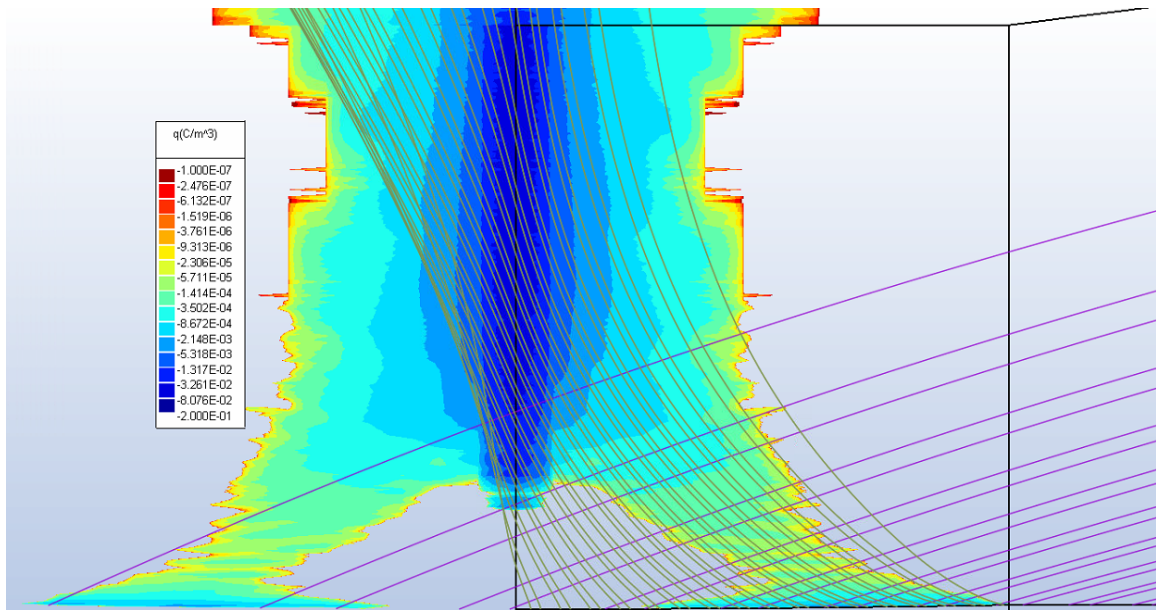


Figure 5.38: 11kV T-I P; 0 mm target recess; 985 μA of cesium; negative charge distribution, radial dimensions stretched. For reference, the black vertical line represents the outer limit of the sample at 0.65 mm from the central axis.

as the rays cross the axis. The rays closest to the axis suffer the most as they cross the axis first and are further repelled by the negative locus, resulting in a poor (high) overall emittance of the negative ions.

11 kV, 1 mm, 500 μA

Moving on to the 1 mm recessed target where the emittance values were much higher, Figure 5.39 shows there is a sharp splitting of the negative ion beam into three directions. Most of the rays stay on the positive (right) side of the axis, some near the axis, while others are defocused. Most of the rays that cross the axis have high radial displacement and angular deviation. This simulation had the lowest emittance of the 11 kV T-I P at 1 mm target recess simulations.

Figure 5.40 shows the positive charge deposition. This is the first example of poor coverage on the surface of the sample. As many rays compress into a small space, they bridge positive charge dominance from the bulk region to the central locus. In this case, the locus peaks at 0.092 C/m^3 .

Figure 5.41 gives the best insight into the three way splitting of the negative ion beam seen in the overview. The rays closest to the axis of symmetry are drawn

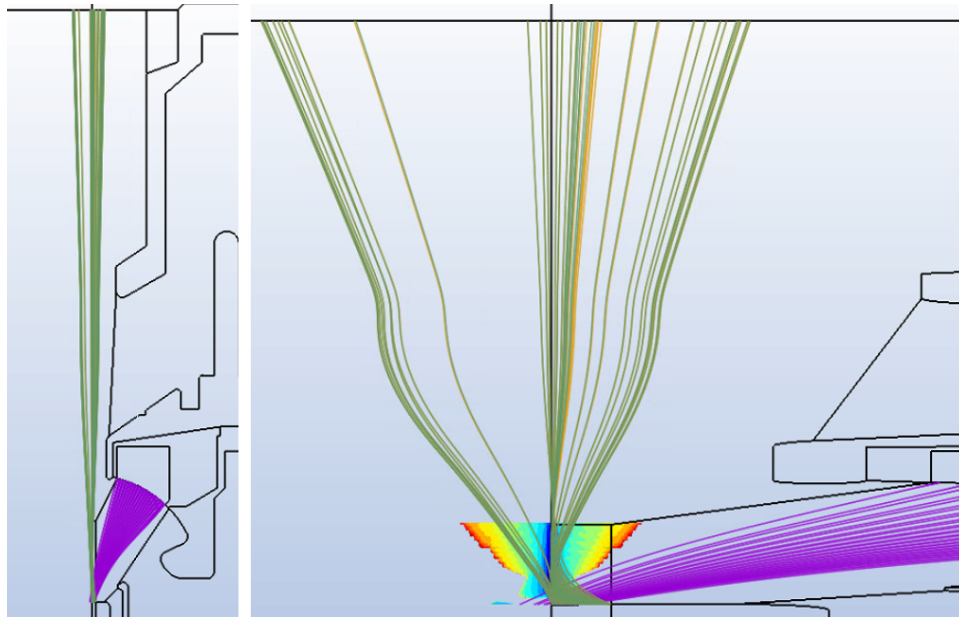


Figure 5.39: 11kV T-I P; 1 mm target recess; 500 μA of cesium; overview: Left is an overview of the simulation while the right shows the same but stretching the radial dimensions to better examine the behaviour of the rays.

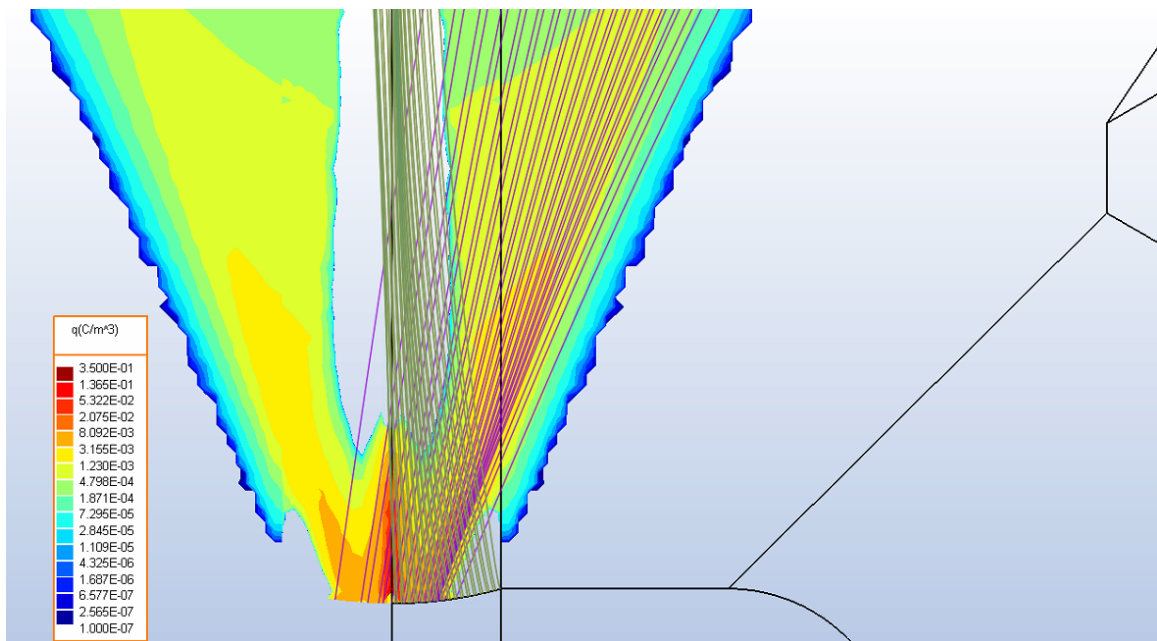


Figure 5.40: 11kV T-I P; 1 mm target recess; 500 μA of cesium; positive charge distribution.

immediately by the positive locus to the negative side of the axis where they are further accelerated away from the axis by the negative locus (peaking at -0.190 C/m^3). The middle rays approach the axis with insufficient radial momentum to surmount the negative locus' potential barrier. The radial velocity decelerates through zero until it is repelled from the axis. This is beneficial compared to the rays that already

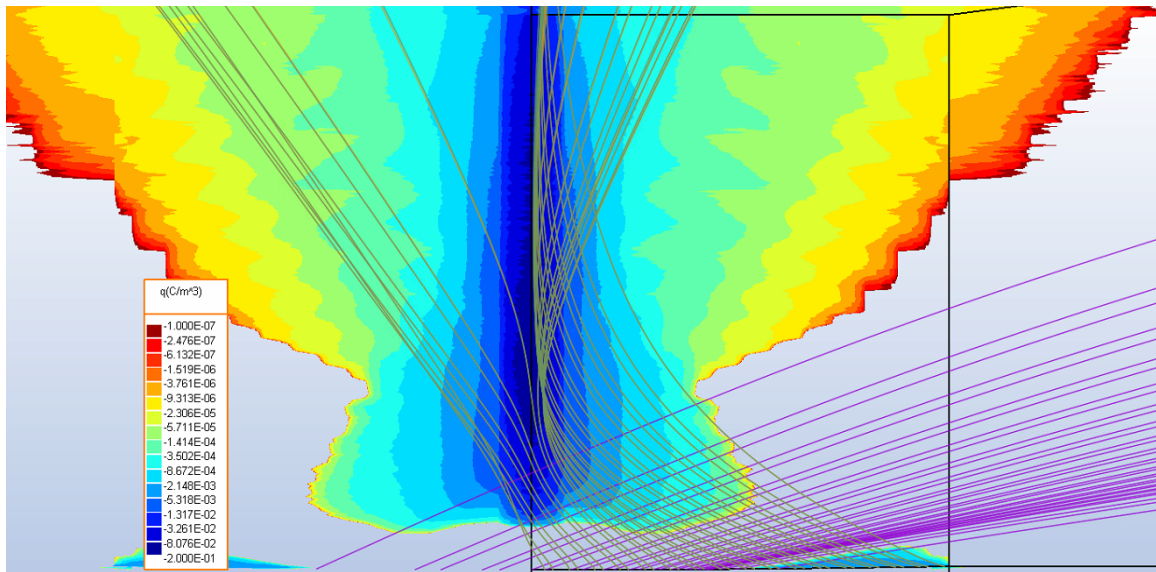


Figure 5.41: 11kV T-I P; 1 mm target recess; 500 μA of cesium; negative charge distribution, radial dimensions stretched. For reference, the black vertical line represents the outer limit of the sample at 0.65 mm from the central axis.

crossed the axis because a significant portion of their flight time is spent radially decelerating before the beam is defocused by accelerating away. The sooner along the flight path this occurs, the worse the rays' radial displacement and angular deviation upon leaving the ion source.

By contrast, the outer most rays are drawn towards the axis by the positive locus with competition from the bulk cesium space charge and the negative locus. These rays straighten out and remain close to the axis for the remainder of their flight through the ion source. Unfortunately, most of these rays are likely a fictitious anomaly of Lorentz-2E being set to emit uniformly-spaced rays, carrying the same current density, normal from the sample surface even if cesium rays do not impinge near their emission site. Otherwise, they would have the best phase space parameters of all negative ion rays. Simulating a more realistic distribution of negative ions based on the impinging cesium distribution is a challenging and significantly more time-consuming affair.

11 kV, 1 mm, 250 μA

Figure 5.42 shows that most of the rays cross the axis with some outer most rays remaining on the positive side of the axis.

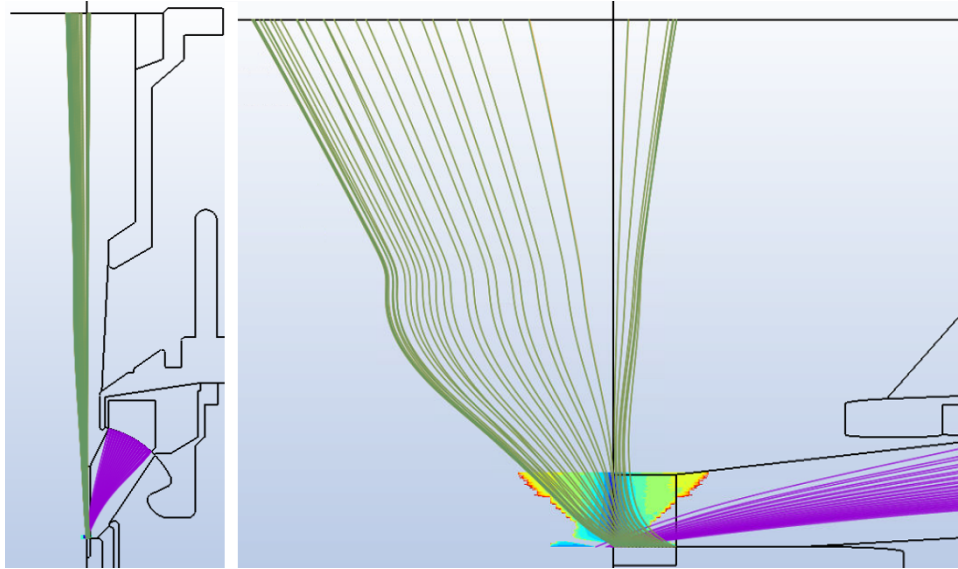


Figure 5.42: 11kV T-I P; 1 mm target recess; 250 μA of cesium; overview: Left is an overview of the simulation while the right shows the same but stretching the radial dimensions to better examine the behaviour of the rays.

The positive space charge density, seen in Figure 5.43, is much more finely

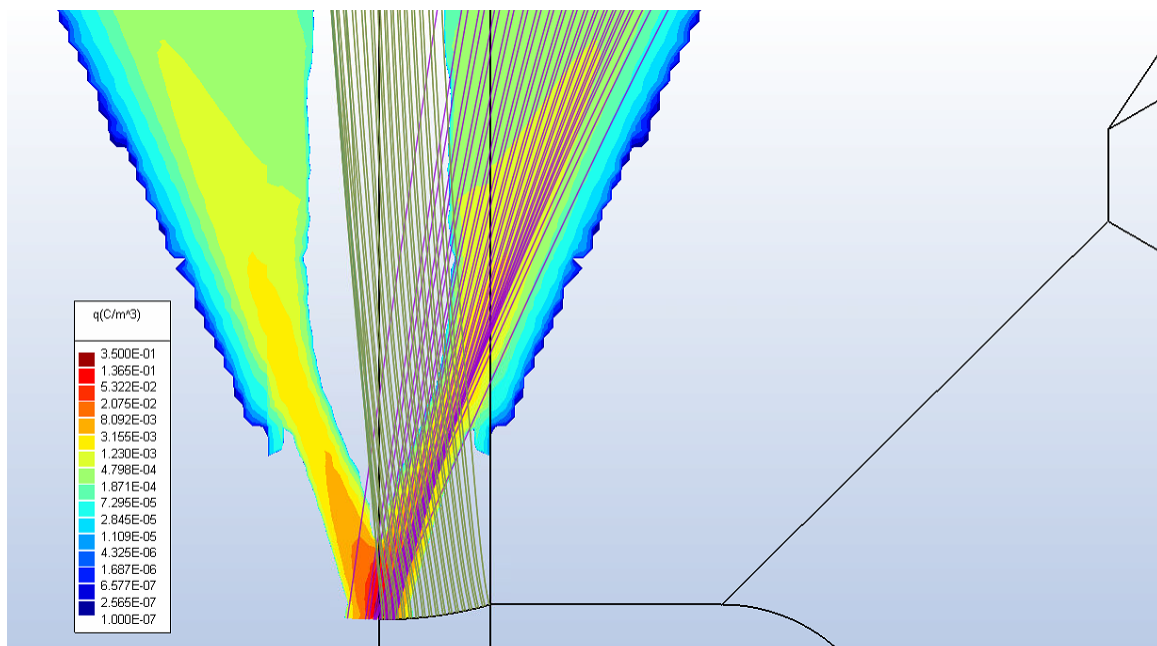


Figure 5.43: 11kV T-I P; 1 mm target recess; 250 μA of cesium; positive charge distribution.

concentrated as the majority of the rays converge on a spot size only a few hundred microns in diameter. Despite having the lowest total cesium current of the four selected examples, the peak of the locus of positive charge is by far the highest at 0.362 C/m^3 . Meanwhile, the bulk charge outside of the negative ion beam is signif-

icantly less.

One additional thing to notice in both Figures 5.40 and 5.43 is that the negative ion rays at the outer edges of the sample are likely a fictitious anomaly of having set the surface of the sample as a uniform emitter (as a first approximation to minimize variables). They would not be present in reality since no cesium impinges on that location of the sample. These fictitious rays tend to have the lowest radial displacement and angular distributions upon exiting the ion source, which means they skew the emittance reported by the simulation to be lower than it likely would be in reality.

As seen in Figure 5.44, the positive locus of charge draws all but the furthest

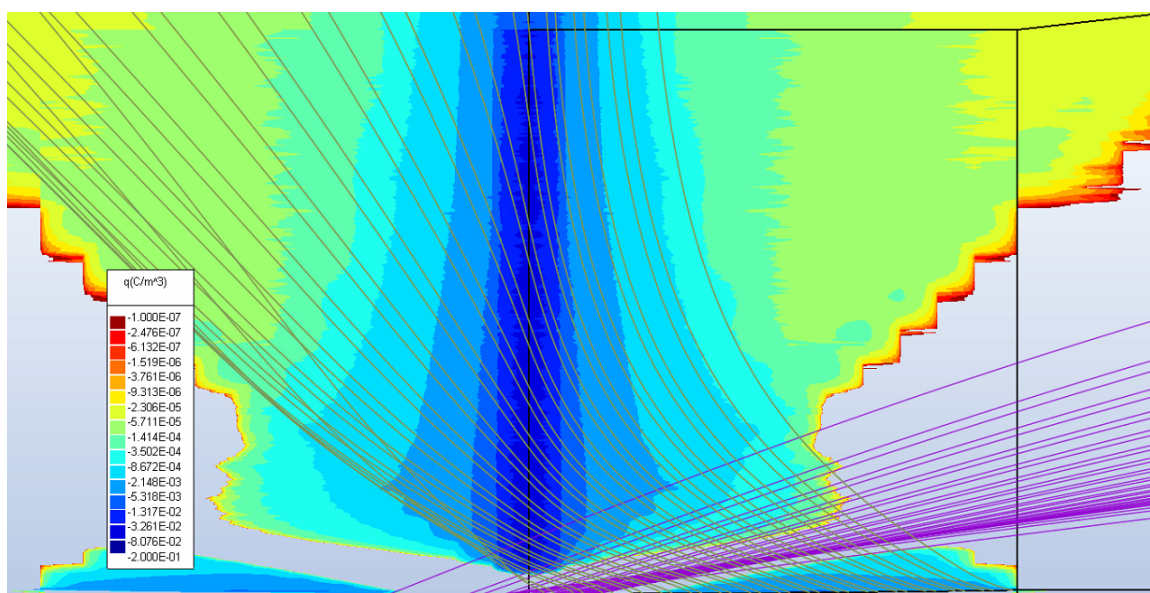


Figure 5.44: 11kV T-I P; 1 mm target recess; 250 μA of cesium; negative charge distribution, radial dimensions stretched. For reference, the black vertical line represents the outer limit of the sample at 0.65 mm from the central axis.

negative ion rays across the axis. They are decelerated slightly by their own negatively charged locus before being accelerated away from the axis on the negative side.

Examining the focusing field

In addition to the aforementioned space charge effects influencing the beam, the raw ambient field acts to mainly defocus the negative ion beam along its trajectory through the interaction region. This effect is slightly mitigated by the initially axis-ward trajectory set by emitting normal to the curved sample surface, the shap-

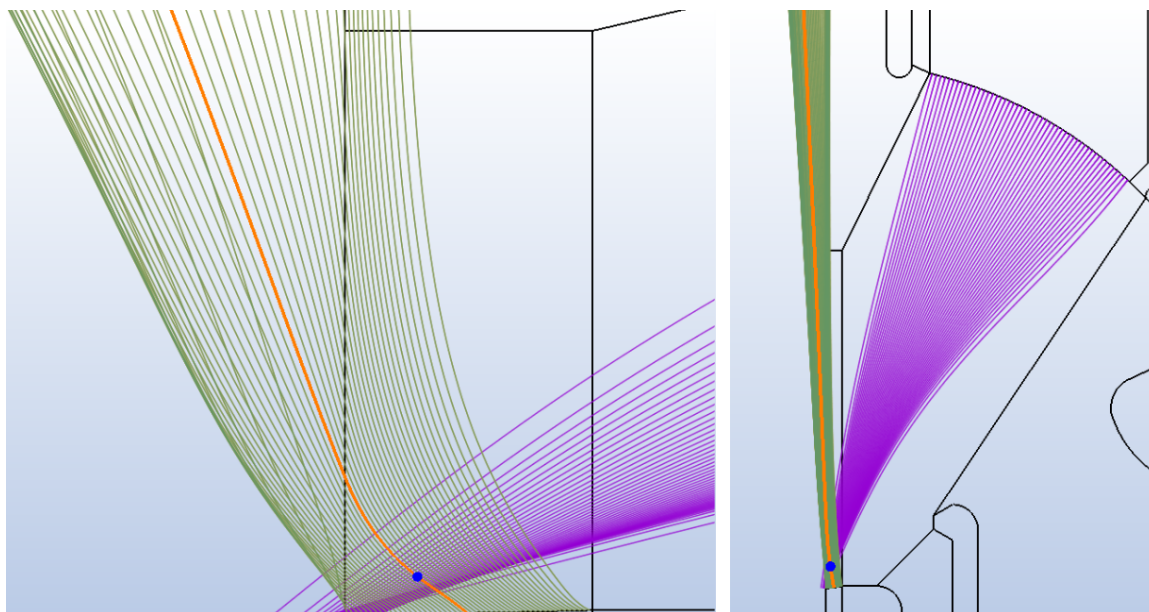


Figure 5.45: 11kV T-I P; 1 mm; 250 μA : Arbitrarily selecting the middle ray (ray 25/50 highlighted in orange) on the negative ion beam, the blue dot represents the last position for which the negative ions experience a force acting radially inwards towards the axis.

ing of the field near the aperture, as well as the locus of positive charge, which is strongest in this selected result. Even with all these mitigating effects, Figure 5.45 shows the last position along the ray's trajectory for which the negative ion experiences a net force acting towards the axis. Beyond this point, and as soon as the ray crosses the axis in a mere few millimetres, the rest of the trajectory through the interaction region is spent in a defocusing field. While some of this may be compensated partially by the Pierce geometry in the extraction region, the emittance upon entering that region appears to be a strong contributor to the emittance upon exiting the ion source.

Contrast with absence of cesium

If one considers the purely fictitious scenario of cesium-less sputter of BeO^- as seen in Figure 5.46, one immediately notices that not a single negative ion ray crosses the axis at any point. This is true for both a 1 mm target recess and unrecessed target. This further emphasizes the importance of space charge effects within the SO-110C ion source.

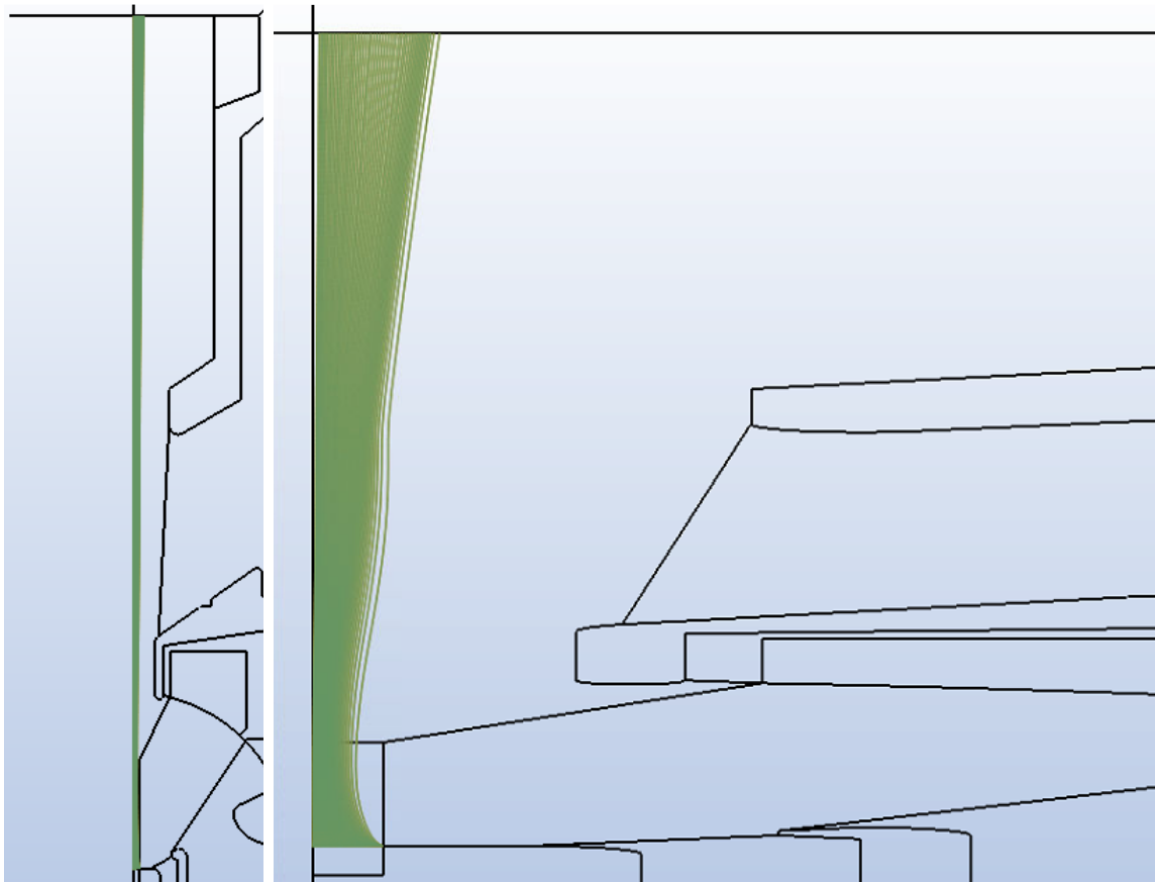


Figure 5.46: 11 kV T-I P; 0 mm; BeO^- emitted with the same ambient field without the presence of cesium.

5.11.4 Summary

From the multi-dimensional comparison of this simulation batch and the experiment that preceded it, the electrodynamics within the ion source can be simplified to four competing processes:

1. The ambient field, which is necessarily designed to focus the positively charged cesium beam onto the sample, is therefore predominantly divergent for negative ions. Only a small region of focusing is provided by the presence of the target aperture.
2. A locus of positive charge forms at the centre of the sample where cesium rays converge near the axis. A consequence of the cylindrical geometry, this buildup of positive charge draws negative ions across the axis. In general, the sooner in time/space they cross, the worse the emittance of the outgoing negative ion beam. This effect decreases with increased radius on the sample. The

magnitude of this locus of charge is more dependent on the cesium focusing than the amount of cesium current emitted.

3. The bulk cesium space charge outside the negative ion beam pulls on the outermost negative ion rays, slowing their convergence. This effect weakens with decreasing radius on the sample and is mostly dependent on the magnitude of cesium current emitted.
4. A locus of negative charge forms as the negative ion beam converges near the axis. This locus acts as a radial potential barrier that can deflect negative ions from the axis. This is beneficial for the focusing of rays that begin and end on the same side of the axis but worsens the divergence of rays that crossed the axis at or before reaching this locus. The ideal case is for the negative ion rays to be drawn gradually near the axis with a waist involving minimal crossover. The further downstream this waist occurs, the better the final emittance. This effect is more a consequence of the three aforementioned effects than being self-caused.

Thus, the initial focusing provided by the curved sample surface, the target aperture shaping of the field, and the magnitude of the positive charge locus are important to ensuring the negative ion beam is contained enough to escape into the extraction region. The coverage of the cesium beam on the sample is also of great importance as it maximizes the sample material accessed for sputtering while also minimizing the overfocusing effect of the positive locus of charge.

Parting comment:

There is one final observation that belongs to no one section: To date, in no simulation of realistic parameters of either carbon or beryllium isotopes has the negative ion beam originating from the sample ever been observed to impinge on the extraction cone. This suggests that losses in transmission are likely either from losses in the interaction region or a consequence of poor emittance later in the accelerator.

Chapter 6

Summary and Outlook

6.1 Summary

The HVEE SO-110C ion source was modelled using IES's Lorentz-2E ion trajectory simulation software. The Rijke code was developed to communicate with Lorentz-2E, to initiate, generate, and run simulations, as well as analyze and record the output data in a variety of formats convenient for plotting or further analysis.

Lorentz-2E incorporates the mutual and self space-charge interaction between the positively charged cesium ion beam and the sputtered negative ion beam. Both mutual and self interactions were shown to be important.

Early simulations suggested that the extraction cone tip plays an important role in confining the diverging field strength on the extracted ions. However, further optimization of this geometry by examining the normalized (for energy) emittance of the beam upon exit from the interaction region and beyond the extraction region may be possible. A multi-electrode gradient transition from ionizer potential to ground may be worth investigating.

The target aperture defocuses the cesium beam near the target and focuses the negative ion beam early in its trajectory. Provided electric discharge is not an issue, protruding this aperture closer to the ionizer could greatly increase the electric field density at the surface of the ionizer, increasing the limit of cesium that can be emitted without increasing the target-ionizer potential difference. Unfortunately, at cesium currents near the limit approximated by Child's Law, the aperture's defocusing effect on the cesium beam may result in more detriment than benefit. At

lower cesium currents where the space charge repulsion is reduced, this defocusing could improve the distribution of cesium on the sample. Excessively protruding the aperture relative to the target will likely result in a similar dampening of the field as was the case when recessing the target relative to the aperture. This is to the detriment of the negative ion emission. Given the complexity of the competing field effects of electrode geometry and space charge from the positive and negative ions, further simulations and experiments are warranted.

In addition to geometric considerations, Brown et al. [39] have shown that using the aperture as an immersion lens by creating a potential difference between target and target aperture can improve the extraction of negative ions. While this would add complexity and additional electrical insulation challenges, it remains an avenue for further innovation.

Modelling of the crater geometry was briefly explored. The emission is highly dependent on the shape of the surface of the sample material. Establishing realistic cratering conditions in simulations remains a challenge.

Simulations and experiments suggest the distribution/coverage of cesium on the sample is critical. In general, the more of the sample that is covered by the cesium beam without rays expanding to miss the sample, the better the extraction and usage of sample material. Rays originating from the outer edge of the ionizer, by geometry tend to carry the most current of cesium. Thus it is important that these rays do not expand to miss the sample.

Target recess simulations and experiments were conducted using ^{12}C graphite blanks and ^{10}Be standard material. At the estimated cesium current of $250\ \mu\text{A}$ routinely produced in the ion source (based on cesium ampule usage time and AMS operation time), the simulation using fixed cesium currents rather than assuming the Child's Law limit could be well approximated. A method to reliably determine the cesium current as a function of the cesium oven temperature and the T-I P would be a strong asset to continued study.

For ^{12}C at low/routine cesium currents (about $250\ \mu\text{A}$), 6 kV T-I P, and 35 keV ion energies, a target recess of 1 mm gave the best long-term measurement stability and usage of target material. This was verified with experiment.

A more expansive test of cesium oven temperature, target recess geometry, and

target-ionizer potential difference resulted in greatly improved emission of ^{10}Be . In a stability batch, samples containing Nishiizumi standard material produced peak currents of $12\ \mu\text{A}$ of $^9\text{Be}^{2+}$ at the high energy offset Faraday cup and achieved a precision of 0.5% in less than an hour of sputtering. This is a great improvement compared to previous measurements of the same material at Lalonde AMS. Higher currents were achieved but in regions where the ion source extraction current became unstable.

From these tests, the interplay between the cesium ion current, target recess geometry, and electrode potential - including their effect on the resultant cesium distribution - were examined. These results show that higher cesium ion currents give a higher flux of cesium on the sample, increasing the sputter rate, but cause the beam to expand by its own space charge at higher currents. This can be compensated in two ways: Higher target-ionizer potential differences or by recessing the target. The former had an issue of secondary electrons, likely created at the ionizer base bore hole impinging on the extraction electrode, causing the extraction current to be unstable. The latter, likely by dampening the extracting field at the surface, reduced the yield of negative ions when recessing the target too far relative to the target aperture.

The simulated electrodynamics of the cesium-negative ion relationship appear to reduce to three competing processes: A locus of positive charge on the axis at the centre of the sample, mainly dependent on the density of cesium rays near the axis, draws negative ions towards the axis. The bulk cesium charge external to the negative ion beam, dependent mainly on the magnitude of the cesium current, draws negative ion rays away from the axis but also slows initially convergent rays to a waist further along their trajectory. The ambient field external to the focusing effect of the target aperture is primarily divergent for negative ions in the interaction region. This provides unavoidable detriment to the phase space of negative ions travelling far from the axis, especially those that cross the axis due to the positive cesium charge locus.

In the paper by HVEE describing the SO-110C ion source, Klein et al. [30] achieved $^9\text{BeO}^-$ currents up to $30\ \mu\text{A}$ and $^{12}\text{C}^-$ currents from graphite samples as high as $400\ \mu\text{A}$. In the acceptance tests during commissioning at Lalonde AMS,

15 μA of ${}^9\text{BeO}^-$ and 200 μA of ${}^{12}\text{C}^-$ were measured in the Faraday cup preceding the accelerator. These results were achieved at higher source output energies. In the time since, routine operation of the source remained at the 35 keV settings inherited from the operation of the SO-110B source. A comprehensive re-tuning of all accelerator components to accommodate a higher energy beam from the ion source has not yet been conducted. Nevertheless, the simulations in this work demonstrated their ability to model and predict improved operating conditions of the source output at energies of 35 keV. The physical insights about the electrodynamics within will also be applicable at higher source energies.

Due to its proximity to the hot ionizer, it is likely that cesium is ionized from parts of the inner shroud resulting in a “halo” of cesium deposition on the surface of the target.

The extraction region appears to be well designed for transmission of negative ions. In no simulation of realistic parameters of either carbon or beryllium isotopes has the negative ion beam originating from the sample ever been observed to impinge on the extraction cone. This suggests that losses in transmission are likely from losses within the interaction region or as a consequence of poor emittance later in the accelerator.

Future simulations could also examine the behaviour of the negative ion beam at varied negative ion mass and current.

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