CALIBRATION OF THE LUX-ZEPLIN DUAL-PHASE XENON TIME PROJECTION CHAMBER WITH INTERNALLY INJECTED RADIOISOTOPES

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CALIBRATION OF THE LUX-ZEPLIN DUAL-PHASE XENON TIME PROJECTION CHAMBER WITH INTERNALLY INJECTED RADIOISOTOPES

A Dissertation Presented
by
CHRISTOPHER NEDLIK

Submitted to the Graduate School of the University of Massachusetts Amherst in partial fulfillment of the requirements for the degree of

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Physics
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ABSTRACT

CALIBRATION OF THE LUX-ZEPLIN DUAL-PHASE XENON TIME PROJECTION CHAMBER WITH INTERNALLY INJECTED RADIOISOTOPES

MAY 2022

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Self-shielding in ton-scale liquid xenon (LXe) detectors presents a unique challenge for calibrating detector response to interactions in the detector’s innermost volume. Calibration radioisotopes must be injected directly into the LXe to reach the central volume, where they must either decay away with a short half life or be purified out. We present an overview of, and results from, the prototype source injection system (SIS) developed at the University of Massachusetts Amherst for the LUX-ZEPLIN experiment (LZ). The SIS is designed to refine techniques for the injection and removal of precise activities of various calibration radioisotopes that are useful in LXe time projection chamber (TPC) experiments such as LZ. We also outline a number of calibration analyses which help to provide a comprehensive understanding of the various detector systems that compose LZ.
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5.10 **Left:** The UMass LXe Detector fully assembled. The brown disc-shaped Kapton polyimide heater is visible at the bottom. **Right:** The fully assembled detector as the cryostat dewar is raised around it to be sealed. One of the custom liquid level sensors (sheathed in braided steel) and the 1/8” OD PTFE outlet tube are visible in the weir spillover channel.
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5.15 The prototype source injection system at UMass Amherst, with the major flow paths labeled. The prototype was designed and constructed at UMass Amherst to develop and practice the procedures for injecting precise quantities of calibration radioisotopes into LXe, in preparation of commissioning the LZ TPC.

5.16 The valve control screen of the UMass LXe detector system’s GUI. The buttons controlling the state of the pneumatically-actuated valves are overlaid onto an image of the prototype Source Injection System P&ID, with each button positioned at the location of the valve that represents it in the diagram. A “Close All” button simultaneously closes all of the pneumatic valves controlled by the interface, and changes the mass-flow controller setpoints to zero.

5.17 The main screen of the UMass LXe detector system’s GUI. All of the sensors are read out in fully customizable live-updating plots, and dedicated buttons set plot and injection procedure parameters in addition to executing the automated injection procedures carried out by the source injection system. The most recent value measured from each sensor is displayed in the array of text-boxes in the top right.
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5.19 Example waveforms from the two PMTs in the UMass LXe detector. **Top:** Example waveforms from a single scatter interaction in the detector’s LXe. **Bottom:** Example waveforms from a two-scatter event in the detector’s LXe, likely a $^{83m}$Kr decay.

5.20 Histograms of data taken by the UMass LXe detector following the injection of $^{83m}$Kr. **Upper Left:** A histogram of the logarithm of the pulse area in the bottom PMT vs. the top PMT for the first pulse in the events. In this parameter space, mono-energetic decays form populations along lines of anti-correlation, with their precise location along those lines depending on the position of the event in the detector. When the two decays of $^{83m}$Kr appear as separate pulses in the event window, the first (33 keV) decay populates this plot. When the two decays occur close together in time and are merged into one (33+9 keV) pulse, a second, 42 keV, population is formed. **Upper Right:** A simple cut selecting $^{83m}$Kr events is applied to the events in the histogram in the top left. Reducing the rate of background with this selection cut allows for a larger useful time range in which the decaying $^{83m}$Kr event rate in the detector can be fitted (appears above background). **Lower Left:** The first-pulse vs. second-pulse areas for the summed top and bottom PMT waveforms. **Lower Right:** The first-pulse vs. second-pulse areas for the summed top and bottom PMT waveforms with the $^{83m}$Kr selection cut (from the top right histogram) applied. The events where the two decays from the $^{83m}$Kr event are merged appear as a separate population than those where the decay is separable.
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5.34 Histograms of data taken with the UMass LXe detector following the injection of $^{220}$Rn. **Left:** A histogram of the logarithm of the pulse area in the bottom PMT vs. the top PMT for the first pulse in the events. In this parameter space, mono-energetic decays form populations along lines of anti-correlation, with their precise location along those lines depending on the position of the event in the detector. The mono-energetic populations of $^{220}$Rn, $^{212}$Bi, $^{216}$Po, and $^{212}$Po $\alpha$-decay events are visible. **Right:** A simple cut selecting $^{220}$Rn and $^{216}$Po events is applied to the events in the histogram on the left. This cut reduces the background rate and random error in the measurement of the injected activity.

5.35 A histogram showing the rate of events passing the $^{220}$Rn+$^{216}$Po selection cut in the UMass LXe detector during an injection of $^{220}$Rn. The injected $^{220}$Rn+$^{216}$Po activity is measured by calculating the difference between the average rate of the selected $^{220}$Rn+$^{216}$Po before and during the injection. The periods of time used to measure both rates are shown by black lines in the plot, at a height corresponding to the average value that they measured. Dips seen in the rate are due to short breaks in the DAQ’s data taking during the transition between 100k-event acquisitions, and are ignored by the rate-measuring algorithm.

5.36 A plot showing the complete set of results from $^{220}$Rn injections into the UMass LXe detector with the prototype SIS. A model (equation 5.4) for the fraction of $^{220}$Rn which survives the transit from the generator to the detector as a function of the carrier GXe flow-rate is fitted to the data, providing a measurement of the $^{220}$Rn transport efficiency, $T_e = 0.163 \pm 0.015$. The residuals from the fit are shown below the results plot.
5.37 A histogram showing the event rate in the UMass LXe detector while at room temperature, filled with Gx, during a continuous injection of \(^{220}\text{Rn}\). The flow rate of Gx through the \(^{220}\text{Rn}\) generator was increased from 100 SCCM to 200 SCCM five minutes after the start of the injection.

6.1 The plumbing and instrumentation diagram for the LZ source injection system.

6.2 A photo of the LZ source injection system. A bottle containing natural methane (CH\(_4\)) can be seen at the left edge of the photo, and three flow-through calibration sources (\(^{83}\text{mKr}\), \(^{131}\text{mXe}\), and \(^{220}\text{Rn}\) can be seen installed on the system near the center of the photo. The calibration-source plumbing is indicated with a red overlay, while the plumbing which is used to flush the calibration isotopes into the circulation system after they are dosed into the dose volume (and which goes through the dose volume), is indicated with a blue overlay. The dose volume is indicated with a green overlay.

6.3 A photo of the first \(^{83}\text{mKr}\), \(^{131}\text{mXe}\), and \(^{220}\text{Rn}\) generators installed onto the LZ source injection system.

6.4 A plot showing the event rate in the cold-Gx filled LZ TPC during a period of time containing multiple \(^{220}\text{Rn}\) injections at a variety of injection flow rates. **Left:** A table summarizing the flow rate and flow duration through the \(^{220}\text{Rn}\) generator over the course of the injections into the LZ circulation system shown in the plot. **Right:** A plot of the measured trigger rate in LZ during the \(^{220}\text{Rn}\) injections described in the table. The changes in trigger rate at the different flow rates have colored labels corresponding to the colored table values.

6.5 A plot summarizing the results of the measured \(^{220}\text{Rn}\) activity injected into the Gx-filled LZ TPC as a function of carrier-Gx flow rate through the \(^{220}\text{Rn}\) generator. The expected activity delivered to the detector is shown by the blue curve, and is seen to model the measured data very poorly. A model with the total transit time as a free parameter is fitted to the data and indicated by the red curve.
6.6 Histograms of TBA versus total pulse area for data taken during the $^{220}$Rn injection into the GXe-filled LZ TPC (left) and on the following day (right). The real time of the data in each histogram is indicated by the black text. The prompt $^{220}$Rn and $^{216}$Po $\alpha$-decays appear as a single bright band during the $^{220}$Rn injection, distinct from the lower-energy background. On the following day, $\alpha$-decays from $^{212}$Bi and $^{212}$Po (stuck to surfaces in the TPC) appear combined with the background $^{222}$Rn-chain alphas. Asymmetries in TBA for the alpha populations are predominantly a reflection of asymmetries in the TPC and PMT-array geometries.

6.7 Histograms of top-bottom asymmetry vs. uncorrected (left) and corrected (right) S1-pulse area in the LZ TPC just after being filled with LXe. The naturally present activation peaks from $^{131m}$Xe, $^{127}$Xe, and $^{129m}$Xe appear as bright bands in the histogram. The uncorrected S1-pulse areas show strong position dependence in each mono-energetic population. An S1-pulse area correction, normalized to the S1-pulse areas at TBA= 0, is applied to the data in the histogram on the right. The TBA in this data is not symmetric about TBA = 0 because of the high reflectivity of the LXe-GXe interface, which results in the majority of photons being collected by the bottom PMT array.

6.8 Histograms of the positions of coincident events in the LZ TPC and LXe skin, during a period of data taking in which $^{127}$Xe was naturally present from activation. Left: The top-bottom asymmetry in the TPC versus in the LXe Skin. Right: The angular position (theta) in the TPC versus in the LXe skin. The artificial population at Skin Theta = 45 degrees is the result of setting it equal to 45 degrees in events with light distributions that cannot be used to properly calculate an angular position. Both histograms demonstrate the coincidence requirement’s ability to selects events which have strongly correlated positions, most likely escaped-$\gamma$-ray $^{127}$Xe-decays.
6.9 Histograms of the corrected S1-pulse area in the LZ TPC over the range of corrected S1-pulse area containing the 33 keV Auger electron/X-ray peak from escaped-\(\gamma\)-ray K-shell \(^{127}\)Xe decays. A model is fit to the data which is the sum of a constant, an exponential, and a gaussian component. The constant+exponential components model the background, while the gaussian component models the 33 keV peak. The fit parameters from the gaussian component are used to measure the number of events in the 33 keV peak. The efficiency of tagging the escaped-\(\gamma\)-ray K-shell \(^{127}\)Xe decays is measured by calculating the ratio of the gaussian-component integral from the fit with a skin coincidence required (right histogram) to the gaussian-component integral from the fit with no skin coincidence required (left histogram). The measured activities of the gaussian populations are reported on each histogram in black text, including the percent of total \(^{127}\)Xe decays which contribute to each population. To determine the contributing percentage, the total \(^{127}\)Xe activity was calculated by integrating a gaussian fit of the 403 keV \(^{127}\)Xe peak in a histogram of corrected-S1-pulse area, and dividing the integral by the total live time of the data, and the fraction of \(^{127}\)Xe decays that are expected to fall into the 403 keV peak (47.6%). ..................................................... 175

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6.13 Histograms of data taken by the LZ TPC following the injection of \( ^{83}\text{mKr} \). **Upper Left:** A histogram of top-bottom asymmetry versus the negative of the drift time for single-scatter (and two-S1, one-S2 events where the S1-pulse areas have been combined). A cut is shown selecting the events between the solid red lines, to remove accidental or otherwise unphysical S1-S2 pairs from the data. **Upper Right:** A histogram of the logarithm of S2-pulse area versus the logarithm of S1-pulse area for single-scatter events (and two-S1, one-S2 events where the S1-pulse areas have been combined). A cut selecting the \( ^{83}\text{mKr} \) events is shown by the solid red lines. **Bottom:** A histogram of the event time stamps versus the negative of the drift time for the \( ^{83}\text{mKr} \) events selected by the cuts in the first two histograms. The \( ^{83}\text{mKr} \) atoms are seen to enter the TPC at the bottom (large negative drift time) and slowly mix into the bulk. The gaps in the data are from periods of time when the DAQ was disabled.

6.14 Histograms produced from LZ TPC data containing \( ^{131}\text{mXe} \), with single-scatter events selected. **Top Left:** A histogram of the logarithm of S2-pulse area versus the logarithm of S1-pulse area. A cut selecting \( ^{131}\text{mXe} \) events is shown with solid red lines, and is applied to the other three histograms. **Top Right:** A histogram of the x position versus y position for the selected \( ^{131}\text{mXe} \) events in the LZ TPC. The division of the TPC into position bins (voxels) in this space is shown by the solid red lines. The apparent holes in the distribution are due to PMTs which were off during this preliminary data-taking period. **Bottom Left:** A histogram of the negative of the drift time versus x position for the selected \( ^{131}\text{mXe} \) events in the LZ TPC. The division of the TPC into position bins (voxels) in this space is shown by the solid red lines. **Bottom Right:** A histogram of the negative of the drift time versus y position for the selected \( ^{131}\text{mXe} \) events in the LZ TPC. The division of the TPC into position bins (voxels) in this space is shown by the solid red lines.
6.15 Histograms of the $^{131m}$Xe S1-pulse areas in four different position bins (voxels) in the LZ TPC. The resulting fit from the iterative gaussian fitting procedure is shown on each histogram in red. The position details of each bin, as well as a description of the bin’s relative position, are included. ................................. 185

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LIST OF ACRONYMS

- **ADM**: Axion Dark Matter
- **BACCARAT**: Basically A Component Centric Analog Response to AnyThing (simulation package)
- **BSM**: Beyond the Standard Model
- **CMB**: Cosmic Microwave Background
- **CP**: Charge-Parity
- **DD**: Deuterium-Deuterium (mode of neutron production by fusion)
- **DER**: Detector Electronics Response (simulation package)
- **ER**: Electron Recoil (scattering event)
- **GXe**: Gaseous Xenon
- **ICV**: Inner Cryostat Vessel
- **LHC**: Large Hadron Collider
- **LUX**: the Large Underground Xenon experiment
- **LXe**: Liquid Xenon
- **LZ**: LUX-ZEPLIN
- **LZap**: LZ Analysis Package
- **NR**: Nuclear Recoil (scattering event)
- **OCV**: Outer Cryostat Vessel
- **OD**: Outer Detector
- **PMT**: PhotoMultiplier Tube
- **PTFE**: PolyTetraFlouroEthylene (Teflon)
- **QCD**: Quantum Chromodynamics
- **ROI**: Region Of Interest
- **SCCM**: Standard Cubic Centimeters per Minute
- **SiPM**: Silicon PhotoMultiplier
- **SIS**: Source Injection System
- **SLPM**: Standard Liters Per Minute
- **SURF**: Sanford Underground Research Facility
- **TPC**: Time Projection Chamber
- **VUV**: Vacuum UltraViolet
- **WIMP**: Weakly Interacting Massive Particle
- **ZEPLIN**: the ZonEd Proportional scintillation in LIquid Noble gases experiment
CHAPTER 1
INTRODUCTION

1.1 History of Evidence for the Existence of Dark Matter

The existence of non-baryonic dark matter is implied by a range of independent astrophysical observations, making it a well established feature of many leading Beyond the Standard Model (BSM) theories in physics today. Though the wide-spread study of the nature of dark matter didn’t begin until after Vera Rubin’s measurements of galactic rotation curves starting in the 1970s, its existence was first inferred at the beginning of the 20th century. Though it was greeted with much skepticism by the scientific community at the time, today, a wealth of evidence for the existence of dark matter has continued to amass from observations of astrophysical systems on many length scales. Some of the areas of study which have contributed most to the body of evidence for BSM dark matter include measurements of galactic rotation curves [1], gravitational lensing of galaxy clusters [2] and galaxy cluster collisions [3], and measurements of anisotropies in the cosmic microwave background [4].

1.1.1 First Inferences of the Existence of Dark Matter

The first time that it was suggested based on observation that the amount of observable matter in the universe is not enough to account for the apparent gravitational interactions of astrophysical bodies was in a series of lectures by William Thomson (known also as Lord Kelvin), the famous mathematical physicist and engineer. In the lecture series, *Baltimore Lectures on Molecular Dynamics and the Wave Theory of Light* published in 1904, Thomson considered the velocity dispersion of stars in
the Milky Way galaxy, making the clever assumption that the stars could be treated as a gas of point-particles under the influence of Newtonian gravity. In doing so, he determined that ”Many of our stars, perhaps a great majority of them, may be dark bodies.” [5] While not a full recognition of the glaring mystery that the existence of dark matter presents to our understanding of physics today, Thomson identified that the understanding of the composition of the Milky Way galaxy was incomplete. A significant amount of mass was unaccounted for.

Several decades later, in 1933, Fritz Zwicky was the next to infer the existence of dark matter after studying the Coma Cluster, a cluster of galaxies containing more than 1000 now-identified galaxies. The galaxies in the Coma Cluster had already been known to exhibit a much larger velocity dispersion than other similar clusters, but by applying the virial theorem to the galaxies on the outer edge of the cluster, Zwicky was able to infer that the mass of the cluster was approximately 400 times greater than the mass that could be inferred from visual observations. Though his measurement turned out to be off by an order of magnitude, by studying the local gravity he had correctly determined that the majority of the gravitational mass in the Coma Cluster was not visible.

In the decades following Zwicky’s measurement, astronomers worked to try to understand his findings. Some argued that Zwicky’s assumption that the Coma Cluster was a virialized system was unjustified, and that the galaxies he measured weren’t permanent members of the cluster bound in a stable orbit, but were instead passing by in an unbound hyperbolic flyby. Others performed their own calculations and were able to confirm the discrepancy that Zwicky found. As a whole, the field of astronomy could neither accept nor fully reject that some mysterious ‘dark’ matter existed in intergalactic space helping to bind galaxy clusters together. It was clear at the time, however, that further measurements would be required to ultimately resolve the mystery that Zwicky had uncovered further.
1.1.2 Galactic Rotation Curves

The evidence that would ultimately convince the scientific community that Zwicky’s discrepancy was pointing to a significant gap in physics knowledge came from high quality measurements of the rotational speeds of spiral galaxies. The first notable result was published in 1970 by astronomer Vera Rubin while working as a staff member at the Carnegie Institution of Washington, and her collaborator Kent Ford, an astronomer and instrument maker. Using an image tube spectrograph that Ford had recently developed, the pair made spectroscopic observations of the Andromeda galaxy with unprecedented quality, ushering in a new era of interest in spiral galaxy dynamics. Rubin and Ford graphed the velocity of orbiting bodies as a function of their radial distance from the galaxy center for the Andromeda galaxy, a plot that is referred to as a galactic ‘rotation curve’. The Andromeda galaxy rotation curve from Rubin and Ford was the first of several that would be published by various astronomers during the 1970s, providing insight into the rotational dynamics of an array of spiral galaxies.

Astronomer Ken Freeman was among the first to realize that the shapes of these rotation curves deviated from what one would expect when accounting for the gravitational influence of the visible matter alone. He concluded that because the measured rotation curves peaked at larger radii than expected, the spiral galaxies studied must be composed of a significant amount of undetected matter, that contributes at least half of the total mass of these galaxies, and which is not distributed exponentially (like the visible matter is) [6]. By the end of the 1970s, it was well established that many observable spiral galaxies had flat rotation curves at high radius, implying the existence of a significant amount of unseen mass far from their centers. A more modern example of the rotation curve discrepancy is illustrated in Fig. 1.1 below, using data presented in [7].
Figure 1.1. The observed rotation curve of the Triangulum Galaxy, M33. The measurements from starlight and the 21 cm hydrogen line are shown in yellow and blue, respectively, and a fit is underlaid. The expected rotation curve obtained by considering only visible matter is shown as a dashed grey line. The major discrepancy between the expected and measured dynamics reveals a significant amount of unaccounted for gravity, implying a significant amount of mass beyond what is visible.
The significance of this new understanding, while at the time not yet explicitly acknowledged, was that the problem of missing mass had now been identified in the dynamics of astrophysical objects at two completely different length (and mass) scales: the scale of galaxy clusters, $\mathcal{O}(10,000,000 \text{ ly})$, from the treatments of Thompson and Zwicky, and the scale of individual spiral galaxies, $\mathcal{O}(100,000 \text{ ly})$, from the spectroscopic measurements of the 1970s. The identification of implied missing mass at these independent dynamical scales is typically considered to be what marks the beginning of dark matter physics as its own field of study. The problem had now been well established with no obvious solutions, and the possibility of new physics at the heart of the problem became a reality. In the decades that followed, evidence for the existence of dark matter would only continue to mount.

1.1.3 Gravitational Lensing

Gravitational lensing is the process by which light originating behind a massive object appears to bend around that object, distorting the image of the light source. As is predicted by the general theory of relativity, spacetime is warped around massive objects, and light follows a straight path through it rather than the light itself being bent. In this way, massive objects act as a lens to light sources behind them. The details of how light propagates through the gravitational lens of a massive object to an observer on the opposite side can be used to infer the mass and mass distribution of the lens object. Gravitational lensing can therefore be used to directly measure the mass of galaxy clusters, and indeed, when such measurements are made, the strength of the gravitational lensing cannot be attributed to the visible matter alone; We see lensing from a combination of visible, and apparently dark, matter.

The most famous example of gravitational lensing providing strong evidence for the existence of dark matter is from measurements made by the Chandra X-ray Observatory of the Bullet Cluster, two galaxy clusters in the immediate aftermath of
a direct collision [3]. The dynamics of the collision can be analyzed independently for each major component of the clusters. The majority of the visible mass in the two colliding galaxy clusters is in the form of hot intergalactic gas, primarily Hydrogen, which is strongly interacting in the collision and results in the emission of x-rays. The rest of the visible mass is in the galaxies themselves, which are largely non-interacting in the collision due to the immense distances between galaxies within each respective cluster. The result of the galaxy cluster collision is therefore the separation of the gaseous and galactic components within each of the clusters; As the intergalactic gas mixes and lags behind, the galaxies of one cluster pass through the other unimpeded. Gravitational lensing of this collision shows that the center of mass of the system does not coincide with the center of mass of the intergalactic gas, where it would be expected in the absence of dark matter. Rather, massive dark matter clumps coincident with the collision-less galaxies are observed to contribute a significant fraction of the mass to the galaxy clusters. Fig. 1.2 shows an image of the Bullet Cluster collision with colors overlaid indicating the distribution of the hot collisional gas, and the total mass distribution inferred from lensing measurements.

1.1.4 Anisotropies in the Cosmic Microwave Background

The Cosmic Microwave Background (CMB) is the relic background radiation produced during the recombination epoch of the early universe. The recombination epoch refers to the time period, starting roughly 300,000 years after the Big Bang, when the universe had cooled enough to allow free protons and electrons to become bound to each other, forming neutral hydrogen atoms. Prior to this, the plasma filled universe was opaque to photons, which scatter off of charged particles in the process known as Thomson Scattering. During the transition from a universe occupied by a dense plasma of charged particles to one occupied by neutral hydrogen gas, the universe became transparent to photons for the first time. The free streaming photons which
Figure 1.2. The galaxy cluster collision 1E 0657-56, known also as the Bullet Cluster. The background shows an optical image of many galaxies, from the Hubble Space Telescope. Overlaid in pink: The distribution of hot collisional gas from the two colliding galaxy clusters, measured via emitted x-rays by the Chandra X-ray Observatory. Overlaid in blue: The mass distribution inferred from gravitational lensing measurements. The center of mass determined from lensing measurements is not coincident with the center of mass of the visible matter in the galaxy clusters, implying the presence of a significant mass of dark matter coincident with the galactic components of the two clusters.
were produced at that time in the universe’s early history and have been propagating through space since are what we observe today as the CMB, red-shifted by the universe’s expansion.

During the recombination epoch of the early universe, dark matter would contribute to the anisotropies in the CMB that we observe today by influencing the production of acoustic oscillations in the existing baryonic matter, the result of the competition everywhere between the inwards forces of gravity from dark and baryonic matter, and the outward force of radiation pressure from photons. The contribution to the acoustic oscillations from dark matter is measurable from the power spectrum of the CMB anisotropies. Cosmological parameter best fits to the CMB power spectrum estimate roughly 5.3 times more dark matter than baryonic matter [4], consistent with the estimates from the host of dynamical astrophysical systems that have been studied independently.

1.2 Dark Matter Candidates

While relatively little is known about the nature of dark matter, there are several features which any dark matter candidate must posses in order to have a feasible cosmological production mechanism, as well as to be consistent with the dark matter distribution and abundance that have been observed in astrophysical systems. These necessary features are detailed briefly in this section:

- **Gravitational interactions with baryonic matter:** The existence of dark matter was first inferred by its gravitational interaction with baryonic matter, and indeed, gravitational interactions with baryonic matter (and lensing of photons) are the only interactions that dark matter has been observed to be capable of.
• **Weak, or no, electromagnetic interactions:** Electromagnetic radiation is the primary mechanism by which baryonic matter dissipates energy in the accretion process that forms compact objects such as stars, planets, moons, and asteroids. Dark matter appears to be incapable of accretion into compact dark-matter objects on timescales comparable to the age of the universe, and instead has only been observed to exist in relatively diffuse clumps. Beyond simply being invisible at all electromagnetic wavelengths, the lack of compact dark-matter objects in the universe provides evidence that dark matter exhibits, at most, only very weak electromagnetic interactions.

• **Stable on age-of-the-universe timescales:** Measurements of the relative abundance of dark matter suggest that the amount of dark matter in the universe has been constant for the last 13.8 billion years, from the earliest moments in the observable universe until now. While the possibility that there is some mechanism by which dark matter is produced at the same rate that it is annihilated remains, the simplest assumption is that dark matter is composed of particles which are stable on time scales comparable to the age of the universe.

• **Cold:** 'Cold' dark matter refers to dark matter with a slow average velocity compared to the speed of light in the early universe. The dark matter 'temperature' in models of the early universe affects the way that structure formation has proceeded as the universe has continued to expand and cool throughout its observable history. In particular, in the cold dark matter model, structures form hierarchically with small length-scale over-densities forming first from the collapse of dark matter under its own self-interactions, and larger structures forming later as these smaller over-dense regions themselves clump together. This is referred to as 'bottom-up' structure formation and can be contrasted with the 'top-down' structure formation that would be expected if dark matter
was ’hot’ in the early universe, fast moving compared to the speed of light. In a hot dark matter paradigm, the largest astrophysical objects would form first, and smaller structures would form later from fragmentation of the larger objects. However, hot dark matter models are unable to explain the formation of galaxy sized dark matter clumps from the uniform dark matter distribution in the early universe that experiments like Plank (2015) [4] have revealed by studying the CMB. Hot dark matter has therefore been excluded from contributing a significant fraction of the total dark matter content of the universe today. Despite this, debate still exists on whether cold dark matter can account for the whole dark matter content of the universe without a ’warm’ component. The debate is fueled by discrepancies between cold dark matter simulations of structure formation and observations of galaxies and their clustering. In particular, the central density distributions of galactic dark matter halos in low mass galaxies are much flatter than the steeply increasing density profiles predicted at small radii by simulations (”cuspy halo problem” [8]). Additionally, far fewer dwarf galaxies than predicted by cold dark matter simulations are observed around larger galaxies (”missing satellites problem” [9]).

Many candidates for dark matter which satisfy the above requirements have been proposed and searched for to varying degrees, but several remain popular for investigation in today’s experimental and theoretical landscape. Below I describe just a few, and by no means all, of the most popular dark matter candidates being investigated today.

1.2.1 Weakly Interacting Massive Particles

If dark matter was created thermally in the early universe, freezing out after the temperature of the early universe decreased to below the dark matter particle’s mass, the relic abundance of dark matter can be used to infer the self-annihilation cross sec-
tion of the dark matter particle. The predicted cross section from the observed relic abundance happens to be roughly consistent with an electroweak-interacting particle of mass \( \sim 100 \text{ GeV} \). Since supersymmetric extensions of the Standard Model of particle physics commonly predict such a particle, this apparent coincidence, often called the "WIMP Miracle", has made the Weakly Interacting Massive Particle (WIMP) a leading candidate for dark matter for the last several decades. The relationship between the relic abundance of dark matter and the self-annihilation cross section in the thermal freeze-out model is shown in Fig. 1.3 from [10]. In addition to gravitational interactions, the traditional WIMP is expected to interact with baryonic matter only through the weak interaction, in which case the WIMP is simply an extension of the Standard Model. This simplest type of WIMP has largely been ruled out, however, for a dark matter particle with \( \mathcal{O}(10-100) \text{ GeV} \) mass, with current experiments setting limits on the WIMP interaction cross-section well below where weak interactions would be expected, assuming that the constraints on the local dark matter density and velocity distribution in the neighborhood of our solar system are accurate.

More recently, "WIMP" has been used generically to describe a dark matter particle which could interact with baryonic matter through some as yet undiscovered new mediator below the scale of weak interactions. The details of this mediator and interaction need not be specified when building an experiment to search for such interactions, since modern detector technologies would be sensitive to many hypothetical new mediators in principle. Any such new mediator below the weak scale would be an example of physics Beyond the Standard Model (BSM), existing in a previously 'hidden sector' of particle physics.

Modern day direct detection experiments search for both flavors of WIMP, since in either case, a flux of WIMP dark matter through the earth should be detectable via scattering from nuclear targets in terrestrial detectors. The body of this thesis is concerned with a specific detector technology, the dual-phase time projection cham-
Figure 1.3. The thermal freeze-out evolution of a 100 GeV dark matter particle as a function of temperature (bottom x-axis) and time (top x-axis) from [10]. The comoving number density (left y-axis) and resulting thermal relic density (right y-axis) are shown on the vertical axes. The solid curve results in an annihilation cross section which yields the correct relic density of dark matter, and the colored regions are for cross sections that differ by a factor of 10, 10², and 10³ from the predicted value. The dashed curve is the number density of a particle that does not freeze out, and remains in thermal equilibrium.
ber, which is being employed by various collaborations around the world to search specifically for WIMP dark matter.

1.2.2 Hidden Sectors

In particle physics today, the 'hidden' or 'dark' sector simply refers to a group of as yet undiscovered hypothetical particles which exist outside of the Standard Model, and only interact with Standard Model particles very weakly through new quantum fields and/or gravity. The hidden sector encompasses BSM WIMPs, but is a more generic descriptor which is not limited to a single particle type, and is therefore popular among theorists. Hidden sector particles are predicted by many string theories, and present the interesting idea that dark matter may be composed of a few, or many different particles which all exist outside of the Standard Model. The idea that dark matter consists of many different fundamental particles remains entirely plausible.

1.2.3 Axions

Axions are hypothetical particles which were originally proposed as a solution to the strong charge+parity (CP) symmetry problem in quantum chromodynamics (QCD): QCD permits CP violation in strong interactions (a difference in the way matter and anti-matter interactions occur), though strangely, no violation has ever been observed. In one possible solution to this problem proposed by Peccei and Quinn, the axion is the boson that results from the introduction of a hypothetical scalar field with non-zero vacuum expectation value that spontaneously breaks a new global symmetry and reduces the CP-violation parameter to zero [11].

Theoretically permissible production mechanisms for the hypothetical axion in the early universe could also explain the matter-antimatter asymmetry that we observe in the universe today, and create the possibility for axions to account for some fraction, or all, of the universe’s cold dark matter content. For cold dark matter to be
composed of axions, the axion mass must be on the order of $\sim 10^{-12} - 10^{-2} \text{ eV}$ [12]. Over much of this mass range the axion is very wave-like, requiring entirely different detection mechanisms than heavier dark matter candidates. If dark matter is primarily composed of axions, the huge number of them required to account for the mass of dark matter that we see in astrophysical systems like our own Milky Way galaxy should be detectable in laboratories on the earth’s surface as a classical (axion) field, and many experiments have been developed to search for it.

1.2.4 Sterile Neutrinos

Sterile neutrinos are the hypothetical right-handed counterpart(s) to the three left-handed neutrinos in the Standard Model, called sterile to indicate that unlike the Standard Model neutrinos, they do not interact via the weak interaction. Because sterile neutrinos interact with other Standard Model particles only through gravity, they may be relatively difficult to detect directly, though there are some constraints which narrow the searchable parameter space. For example, for sterile neutrino dark matter to result in bottom-up structure formation in models of the early universe, it has been shown that the sterile neutrino must have approximately keV scale mass [13]. Experiments at FermiLab [14] and CERN [15] have searched for sterile neutrino production and decay, and have seen no evidence of detection yet, setting limits on the interaction strength. Beyond these, many of the other features of the hypothetical sterile neutrino are unknown, though despite the relative difficulty in detecting them, they remain an interesting dark matter candidate.

1.2.5 Modified Newtonian Dynamics

Modified Newtonian Dynamics (MOND) refers to the class of theories which attempt to solve the dark matter problem with a modification to newtonian gravity in the regime of extremely small accelerations, rather than by the introduction of an exotic new particle. While certain MOND theories have been successful at explaining
the dynamics of rotating galaxies and other galaxy scale dynamics, so far they have failed to simultaneously account for the dynamics and mass distributions in galaxy clusters, like the Bullet Cluster. MOND theories have been unable to produce a successful and comprehensive cosmological model without a dark matter component. Perhaps MOND theories can contribute to explaining some of the outstanding problems in dark matter physics, but at present, they have not eliminated the need for a dark matter particle generally.

1.3 Local Dark Matter Distribution

For dark matter detection experiments on earth to be viable, a flux of dark matter particles passing through the earth that is capable of interacting with a terrestrial detector is required. Consistent with observations of other spiral galaxies, the best observational evidence suggests that the Milky Way galaxy (within which we find ourselves) is embedded in a large, diffuse, and roughly spherical, though perhaps slightly prolate [16], dark matter 'halo'. The dark matter halo of the Milky Way galaxy appears to be concentric with the galaxy’s visible component, and to extend to radii well beyond the visible matter which composes the Milky Way’s spiral arms. The length scale of the dark matter halo is, however, poorly constrained at present.

Simulations predict that at the radial distance of our solar system from the galaxy’s center, dark matter in the halo is approximately smoothly distributed [17]. The density of the dark matter halo at the radial distance of our solar system is model dependent, but assuming a spherical halo, has been constrained to 0.2-0.4 GeV/cm² depending on the halo’s length scale [18]. A density of 0.3 GeV/cm² is typically assumed when attempting to calculate the expected dark matter flux through the earth for a given dark-matter-particle mass.

The velocity distribution of dark matter particles in the halo is typically assumed to be Maxwellian. Recent results from the Gaia satellite estimate the average orbital
velocity of particles in the dark matter halo at the radius of our solar system to be 210 km/s isotropically, in all orbital planes [16], compared to our solar system’s orbital velocity of 230 km/s around the galaxy’s center. The current best models, therefore, predict an ever-present flux of dark matter particles through the earth. While the dark matter flux through the solar system is expected to be roughly constant, an annual modulation in the flux through the earth is expected as the orbital velocity of the earth around the galaxy’s center varies (and therefore the velocity of the earth relative to the dark matter halo varies too) during the earth’s orbit around the sun. This flux of dark matter particles through the earth interacts extremely rarely, if at all, with the baryonic matter that composes it, but dark matter detectors on earth like the LUX-ZEPLIN experiment with which this thesis is primarily concerned, aim to detect these exceedingly rare interactions in specialized detectors.

1.4 Laboratory Based Dark Matter Detection

Experiments designed to detect the presence of dark matter fall into three general categories. These are direct detection experiments (like the LUX-ZEPLIN experiment) which also include searches for axions, missing-mass searches at particle colliders, and indirect detection. Below I give a cursory overview of these experimental dark matter detection approaches.

1.4.1 Direct Detection

Direct detection describes a range of experiments which aim to detect scattering of galactic WIMP dark matter off of nuclei in terrestrial detectors. These detectors are designed to measure the energetic products of such a scatter, which include light (photons), free charge (electrons), and material vibrations (phonons). Common interaction targets in direct detection experiments include noble liquids such as xenon or argon, organic liquid scintillators, and scintillating or semiconducting crystals. To
reduce signal backgrounds, direct detection experiments are often located deep underground to shield from cosmic radiation, and use radio-pure materials to achieve low levels of in-situ radiation. Dozens of direct detection experiments have constrained the parameter space for WIMP dark matter over the last several decades, and continue to operate at ever-larger scales, and/or with ever-lower energy thresholds.

1.4.2 Axion Searches

Axion searches take advantage of the fact that in the presence of a strong static magnetic field, axion dark matter (ADM) acts like an effective current density, and can be transformed into photons. This mechanism, called the Primakoff effect, can be exploited using a resonant cavity, or axion haloscope. The resonant cavity has been the most successful technology for ADM searches thus far. In such a detector, the resonant frequency of the cavity is tuned to a specific axion mass, and the electromagnetic coupling of the axion is detectable as a resonance. Other types of experiments have been designed to exploit the Primakoff effect as well, and include transforming photons into axions which propagate through solid metal before being transformed back into photons for detection, searching for polarization changes in photons propagating through a magnetic field, and searching for resonances in Josephson Junctions. ADM searches have been making quick progress in recent years, and the very active field is a promising sign of continued progress in the near future.

1.4.3 Collider Searches

Searches for dark matter in particle colliders differ from direct detection experiments in that dark matter does not interact with the detector materials in a collider search. Instead, collider searches like those performed with the Large Hadron Collider (LHC) look for missing momentum in the event reconstruction of a particle collision as the signature of dark matter. While direct detection experiments rely on dark matter to scatter off of Standard Model particles, collider searches look for Standard Model
particles in high energy collisions to produce dark matter through the same as yet unknown mediator(s) that motivate the BSM WIMP. When dark matter is produced in such a collision, it would escape the collider undetected, though the characteristic amount of missing energy carried away by the WIMP would allow it to be identified as a new particle. Supplementing the current searches for dark matter production with beams of ever-higher energy, searches are now underway at the 'intensity frontier', using lower-energy beams to produce a comparatively enormous number collisions.

1.4.4 Indirect Detection

Indirect detection dark matter experiments look for signatures of dark matter outside of our solar system, primarily from telescopic observations, by searching for excess Standard Model particles and/or anti-particles, produced when dark matter is annihilated or decays in astrophysical systems. This particle excess could be in the form of neutrinos, positrons, gamma-rays, X-rays, or something else entirely. Indirect detection experiments have served most notably to constrain the dark matter annihilation cross-section, placing ever stricter limits across a wide range of dark matter masses. The main challenges for indirect detection experiments are that the signals that they search for are also produced by decays and annihilation of many forms of baryonic matter, and worse, dark matter distributions are typically coincident with distributions of baryonic matter in astrophysical systems, making background free searches impossible. Therefore a very comprehensive understanding of the background present from decay and annihilation of baryonic matter is required.
CHAPTER 2

DUAL PHASE XENON TIME PROJECTION CHAMBERS

The dual-phase xenon (Xe) Time Projection Chamber (TPC) is a particle detector capable of full 3-D position and energy reconstruction of interactions between incoming particles/radiation and a liquid Xe (LXe) target. Particularly useful for a WIMP search experiment, the dual-phase LXe TPC is able to discriminate between scattering interactions from the LXe’s atomic nuclei and electrons, so called Nuclear Recoil (NR) and Electron Recoil (ER) events. In recent years, dual-phase Xe TPCs have led the field of direct dark matter detection in limit setting for the $\mathcal{O}(10-100 \text{ GeV})$ spin-independent WIMP interaction cross-section. In the last decade, continuous improvements in sensitivity and reach have been achieved primarily by a combination of an increase in the scale of such detectors, and a reduction of the intrinsic background from naturally occurring radioactivity in detector materials. This effort has been led recently by the LUX [19] and LUX-ZEPLIN (LZ) [20] collaborations, the XENON collaboration [21] and [22], and the Panda-X collaboration [23].

Liquid nobles, like xenon and argon, are excellent targets for WIMP detection because they are easy to purify and are transparent to the scintillation light that they produce following an interaction. Xenon is a particularly good choice due to its large atomic mass and high density in the liquid phase, $\sim 2.9 \text{ kg/L}$, which provides a large target for WIMP interactions and a high stopping power for incoming particles and radiation. Additionally, xenon has naturally occurring isotopes with odd numbers of neutrons which provide sensitivity to spin-dependent WIMP interactions, but has no naturally occurring long-lived radioisotopes. Because of these features, ton-scale
dual-phase Xe TPCs are used to search for other rare interactions as well, including neutrinoless double beta decay and supernova neutrinos.

2.1 Basic Detection Principles and Xenon Microphysics

In a dual-phase LXe TPC, the LXe target material is contained within a highly reflective and radiopure cylindrical chamber of polytetrafluoroethylene (PTFE, or Teflon), and is instrumented at the top (gas phase) and bottom (liquid phase) with arrays of light sensors such as photomultiplier tubes (PMTs) or silicon photomultipliers (SiPMs). High reflectivity inside of the TPC is critical to achieve high light-collection efficiency for the light-sensing arrays, while radiopurity of materials reduces the rate of WIMP-like background interactions (WIMP-like background events are produced from the decay products of naturally occurring uranium and thorium isotopes present in trace amounts in all materials). The cylindrical detector volume is filled with LXe, leaving a thin region of gaseous Xe (GXe) at the top, in which the top array of light sensors are positioned. Metal wire grids near the top and bottom of the TPC establish an electric field along the cylindrical (Z) axis of the TPC, and metal field-shaping rings are embedded in the PTFE walls to improve the uniformity of the electric field. A metal wire grid positioned just below the LXe surface and another positioned in the GXe just above the LXe surface establish a stronger ‘extraction’ electric field, which facilitates the emission of free electrons from the liquid bulk into the gas space.

When an incident particle scatters off of a xenon nucleus or bound electron in the LXe bulk, momentum transferred from the incident particle creates excited Xe atoms ($\text{Xe}^*$), freed electrons, and heat. $\text{Xe}^*$ atoms are created either directly or through the recombination of ionized electrons with $\text{Xe}^+$ ions created in the interaction. $\text{Xe}^*$ atoms combine with neutral ground-state Xe atoms to form molecular dimers ($\text{Xe}_2^*$) which decay to the neutral ground-state through the emission of a 175 nm (Vacuum-
Ultraviolet (VUV) photon on an $\mathcal{O}(10-100 \text{ ns})$ timescale. This prompt light emission produced from the interaction in the LXe bulk, called scintillation, is directly detected by the light-sensing arrays, and is the primary signal (S1) detected from an interaction. The energy converted to heat (not measured) in a scattering event is negligible for ER events, but significant for NR events.

Many of the ionized electrons created during an interaction in the LXe do not recombine with Xe$^+$ ions because of the strong electric field established along the cylindrical (Z) axis of the TPC. Instead, these freed electrons drift upwards under the influence of the electric field and are emitted across the liquid surface by the extraction field. Once in the GXe the electrons accelerate, producing electroluminescence photons (proportional to the number of extracted electrons) from the de-excitation of Xe$_2^+$ dimers, themselves produced in interactions between the accelerating electrons and GXe atoms. These (S2) photons, a secondary (in time) signal from the initial interaction in the LXe, are detected primarily by the top array of light sensors. WIMP-like events, which scatter a single time in the TPC, produce signals with one S1 and one S2 pulse, though multiple-scatter events in the TPC produce signals with multiple S1 and/or multiple S2 pulses depending on the details of the interaction.

In TPCs which use PMTs to detect light, the scintillation and electroluminescence photons, S1 and S2, are typically measured in units of photoelectrons emitted from the PMT faces (phe), or the inferred number of photons detected by the PMT faces (phd) after accounting for the double photo-electron emission probability. The time separation between the detection of S1 and S2 photons, called drift time, is used to determine the position of the scattering event along the cylindrical (Z) axis of the TPC, and the distribution of light collected by the PMT arrays is used to determine the transverse (X, Y) position. Combining these two measurements, full 3-D position reconstruction is achieved for scattering events that occur within the TPC. A pictorial
representation of the production of S1 and S2 photons following a scattering event is shown in Fig. 2.1.

2.2 Energy Reconstruction

When an interaction occurs in the TPC, the relative amount of deposited energy which goes into producing scintillation light (S1 channel) versus freed electrons (S2 channel) depends on the fraction of electrons that recombine with the xenon atom, forming Xe* excimers, in the aftermath of the interaction. The recombination fraction varies and depends on the type of interaction (NR or ER), energy of the incident particle, and the local electric field strength. Despite the electric field dependence on the relative signal production in the two channels, the sum of the energy-normalized S1 photons and freed electrons will be constant for all events of the same type. This is simply a statement of the fact that the scintillation photons and free electrons produced must share the total deposited energy; They are anti-correlated. In the case of ER events in LXe, the energy lost to heat is negligible and can be ignored. If ER events from different mono-energetic sources are displayed on the axes S1/E versus S2/E, where E is the total energy deposited in both channels, these events will lie on a straight line; This is known as a Doke plot. The x and y intercepts of the line formed by the various mono-energetic sources are equal to the average number of PMT-photo-electrons emitted (phe), or the average number of photons detected (phd), per keV for ER S1s and S2s, respectively. By multiplying the x and y intercepts by the xenon work function, W, which has been measured to be $13.7 \pm 0.2 \text{ eV/quanta}$ [25], the average number of phe or phd per photon and per electron propagated from the interaction site is obtained (depending on the units used to measure the S1 and S2 pulse area). These constants which characterize the global detector 'gains' are named gain-1 (g1) and gain-2 (g2), respectively. One can accurately measure g1 and g2 by plotting the mean S1/E versus mean S2/E for a variety of mono-energetic calibration
Figure 2.1. The basic signal production and measurement process in a dual-phase Xe TPC, from [24]. The sum of all PMT signals, as measured by arrays of PMTs (pictured as colored circles) at the top and bottom of the TPC, is shown on the right at the corresponding height of the production process. S1 photons and freed electrons are produced during an ER or NR event in LXe. An electric field drifts the freed electrons upwards where they are emitted across the liquid surface and accelerated in the GXe to produce S2 photons via electroluminescence. The distribution of S2 light on the top array (shown with PMT colors, red indicating a large signal) provides (X, Y) position reconstruction, while the time separation between S1 and S2 determine the Z position of the initial scatter.
sources and then calculating the x and y intercepts of a straight line best fit to the data. An example Doke plot from [26], showing data from LUX, is shown in Fig 2.2. If $g_1$ and $g_2$ are known, the energy of an ER scattering event can be accurately reconstructed in units of keVee (electron-recoil equivalent keV) from $S_1$ and $S_2$ (with position-dependent corrections applied) using the relationship:

$$E = W \left( \frac{S_1}{g_1} + \frac{S_2}{g_2} \right)$$

(2.1)

where $W$ is the work function for xenon. Reconstructing ER event energies using these global $g_1$ and $g_2$ measurements is standard in TPC-based dark matter detection experiments.

In the case of NR events, the prescription is modified slightly, requiring the addition of the energy dependent Lindhard factor ($\mathcal{L}$) [27] to account for the fact that the energy lost to heat in the scattering event is not negligible in this case. The reconstructed energy is then given in keVnr (nuclear-recoil equivalent keV) by:

$$E = \mathcal{L}^{-1} W \left( \frac{S_1}{g_1} + \frac{S_2}{g_2} \right)$$

(2.2)

where the Lindhard factor can be determined from calibration data.

### 2.3 NR/ER Discrimination

Central to the successful identification of a WIMP scattering event in a dual-phase Xe TPC is the ability to distinguish between electronic and nuclear recoil events. WIMPs are much more likely to coherently scatter off of a xenon nucleus than a bound electron because of the enhanced cross-section that the many nucleons provide. Additionally, electronic interactions constitute the majority of the background events in Xe TPCs, and make a search for a rare WIMP-electron scatter much more difficult. For these reasons, WIMP search experiments typically look for
Figure 2.2. A Doke plot showing the mean of $S1/E$ vs $S2/E$ for a range of calibration sources used in LUX, from [26]. The gains, $g1$ and $g2$, from the best fit are in units of phe per scintillation (S1) photon produced, and phe per free electron produced, at the interaction site.
nuclear WIMP interactions. The ability to discriminate between electron and nuclear recoil events is possible in practice because of a difference in the ratio of ionization electrons to scintillation photons produced at the interaction site between the two interaction types.

A TPC’s ability to discriminate between ER and NR events can be studied by plotting the logarithm of $S_2/S_1$ as a function of $S_1$ as in Fig. 2.3, from [24] (or similarly, the logarithm of $S_2$ as a function of $S_1$). In this parameter space the two interaction types form distinct bands, with ER events producing more initial...
ionization and less direct excitation (leading to less S1 from scintillation) than in NR events. To reject ER events in practice, a contour below which some fraction of the NR events lie is chosen, often 50% (the NR median). The fraction of ER leakage below the chosen NR contour is used to define the discrimination ability of the detector. In the case of 50% NR rejection, all events above the NR band median are rejected and the discrimination value is defined as the percentage of ER events which are rejected this way. In past dual-phase Xe TPC experiments, a 50% NR rejection has typically resulted in an ER event rejection greater than 99.5%. Because ER discrimination is not perfect, great effort goes into minimizing low energy ER backgrounds during the construction and operation of dual-phase Xe TPCs to achieve maximal sensitivity to rare low-energy NR interactions.
CHAPTER 3

LUX-ZEPLIN

The LUX-ZEPLIN (LZ) experiment is a WIMP-dark-matter direct detection experiment with a dual-phase Xe TPC at its core, boasting the largest collection xenon atoms ever amassed, approximately 10 tonnes. LZ is located 4850 feet underground (4300 m.w.e.) in the Davis Cavern of the Sanford Underground Research Facility (SURF) in Lead, SD, where the LUX experiment was previously housed. LZ is designed to achieve the greatest sensitivity to spin-independent $O(10-100$ GeV) WIMP-scattering interactions of any experiment to date by the end of its first dedicated WIMP search run. At the time of writing, LZ has completed a successful commissioning campaign, and has collected the critical calibration data required to consider a dedicated dark matter search. The data is actively being studied to determine if additional calibrations are needed before the first science exposure can begin.

The dual-phase Xe TPC at the core of the LZ experiment is surrounded by a LXe ‘skin’, inside of an ultra-pure-titanium (low radioactivity) cryostat, the Inner Cryostat Vessel (ICV). The ICV is suspended inside of a second, ‘outer’, ultra-pure-titanium cryostat vessel (the OCV) which contains an insulating vacuum that thermally isolates the ICV (at LXe temperature, $\sim 170$ K) from the room temperature OCV. The OCV stands inside of a water tank, and is surrounded on all sides by acrylic vessels filled with Gadolinium-loaded organic-liquid-scintillator, called the Outer Detector (OD), also within the water tank. A drawing of the LZ experiment and its major components is shown in Fig. 3.1.
3.1 The LZ TPC

The LZ TPC contains approximately 7 tonnes of LXe within in a 1.46 m diameter by 1.46 m tall cylindrical volume. The walls of the TPC are constructed from stacked PTFE rings with titanium field shaping rings embedded between the PTFE ring layers, comprising the 'field cage'. Arrays of 3-inch diameter (Hamamatsu R11410-22) PMTs, developed for operation at LXe temperatures and optimal sensitivity to VUV photons from Xe scintillation, compose the top and bottom surfaces in the TPC. These arrays contain 253 (top) and 241 (bottom) PMTs, respectively, held in titanium structures whose surfaces are entirely covered in PTFE. The upward looking bottom array (immersed in the LXe) is arranged in a close-packed hexagonal pattern to maximize PMT coverage, while the downward looking top array (in the GXe region) is arranged in a close-packed hexagonal pattern that transitions to a circular pattern near the perimeter to optimize position reconstruction (from S2) for
events near the walls, a primary source of background. The height of the LXe, or LXe level, is set by three weirs spaced equally around the perimeter of the TPC, positioned at a height between the gate and anode grids. The bottom, cathode, gate, and anode grids, which establish the drift field and extraction field along the cylindrical (Z) axis of the TPC, are visible in Fig. 3.2, a drawing of the inside of the fully assembled LZ TPC. The region below the cathode grid (and above the grounded bottom PMT array) is known as the reverse field region. In the reverse field region S1 is observed normally, but with no charge collection (being outside of the drift field), no S2 is observed. Key dimensions and parameters of all four grids in the TPC, from [20], are listed in Table. 3.1. Photos of the fully assembled TPC and the top PMT array are shown in Fig. 3.3, and key dimensions and projected parameters of the LZ TPC from [20], [24], and [28] are shown in Table. 3.2.
Figure 3.3. Photos by Matthew Kapust, Sanford Underground Research Facility. **Left:** The fully assembled LZ TPC. **Right:** The top PMT array before being mounted onto the TPC. PTFE (highly reflective at LXe temperatures) covers the surfaces of the titanium support frame between the PMT faces to maximize light collection efficiency.

**Table 3.1.** Table of key grid dimensions and design parameters (all 90° woven 304SS meshes). The columns report the design voltage, voltage applied during the detector-commissioning data taking detailed in chapter 6, wire diameter, wire pitch, and total number of wires

<table>
<thead>
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</thead>
<tbody>
<tr>
<td>Anode</td>
<td>+5.75</td>
<td>+4.50</td>
<td>100</td>
<td>2.5</td>
<td>1169</td>
</tr>
<tr>
<td>Gate</td>
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<td>−4.50</td>
<td>75</td>
<td>5.0</td>
<td>583</td>
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<tr>
<td>Cathode</td>
<td>−50.0</td>
<td>−32.0</td>
<td>100</td>
<td>5.0</td>
<td>579</td>
</tr>
<tr>
<td>Bottom</td>
<td>−1.5</td>
<td>−1.25</td>
<td>75</td>
<td>5.0</td>
<td>565</td>
</tr>
</tbody>
</table>
Table 3.2. Table of key TPC dimensions, predicted parameter values, and preliminary parameter values during the detector-commissioning data taking detailed in chapter 6.

<table>
<thead>
<tr>
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<tr>
<td>TPC active height [m]</td>
<td>1.46</td>
</tr>
<tr>
<td>TPC inner diameter [m]</td>
<td>1.46</td>
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<tr>
<td>Active LXe mass [kg]</td>
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<table>
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<th>Predicted/Projected TPC Parameters</th>
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<tbody>
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<td>PTFE-LXe(GXe) reflectivity</td>
<td>0.977(0.85)</td>
</tr>
<tr>
<td>LXe(GXe) photon absorption length [m]</td>
<td>100(500)</td>
</tr>
<tr>
<td>PMT quantum efficiency*</td>
<td>0.309</td>
</tr>
<tr>
<td>Predicted g1 [phd/ph]</td>
<td>0.119</td>
</tr>
<tr>
<td>Predicted g1_{gas} [phd/ph]</td>
<td>0.102</td>
</tr>
<tr>
<td>Predicted Single electron size [phd]</td>
<td>83</td>
</tr>
<tr>
<td>Predicted S2 electron extraction efficiency</td>
<td>0.95</td>
</tr>
<tr>
<td>Predicted g2 [phd/e]</td>
<td>79</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Preliminary Parameter Values from Detector Commissioning</th>
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</tr>
</thead>
<tbody>
<tr>
<td>g1 [phd/ph]</td>
<td>0.1045</td>
</tr>
<tr>
<td>g1_{gas} [phd/ph]</td>
<td>0.0753</td>
</tr>
<tr>
<td>Single electron size [phd]</td>
<td>64</td>
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<tr>
<td>S2 electron extraction efficiency</td>
<td>0.93</td>
</tr>
<tr>
<td>g2 [phd/e]</td>
<td>59.6</td>
</tr>
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</table>

*After accounting for dual-photoelectron emission
3.2 The LXe Skin

Approximately two tonnes of LXe 'skin' (optically isolated from the TPC) surrounds the sides and bottom of the TPC within the ICV. This LXe volume is required for dielectric insulation of the TPC, but is also instrumented with its own dedicated PMTs to create a standalone S1-only detector which actively vetos neutron and γ-ray interactions that are coincident with TPC signals. The ability to veto events with multiple scatters in LZ is one of the key ways that background events are rejected when searching for WIMPs, which will only scatter once in LZ’s xenon because of the WIMP’s extremely small interaction cross-section.

In the LXe skin, PMTs are positioned in three different locations. Near the top of the side skin but below the LXe surface, 93 one-inch (Hamamatsu R8520-406) PMTs surround the outside of the TPC, looking down on the side skin from above. At the bottom of the side skin, 20 two-inch (Hamamatsu R8778) PMTs attached to the inner wall of the ICV look upwards at the side skin from below. Finally, a ring of 18 additional two-inch (Hamamatsu R8778) PMTs attached to the bottom of the TPC collect light in the 'dome' region, underneath the TPC, with 12 of the PMTs looking radially outwards, and 6 looking radially inwards. To improve light collection efficiency in the Xe skin, where photons scatter many times on average before being detected, all of the PMTs in the skin are fully contained in PTFE housings, and the inner ICV wall is tiled with a thin layer of PTFE. The locations of the lower side-skin and dome PMTs are shown in the drawing and photos in Fig. 3.4, from [29] (the position of the upper side-skin PMTs are visible in Fig. 3.2).

3.3 The Circulation System

The primary function of the online xenon purification system, or 'circulation' system, is to constantly remove non-noble impurities from LZ’s xenon. A radon (Rn)
Figure 3.4. **Upper Left:** Cross-sectional drawing of the dome and lower side-skin showing the position of the PMTs there. **Lower Left:** Photo of the ring structure which holds the dome PMTs just below the bottom of the bottom TPC PMT array, before the fully assembled TPC was lowered into the ICV. **Right:** Photo of the inner wall of the ICV from above, lined with PTFE tiles. The 20 bottom side-skin PMTs are installed around the perimeter. The PTFE tiles have holes drilled in them which fit over low-profile titanium buttons, epoxied to the ICV wall. PTFE screws which attach PTFE washers to the buttons are visible in the photo.
Figure 3.5. A diagram of the online xenon purification system in LZ. The main circulation path which purifies the Xe in LZ using a heated-zirconium getter is shown in blue. The radon removal system paths are shown in black.

removal system also provides a low level of Rn removal and control. An overview of the major systems and paths through the circulation system is shown in Fig. 3.5.

As a constant flow of LXe from circulation enters the bottom of the ICV, LXe in the TPC spills over the three weirs in the extraction region, at a height between the gate and anode grids. The weir spillover LXe is collected in the weir drain pipe and flows horizontally out of the ICV, through the water tank and towards the LXe tower.

The LXe tower is a free-standing vacuum-insulated cryogenic vessel outside of the water tank, containing the "reservoir vessel", "two-phase heat exchanger", and "subcooler vessel". LXe from the ICV is collected in the reservoir vessel where a standpipe design decouples the liquid level there from that in the weir drain line. LXe
flows from the bottom of the reservoir vessel into the two phase heat exchanger where it is vaporized by thermalizing with purified GXe on its way towards the ICV. On the other side of the two-phase heat exchanger, the purified GXe begins condensing and flows into the subcooler vessel where any remaining GXe is separated from the newly condensed LXe. In the subcooler vessel, the LXe is cooled to below its saturation temperature via a liquid nitrogen (LN$_2$) thermosyphon-coldhead. Once cooled, the LXe flows horizontally back through the water tank and enters the LXe skin and TPC through the bottom of the ICV. A purity monitor in the subcooler vessel monitors the concentration of electronegative impurities in the LXe entering the ICV.

When LXe is vaporized in the two-phase heat exchanger after exiting the ICV, the cold GXe is pulled out of the LXe tower and into two circulation compressors arranged in parallel. The compressors push the now-room-temperature GXe through a heated-zirconium getter, the active purification component in the circulation system which removes non-noble impurities from the GXe. After being purified, the GXe is pushed by the compressors into the condensing side of the two-phase heat exchanger in the LXe tower, where it follows the path back to the ICV described in the previous paragraph. The LZ online purification system is designed to continuously circulate Xe through the circuit described in this section at flow rates up to 600 standard liters per minute (SLPM), purifying the full 10 tonnes of Xe in $\sim$2 days per single pass.

Several cable conduits (pictured in Fig. 3.5) guide the many cables within the ICV to isolated GXe spaces where they are connected to breakout feed-throughs and guided out of the ICV and water tank. The Rn removal system pulls GXe in these isolated spaces at a rate of 0.5 SLPM into a charcoal column containing 10 kg of synthetic charcoal (Saratech Spherical Adsorbant, Blücher GmbH [30]) at 190 K. The radon emanation rate of the charcoal was reduced by etching with nitric acid (HNO$_3$) and rinsing with distilled water. The Rn removal system is designed to retain $^{222}$Rn atoms for three half-lives, 12.7 days, after which 90% of the $^{222}$Rn atoms will
have decayed. GXe leaving the Rn reduction system is pulled by the circulation compressors into the main circulation loop, upstream of the heated getter.

3.4 The Outer Detector

The Outer Detector (OD) is designed to tag neutron scattering events such as those from (\(\alpha, \text{n}\)) processes, where an \(\alpha\)-particle emitted from the decay of a heavy atom interacts with a light nucleus in a material, resulting in the emission of a neutron. (\(\alpha, \text{n}\)) reactions occur frequently from alphas produced by naturally occurring \(^{238}\text{U}\)- and \(^{232}\text{Th}\)-chain radioisotopes in materials such as PTFE.

In the OD, gadolinium-doped liquid scintillator is contained within segmented acrylic vessels which surround the OCV on all sides inside of the water tank containing the entire detector system. When a neutron captures on gadolinium, \(\gamma\)-rays are emitted which induce scintillation light from the liquid scintillator, and PMTs inside the water tank detect photons produced from the interaction. The OD enables the capture and tagging of neutrons within a time window that allows for correlation with (and veto of) any corresponding NR scatters in the TPC.

To maximize tagging efficiency, the thickness of the acrylic tanks was designed to be as thin as structurally possible, reducing the fraction of neutrons that capture on hydrogen in the acrylic (producing a single 2.2 MeV \(\gamma\)-ray) to an estimated 10%. To maximize light collection efficiency in the water tank, the OCV is surrounded with (reflective) Tyvek, and a Tyvek curtain is positioned behind, as well as above and below, the PMTs. The acrylic tanks, water-tank PMTs, and Tyvek surfaces are all visible in the diagram in Fig. 3.1. The final design of the OD is estimated to have a neutron tagging efficiency that is greater than 95% [29]. The fully assembled (but not filled) OD, surrounded by Tyvek and PMTs is pictured in Fig. 3.6.
Figure 3.6. The Outer Detector fully assembled, but not yet filled. The acrylic tanks which hold liquid scintillator are seen surrounding the Outer Cryostat Vessel. The neutron calibration conduits (nitrogen filled tubes which allow neutrons to be fired into the TPC from outside the water tank) can be seen traversing the water tank and Outer Detector vessels. The PMTs and PMT ladders are shrouded in reflective Tyvek to maximize light collection efficiency in the Outer Detector.
3.5 Backgrounds

Backgrounds in LZ fall into two broad categories, electron recoil (ER) and nuclear recoil (NR) events, which appear as two distinct bands in a plot of S2-pulse area versus S1-pulse area. The ER and NR bands overlap at low energies, in the WIMP search ROI, making background mitigation extremely important in LZ. Backgrounds which can’t be completely mitigated must be thoroughly understood to maximize the sensitivity of a WIMP search. Many aspects of the LZ experiment have been designed, or are naturally able, to significantly reduce backgrounds in the TPC. Some of the major background reduction features and techniques include: underground operation within a water tank to mitigate cosmogenic backgrounds and high-energy γ-rays from the rock overburden, a target LXe mass which is large enough to self-shield from external radiation, active vetoing of events with coincident scatters in the LXe skin and OD, and the ability to perform S2/S1-based ER rejection (described in section 2.3). A plot of S2 versus S1-pulse area in the WIMP search ROI, as well as summaries of the expected backgrounds in the LZ TPC, are shown in Fig. 3.7, from [20], for a 5.6 tonne fiducial LXe mass in LZ. A brief discussion of each of the various types of backgrounds in LZ is presented in this section.

3.5.1 Naturally Present Radioisotopes in Materials

Naturally occurring radioisotopes present in the materials used to build LZ are the largest source of background events in the LZ TPC. Particularly problematic are the γ-emitting radioisotopes $^{40}$K, $^{137}$Cs, and $^{60}$Co, as well as the many decay topologies produced from $^{238}$U, $^{235}$U, $^{232}$Th, and their progeny. The uranium and thorium chains produce neutrons (NR backgrounds) from spontaneous fission and ($\alpha$, n) reactions, while outgassing of radon and krypton from detector materials produce ER backgrounds in the LXe bulk. After outgassing as (chemically inert) radon, $\alpha$-emitting radon daughters can become re-distributed in the TPC and contribute to ER
Figure 3.7. **Left:** The simulated background events from a 1000 live-day exposure with a 5.6 tonne fiducial volume in the LZ TPC, from [20]. The ER and NR bands are shown in blue and red, respectively, with the mean indicated by the solid line, and 10% and 90% contours indicated by the dashed lines. In LZ, $^{214}$Pb is the dominant source of ER-band background events. **Right:** Expected NR (upper right) and ER (lower right) background rates in the LZ TPC for a 5.6-tonne fiducial volume for single scatter events with no coincident events in the LXe skin or OD. No detector efficiency or WIMP-search ROI cuts have been applied. Contributions from detector components, surface contamination and environmental backgrounds are summed together into a single component labeled "Det. + Sur. + Env."
and NR backgrounds when deposited on certain material surfaces. $^{222}$Rn emanated from detector materials is the dominant individual contributor to backgrounds in LZ, producing beta emissions from ground-state $^{214}$Pb decays (with no associated $\gamma$-radiation) in the $^{222}$Rn sub-chain.

3.5.2 Xenon Contaminants

Non-noble contaminants can be purified out of xenon quickly and efficiently, in bulk, through the use of a heated-zirconium getter. Removal of naturally present noble elements from xenon in bulk, most importantly $^{85}$Kr, is considerably more difficult, requiring the exploitation of minor differences in the physical chemistry of the different noble atoms. The krypton removal process for the xenon used in LZ was performed at SLAC using charcoal chromatography, a technique which separates krypton from xenon using the difference in their mobility through porous media. The krypton removal effort at SLAC reduced the $^{nat}$Kr concentration of LZ’s xenon to less than 0.15 ppt g/g, and the $^{nat}$Ar concentration to less than 1 ppb g/g. The remaining trace amounts of $^{222}$Rn, $^{220}$Rn, $^{nat}$Ar, and $^{nat}$Kr contribute to LZ’s backgrounds at the levels estimated in Fig. 3.7.

A different technique for purifying xenon in bulk, which has been demonstrated by the Xenon collaboration is cryogenic distillation [31]. Cryogenic distillation takes advantage of the difference in vapor pressures to separate krypton from xenon and has the added advantage of being integrable into LXe detector systems. Cryogenic distillation allows for active purification of the xenon while operating, unlike charcoal chromatography which must be performed in advance. Both charcoal chromatography and cryogenic distillation have been demonstrated to reduce the concentration of $^{85}$Kr to a low enough level such that Kr is a sub-dominant contributor to the background.
3.5.3 Surface Contaminants

During the manufacture and assembly of the many components which compose LZ, radioactivity will have accumulated on material surfaces through electrostatic attraction of generic dust, and through the plate-out of airborne $^{222}$Rn-daughters. The same radioisotopes described in section 3.5.1 are present in dust, and contribute to the same $\gamma$-induced neutron emission processes described there. Plate-out can lead to NR backgrounds through neutron production in $(\alpha, n)$ reactions, and through $^{210}$Pb sub-chain ions originating at the TPC edges being mis-reconstructed as NR events within the fiducial volume if position reconstruction near the edges is sufficiently bad. The latter is the main motivation for a radial fiducial volume cut in the WIMP-search analysis, which ignores the outer-most few centimeters of xenon in the TPC where backgrounds are the highest. To mitigate surface contamination, the assembly of the LZ TPC was completed in a reduced-radon cleanroom in the Surface Assembly Lab at SURF.

3.5.4 Laboratory and Cosmogenic Backgrounds

The largest source of background in LZ that originates from outside of the water tank is the flux of $\gamma$-rays produced in the rock that makes up the cavern walls. The $\gamma$-ray flux in the Davis cavern has been carefully measured in [32]. Another background source, cosmic muons, interact with the rock-overburden to produce electromagnetic and hadronic showers. Events from these particle showers typically scatter multiple times in the TPC, xenon skin, and OD, and are therefore easily vetoed.

Cosmogenic activation of the xenon in LZ, from exposure to cosmic rays at the earth’s surface while above ground, results in the production of several short-lived xenon radioisotopes of which $^{127}$Xe ($T_{1/2} = 36.4$ d) is the most problematic. These activation products are also produced from neutron activation during the Deuterium-Deuterium fusion (DD) neutron calibration, and to a lesser extent, during
Figure 3.8. **Left:** The simulated number of total decays in the TPC, skin, and OD resulting from the activation products produced in a 2 day DD neutron calibration. **Right:** The simulated number of total decays in the TPC, skin, and OD resulting from the activation products produced in a 9 hour AmLi neutron calibration. Both plots are taken from [33] the Americium-Lithium (AmLi) neutron calibration of LZ. The simulated number of events produced by the various activation isotopes resulting from these calibrations in LZ is shown in Fig. 3.8. The $^{127}$Xe decay process is described in detail in section 4.1.5, but is also described briefly here.

$^{127}$Xe undergoes electron capture, generating electron cascades as higher orbital electrons descend to lower orbitals to fill the vacancy created in the process. The electron capture produces 33.2 keV, 5.2 keV, 1.1 keV, and 186 eV of Auger electrons and/or X-ray radiation for K-shell, L-shell, M-shell, and N-shell captures, respectively [34]. These Auger electrons/X-rays are accompanied by one or more $\gamma$-rays with total energy equal to 619 keV, 375 keV, or 203 keV, produced in the subsequent decay of the excited-state $^{127}$I nucleus, allowing most $^{127}$Xe decays to be rejected by coincidence tagging. In $^{127}$Xe decays where the associated $\gamma$-radiation escapes the TPC and is not tagged by the xenon skin or OD, the Auger electrons/X-ray radiation left behind can produce low-energy ER background events in LZ. The relatively short half-life of $^{127}$Xe, and the $\mathcal{O}(1 \text{ cm})$ mean free path of these $\gamma$-rays in LXe (which confine these
escaped-gamma events to the edges of the TPC) prevent $^{127}$Xe from contributing significantly to the WIMP-search backgrounds ultimately.

The largest contribution to backgrounds from cosmogenic activation in detector materials comes from $^{46}$Sc ($T_{1/2} = 83.8$ d) produced in the 2.5 tonnes of titanium used in the construction of LZ. The beta-decay of $^{46}$Sc is followed by the emission of two $\gamma$-rays of energies 1,120 keV and 889 keV, making it easy to veto with coincidence tagging and rendering this background negligible in LZ [35].

### 3.5.5 Rare Events and Coincident Interactions

Solar $pp$, $^7$Be, and CNO neutrinos can produce single scatter ER events in LZ, while solar $^8$B and $^3$He–proton fusion ($hep$) neutrinos, as well as diffuse supernova neutrinos (DSM) and atmospheric (Atm) neutrinos can produce NR events. Because of the neutrino’s extremely small scattering cross-section, neutrino interactions in LZ will have no corresponding veto signal (will scatter only once), making a detailed understanding of the interaction rates critical for interpreting results in the WIMP-search region of interest. Event rates from neutrino interactions in LZ, shown in Fig. 3.7, are calculated by combining the flux and spectra from [36] with up to date oscillation parameters from [37].

Another source of single scatter ER events in LZ is from the two-neutrino double beta decay ($2\nu\beta\beta$) of $^{136}$Xe (8.9% isotopic abundance), which has $Q = 2458$ keV. The rate of this decay has been precisely measured in EXO-200 [38] and KamLAND-Zen [39].

Finally, rare event topologies and coincidences also contribute to the WIMP-search background in LZ, though are subdominant to the other ER and NR backgrounds considered in this section. Three rare non-standard topologies in particular have been identified as probable enough in LZ to require consideration. First is multiple scattering of $\gamma$-rays, where one scattering vertex is located in LZ’s reverse field region
(below the cathode grid) and the second is located above the cathode, in the drift field. In such a multiple scatter, the S1 from the vertex in the reverse field region is observed normally, but the charge is not collected, lowering the S2/S1 ratio measured and moving the event towards the NR band in a plot of the logarithm of S2/S1 versus S1. A fiducial cut in the TPC reduces the contribution of these rare events to well below one event in a 1000d run [20].

The second rare and non-standard background topology that is considered in LZ is the production of fake S1-only signals from accidental coincidences between multiple PMT dark counts, which may combine with a coincident S2-only event to create a plausible low energy S1-S2 pair in the NR band. For a 3-fold PMT coincidence requirement and a simulated 1 mHz S2-only rate, less than 0.2 of these events are expected in a 1000d run [20].

The final rare and non-standard background topology that is considered is from S1-like Cherenkov light generated in the quartz windows of the PMTs. Such S1-like signals are produced from Compton electrons or energetic betas originating in $^{40}$K decays in the PMT materials. These S1-like signals can also combine with S2-only events to produce low energy S1-S2 pairs with S2/S1 ratios that cause them to appear in the NR band. The majority of these coincidence events can be identified from their PMT hit pattern and PMT hit timing, with all of the light being detected in an extremely short time window and largely in only one PMT. For a simulated S2-only rate of 1 mHz, 0.2 background events from such events are expected in a 1000d run [20].
CHAPTER 4
INTERNAL CALIBRATION OF THE LZ TPC

As discussed in previous chapters, LXe’s high density is one of several features that makes it an excellent target for a WIMP search experiment. The mean interaction length in LXe for MeV neutrons [40] and gamma rays [41] (both $\mathcal{O}(10 \text{ cm})$) is much shorter than the typical length scale of contemporary LXe TPCs such as LZ’s, which boasts a ∼1.46 meter diameter and height. In a detector of the scale of the LZ TPC, an outer layer of LXe (defined in data analysis) shields an extremely low background fiducial region from events originating primarily in detector materials. The mean interaction length for a range of neutron and photon energies in LXe is shown in Fig. 4.1.

In LZ, this self-shielding strategy is part of a much larger effort to reduce backgrounds in the TPC to unprecedented levels, but it also makes low-energy electron recoil calibration of the fiducial region practically impossible using external calibration sources. Instead, gaseous radioisotopes must be injected into the LXe itself, where they will mix to provide homogenous distributions of electron-recoil events. Improving the precision of this strategy, which has been demonstrated in the Large Underground Xenon (LUX) experiment, is one of the main focuses of the work presented in this thesis.

4.1 Internal Calibration Source Motivations

The radioisotopes that are internally injected into the LZ LXe provide a range of calibrations which are summarized in the table in Fig. 4.2. The details and utility of
Figure 4.1. Mean neutron (left) and photon (right) interaction length in liquid xenon for a range of energies.

<table>
<thead>
<tr>
<th>Decay Mode</th>
<th>Half Life</th>
<th>Energy</th>
<th>Deliverable</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{83m}$Kr</td>
<td>IC</td>
<td>1.83 h</td>
<td>32.1 keV and 9.4 keV TPC Position Corrections, TPC Flow Mapping</td>
</tr>
<tr>
<td>$^{137m}$Xe</td>
<td>IC</td>
<td>11.9 d</td>
<td>163.9 keV TPC Position Corrections, LXe Skin</td>
</tr>
<tr>
<td>$^{222}$Rn</td>
<td>$\alpha / \beta / \gamma$</td>
<td>Various</td>
<td>Various ER band, LXe Skin, TPC Flow Mapping</td>
</tr>
<tr>
<td>$^7$H</td>
<td>$\beta$</td>
<td>12.3 y</td>
<td>$Q = 18.6$ keV High Stats ER band</td>
</tr>
<tr>
<td>$^{14}$C</td>
<td>$\beta$</td>
<td>5730 y</td>
<td>$Q = 156.4$ keV High Stats ER band</td>
</tr>
</tbody>
</table>

Figure 4.2. Summary of the internally injected calibration sources in LZ.
each of the internally injected sources (and the naturally present $^{127}$Xe) are described in this section.

4.1.1 $^{83m}$Kr

$^{83m}$Kr is a 41.5 keV monoenergetic ER source outside of the WIMP-search region of interest (ROI) in LZ, with a conveniently short half life of 1.83 hours. Its keV-scale decay energy is comparable to the few-keV energy thresholds of liquid noble TPCs generally. Like xenon, $^{83m}$Kr is noble, making it easy to purify with a heated-zirconium getter, and allowing it to mix evenly into the LXe bulk (if the mixing timescale of the detector is short compared to the $^{83m}$Kr half-life). For all of these reasons, $^{83m}$Kr is an excellent choice for a calibration source in LZ. Additionally, the LXe (and liquid argon) response of $^{83m}$Kr has been studied extensively, as in [42] (and [43]). The decay scheme of $^{83m}$Kr is shown in Fig. 4.3.

$^{83m}$Kr decays in two main steps, through internal conversion followed by emission of Auger electrons and/or X-rays, which produce a 32.1 keV (1.83 h half life) and a 9.4 keV (154 ns half life) emission. In LZ, these peaks are sometimes separable by the pulse finder (2 S1s, 1 S2), but otherwise show up as a single (1 S1, 1 S2) larger energy deposit. In either case, the monoenergetic sum of the two decays allows for the production of high-resolution 3-D maps of S1 and S2 detector response. By producing maps of position-dependent detector efficiencies, corrections to S1 and S2 areas as a function of position can be calibrated. Position-dependent effects include light collection efficiency in the case of S1, and electron drift, electron extraction, and light production efficiency in the case of S2, which may also be time dependent as the LXe purity changes over time. Regular injections of $^{83m}$Kr into the LXe of LZ to produce these critical detector response maps are therefore necessary, contributing significantly to accurate event-energy reconstruction over the course of LZ’s data taking.
Figure 4.3. $^{83}\text{mKr}$ decay scheme from [44], showing its possible emissions. $^{83}\text{mKr}$ decays in two steps, with a 32.1 keV emission (1.83 h half life) followed promptly by a 9.4 keV emission (154 ns half life), and results in a stable $^{83}\text{Kr}$ atom. $^{83}\text{mKr}$ is detected in LZ as either a 2-S1, 1-S2 or a 1-S1, 1-S2 event, depending on the time separation between the two emissions in the decay.
The 1.83 hour half life of $^{83m}$Kr, while convenient because it decays away quickly after it is introduced, results in the injected activity never becoming fully homogenous before decaying away for discrete (all-at-once) injections in large LXe detectors like LZ. The fluid dynamics of the LXe bulk, driven by thermal gradients, are difficult to predict in general. The timescale for the $^{83m}$Kr to become uniform in any given detector must therefore be measured directly. A uniform distribution is not required to perform the position-dependent calibrations that $^{83m}$Kr will be used for in LZ, but if there are regions of the LXe that have a very low $^{83m}$Kr activity following an injection, an additional source which can produce the same calibrations may be useful or necessary. In LZ, $^{131m}$Xe can be used for this purpose.

4.1.2 $^{131m}$Xe

As a LXe TPC calibration isotope, $^{131m}$Xe serves a similar role to $^{83m}$Kr in that it is a monoenergetic ER source (outside of the WIMP-search ROI in LZ) in addition to also being noble, making it easy to purify with a heated-zirconium getter, and allowing it to mix evenly into the LXe bulk. With an 11.8 day half life, injected $^{131m}$Xe has significantly more time to become uniformly distributed in the LXe than $^{83m}$Kr. The decay of $^{131m}$Xe results in a stable $^{131}$Xe atom and the emission of a 164 keV gamma via internal conversion. Injected $^{131m}$Xe can therefore be used to produce the same high resolution 3-D maps of detector response that are produced with injected $^{83m}$Kr, albeit at higher energy, with the advantage of guaranteed uniformity in the LXe. $^{131m}$Xe is also one of the primary calibration sources for the xenon skin in LZ, since the 164 keV emission is comparable to the $\sim 100$ keV$_{ee}$ threshold of the LXe skin.

4.1.3 $^{220}$Rn

$^{220}$Rn can provide a variety of calibrations in LXe TPCs that supplement those which can be performed with the naturally occurring $^{222}$Rn chain background. $^{220}$Rn produces charged and neutral daughters that undergo both alpha and beta decays,
analogous to those in the $^{222}$Rn chain, but with the advantage of having no long lived progeny. Being noble, $^{220}$Rn is easy to purify by passing it through a heated-zirconium getter, and mixes evenly into the LXe bulk. The $^{220}$Rn-chain decay time is dominated by the 10.6 hour $^{212}$Pb half life, which follows from the very short 55 second $^{220}$Rn and 145 millisecond $^{216}$Po half lives. The $^{220}$Rn decay chain is shown in Fig. 4.4 with the decay modes and half lives indicated.

The very short half lives of $^{216}$Po (145 ms), $^{212}$Po (299 ns), and $^{208}$Tl (3.1 min) allow for the possible identification of ‘coincident’ pairs of decays in LZ from their spatial and temporal correlation, in this case $^{220}$Rn+$^{216}$Po, $^{212}$Bi+$^{208}$Tl, and $^{212}$Bi+$^{212}$Po. The ability to identify pairs of decays from the same atom enables the possibility of LXe flow mapping, where the difference in the position of the atom at the time of the two decays, along with the time between the decays, gives a measurement of the velocity of the LXe flow that carried the atom. The ability to identify pairs of decays
also allows for a measurement of the fraction of alpha and beta decay daughters which are produced with net-charge, if the LXe convective flow velocity is slow enough (less than $\sim 1$ mm/s, the electric field induced drift velocity of a heavy ion like $^{212}\text{Bi}$ in LZ). The charged-fraction of alpha and beta decay daughters has been measured previously in LXe in the EXO-200 detector [45], and in LAr in the Darkside-50 detector [46]. Finally, the identification of coincident pairs enables the study of several position-dependent effects including: removal processes of non-noble atoms from the LXe bulk, mapping of where Rn-daughters naturally become distributed in the detector, and S2 response of events on the TPC walls. These studies are all of considerable importance because they contribute to characterizing the $^{222}\text{Rn}$ chain background by exploiting the $^{220}\text{Rn}$ chain’s analogous behavior. Alpha decays from the $^{220}\text{Rn}$ chain also provide a useful higher energy calibration of the LXe skin.

The injection of $^{220}\text{Rn}$ into LXe detectors differs from injections of the other radioisotopes presented here because of its significantly shorter half life (55 s). For detectors with sufficiently complex or large pathways from the calibration source to the TPC, some or all of the $^{220}\text{Rn}$ can decay in transit, resulting in the delivery of nearly pure $^{212}\text{Pb}$ to the TPC. While the lack of $^{220}\text{Rn}^{+}\text{216Po}$ coincident pairs in such detectors limits some of the usefulness of the $^{220}\text{Rn}$ source, the calibrations described above are potentially still achievable using a combination of $^{212}\text{Pb}$ daughters and the background $^{222}\text{Rn}$ chain decays. Additionally, low-energy ground-state decays from $^{212}\text{Pb}$ can be used as a lower risk alternative to long-lived $^3\text{H}$ for calibrating the low energy ER band near the TPC’s energy threshold (the WIMP-search energy ROI). The ground-state decay of $^{212}\text{Pb}$ (where no $\gamma$-radiation is emitted) occurs for 11.9% of $^{212}\text{Pb}$ decays [47]. The theoretical ground-state decay spectrum from $^{212}\text{Pb}$ [48] and $^3\text{H}$ are shown in Fig. 4.5 for comparison.

In the xenon circulation system of LZ, the transit time for the calibration radioisotopes from generator to TPC is calculated to be several minutes, in which case the
Figure 4.5. The theoretical $\beta$-decay energy spectra from $^3$H and ground-state $^{212}$Pb decays [48]. The $^{212}$Pb $\beta$ spectrum is much less concentrated at low energies than the $^3$H spectrum, but has the benefit of being short-lived, allowing it to decay away naturally rather than requiring removal by purification once injected.
majority of the $^{220}$Rn atoms are expected to decay away before reaching the TPC. Despite this, results from the first injection with the $^{220}$Rn source in LZ saw $^{220}$Rn atoms surviving the transit to the TPC, evident from their characteristic prompt alpha decay. The $^{220}$Rn injection results in LZ are detailed in section 6.9.

4.1.4 $^3$H & $^{14}$C

$^3$H is a beta emitter with $Q = 18.6$ keV, making it an ideal candidate for a low-energy ER calibration in LXe TPCs. The much lower $Q$-value makes $^3$H a more natural choice than $^{212}$Pb for an ER calibration near threshold, achieving the same number of useful calibration events with a much lower total event rate. Additionally, a calibration with $^3$H provides an energy specific calibration from its spectral shape. $^3$H will be injected into LZ in the form of tritiated methane (CH$_3$T) after the completion of LZ’s first science run. Injected $^3$H must be purified out of the detector rather than being allowed to decay away because of its long 12.3 year half life.

$^{14}$C is a beta emitter like $^3$H, with $Q = 156.5$ keV, effectively extending the range of an ER band calibration from $^3$H to higher energies in addition to providing an energy specific calibration from its spectral shape. Like $^3$H, $^{14}$C will be injected into LZ as a methane molecule, $^{14}$CH$_4$, and will be removed at the same rate as the methane-based tritium, CH$_3$T, by purification in the circulation system.

4.1.5 $^{127}$Xe

As described in section 3.5.4, $^{127}$Xe is not internally injected but is naturally present in LZ from cosmogenic activation, and is also produced in situ by neutron activation during DD and AmLi neutron calibrations. $^{127}$Xe decays by electron capture, and generates Auger electrons and/or X-rays as higher orbital electrons descend to lower orbitals to fill the vacancy created in the decay. The electron capture comes from the K shell in 83% of decays, the L shell in 13% of decays, the M shell in 3% of decays, and the N shell in less than 1% of decays, producing 33.2 keV, 5.2 keV, 1.1
keV, and 186 eV emissions of Auger electrons and/or X-ray radiation respectively [34]. These emissions are accompanied by 619 keV, 375 keV, or 203 keV emissions of γ-ray radiation, produced in the subsequent decay of the excited-state $^{127}$I nucleus. As a calibration source, $^{127}$Xe provides a range of low-energy mono-energetic ER peaks when the associated γ-rays from the decay deposit their energy outside of the TPC, leaving only the low energy Auger electrons/X-rays to deposit energy in the TPC. These low-energy Auger electron/X-ray deposits provide useful mono-energetic calibration peaks spanning the WIMP-search ROI and reaching all the way down to 186 keV, providing the lowest energy calibration peaks in LZ. However, because of the $\mathcal{O}(1 \text{ cm})$ mean free path of the γ-rays that follow the $^{127}$Xe decay, mono-energetic ‘escaped-γ-ray’ $^{127}$Xe events occur exclusively near the walls of the TPC, limiting their usefulness. The detailed decay scheme of $^{127}$Xe and the measured probabilities of the various electron shell captures in LUX are shown in Fig. 4.6.

4.2 Internal Calibration Analyses of Simulated LZ and Real LUX Data

The internal calibrations made possible by the variety of sources described in the previous section are central to gaining a complete understanding of LZ data. These calibrations produce large samples of well understood interactions in the detector across a range of energies and interaction types, allowing the detector response to be fully characterized. In this chapter I present several example analyses that were performed with simulated LZ data, and with real data from the LUX experiment, in preparation for the beginning of LZ data taking.

4.2.1 Simulating LZ Data

Prior to the start of LZ data taking, simulated data played a critical role in the development and refinement of the analyses that would eventually be used to
Figure 4.6. **Top:** Table of electron capture probabilities from the various orbitals in the $^{127}\text{Xe}$ electron cloud, from [34], with the measured probabilities in LUX shown. **Bottom:** Decay scheme of $^{127}\text{Xe}$ with units of keV, from [34]. The percentages above the transition arrows indicate the $\gamma$-ray intensity.
study the real data collected by LZ. The code for simulating particles and their interactions in LZ, BACCARAT (Basically, A Component-Centric Analog Response to AnyThing) [49], builds upon the simulation code which was originally developed for the LUX experiment. BACCARAT tracks particles using Geant4 [50] and identifies their interaction points in the simulated LZ detector. The Geant4 toolkit contains pre-defined physics lists which provide options for modeling various processes, but also contains the functionality to allow user-defined processes to be integrated into the physics of the simulation. BACCARAT uses this functionality to simulate LZ data, deploying several custom modules which improve the accuracy of the xenon microphysics simulated in the particle interactions [49]. Of particular importance, the physics of the Noble Element Simulation Technique (NEST) [51], the most comprehensive simulation of the excitation, ionization, and corresponding scintillation and electroluminescence processes in liquid noble elements, are integrated into BACCARAT this way.

Following the simulation of the xenon interactions, simulations of light and charge propagation with BACCARAT determine the pattern of photons incident on the PMT faces in LZ, and this information is fed into a second package, the Detector Electronics Response (DER). The DER is a software package which simulates the PMT signal generation and subsequent signal processing by the analogue front-end electronics and digitizers in LZ. Raw photon hits are read from BACCARAT to create simulated digitized waveforms. These waveforms are passed through the LZ Analysis Package (LZap), which performs pulse and event reconstruction, to provide the practice data for analyses presented in this chapter [49]. The data analyzed in this chapter used a simulated LZ electric field map with a mean value of 305 V/cm, and the predicted/projected parameters listed in Table. 3.2.
4.2.2 Simplistic S1 Area Correction in LZ

For events of a given energy and type, the pulse area of the measured S1 and S2 signals will vary systematically as a function of position in the LZ TPC because of the position dependence of light and charge collection efficiency. Reasons for this position dependence include: non-uniformities in the TPC geometry, PMT saturation for events near the bottom array, signal loss due to impurities in the LXe, and non-uniformities in the electric field. One of the most general goals of the LZ internal calibrations campaign is to correct for these systematic effects. This is done in LZ by mapping the position dependence of S1- and S2-pulse area size using the homogenous distributions of mono-energetic decays that internal source injections provide. In this section I present a correction to S1-pulse area as a function of position, demonstrated using simulated LZ data containing $^{83m}\text{Kr}$ and $^{131m}\text{Xe}$ injections.

First, all events with one S1 and one S2 (single scatter events), or with two S1s and one S2 ($^{83m}\text{Kr}$-like events), were selected. For two-S1 and one-S2 events, a single S1-pulse area was calculated by adding the two S1-pulse areas together; This made the $^{83m}\text{Kr}$ events in which the two S1s were not merged effectively identical to the single scatter $^{83m}\text{Kr}$ events in the data, allowing both topologies to be considered simultaneously. Within this data, the $^{83m}\text{Kr}$ population ($\sim 883,000$ simulated $^{83m}\text{Kr}$ decays, uniformly distributed in the TPC) appears as a bright peak in S2- versus S1-pulse area. The $^{83m}\text{Kr}$ population was selected with a cut in this space (upper left of Fig 4.7). The TPC volume was then divided into equal sized bins in the negative of drift time versus radius squared ($R^2$) (upper right of Fig 4.7), where (the negative of) drift time is a proxy for Z position of the event in the TPC, and $R^2$ describes the distance of the event from the central axis of the TPC. In each of these position bins (voxels), the S1-pulse areas from events in the selected $^{83m}\text{Kr}$ population were used to fill a histogram which was subsequently fit with a gaussian. The mean of the
gaussian fits provide a measurement of the mean $^{83m}$Kr S1-pulse area in each position bin (voxel).

To avoid non-gaussian features and backgrounds in the selected populations, the gaussian fitting was performed iteratively on the histograms of S1-pulse area in each position bin (voxel). First a gaussian was fit to the entire range of the histogram, approximating the distribution of pulse areas only very roughly. A second gaussian is then fit to the data in the histogram within two standard deviations of the mean from the first gaussian fit. A third gaussian fit is performed on the data within two standard deviations of the mean from the second gaussian fit. This iterative fitting over a range determined by the previous fit is performed until six total gaussians have been fit. The result of this iterative fitting procedure is that the fit means converge to the location of the peak in the S1-area histogram. Though the extracted parameter is the mean from the final gaussian fit, in practice, this iterative gaussian fitting locates the peak of the fitted distribution. Example fits to the S1-pulse area histograms from four different TPC position bins (voxels) are shown in Fig 4.7 (bottom left).

The $^{83m}$Kr S1-pulse area means from the iterative gaussian fits in each position bin (voxel) were used to fill a new 2-D histogram of the negative of drift time versus $R^2$, and the histogram was normalized by dividing each bin value by the $^{83m}$Kr S1 mean from the bin which corresponds to the TPCs geometric center. This map of mean $^{83m}$Kr S1-pulse area relative to the TPC center constitutes the S1 area 'response map', and provides the value by which the S1-pulse area of any event in the TPC should be divided to correct for position dependence. The response map is shown in the bottom right of Fig 4.7.

In practice, the S1 area correction factor for a given event in the TPC is found by performing bilinear interpolation on the response map at the position (in -drift time vs $R^2$) of the event in consideration. Dividing the S1 area by the resulting correction factor gives the corrected S1 area, $S_{1c}$. The applied S1-area correction is shown in
Figure 4.7. Histograms produced from simulated LZ TPC data. **Upper Left:** A 2D histogram of the logarithm of S2-pulse area vs. the logarithm of S1-pulse area. The $^{83\text{m}}$Kr population is visible as a clear peak above the background events, and is selected in this analysis with cuts on S1- and S2-pulse area shown by the red box. **Upper Right:** A 2D histogram of -drift time (a proxy for Z position in the TPC) vs. radius of the event from the central TPC axis, squared. Red lines are overlaid indicating the division of the TPC geometry into the position bins (voxels) where separate measurements of the mean S1 area of the selected $^{83\text{m}}$Kr events are made. **Lower Left:** Example gaussian fits to the $^{83\text{m}}$Kr S1 area histograms from four of the TPC position bins (voxels) in this analysis. The position-bin centers are indicated with text in each histogram. **Lower Right:** The S1 area ‘response map’, which contains the mean $^{83\text{m}}$Kr S1 area from each of the TPC position bins (voxels), normalized to the TPC’s geometric center. The S1 area response map indicates that the S1 light collection efficiency is highest near the bottom of the TPC and near the TPC’s radial center.
Fig. 4.8 for peaks from $^{131m}$Xe and $^{127}$Xe present in the same data set which contained the selected $^{83m}$Kr events. The $^{131m}$Xe and $^{127}$Xe peaks can be seen to become more resolved as a result of applying the S1-area correction.

This analysis demonstrates the ability to perform a simple S1-area correction on simulated LZ data using a procedure which can be directly applied to real data from LZ. In practice, this analysis served as a prototype S1-area correction that was developed further before being applied to LZ data. The improved S1-area correction that is now applied to real data from LZ uses a fully 3-D position binning in x, y, and -drift time, and is detailed in section 6.7.

4.2.3 Position-dependent Doke Plots in LZ

If the detector gains, $g_1$ and $g_2$ (the average number of detected photons [phd] per interaction-site photon and electron, respectively), are known at the position where an event occurs in the TPC, the energy of the event can be reconstructed. The reconstructed energy is calculated from the S1- and S2-pulse areas using the relationship $E = W \left( \frac{S_1}{g_1} + \frac{S_2}{g_2} \right)$, where $W$ is the work function for xenon and has been measured to be $13.7 \pm 0.2$ eV/quanta [25].

Historically, $g_1$ and $g_2$ are measured after the S1- and S2-pulse areas are corrected to account for position-dependent effects, resulting in gains that describe the full position-corrected TPC (described in section 2.2). One downside to defining and measuring $g_1$ and $g_2$ in this way is that the measured values are de-coupled from the fundamental physics quantity that they describe: the number of photons detected per interaction-site photon, and electron, produced. This is because the measured $g_1$ and $g_2$ are pre-scaled by the arbitrary normalization that is chosen for the S1- and S2-pulse area corrections. (In the standard procedure for correcting S1 or S2 pulse area, a position in the TPC is chosen and the pulse areas at all other positions in the TPC are made to be equal to those at the chosen position for events of the
Figure 4.8. Histograms produced from simulated LZ TPC data. **Top:** 1D histograms of S1-pulse area (left) and corrected S1-pulse area (right) for a range of S1-pulse areas that contains the 164 keV $^{131m}$Xe and 236 keV $^{127}$Xe peaks. **Bottom:** 2D histograms of -drift time vs. S1-pulse area (left) and -drift time vs. corrected S1-pulse area (right), demonstrating how the S1-area correction removes variation in S1-pulse area as a function of drift time (z position) from the monoenergetic 164 keV $^{131m}$Xe and 236 keV $^{127}$Xe peaks.
same energy. In LZ, these positions are the geometric TPC center for S1, and the radial center at the top of the TPC [the liquid surface] for S2). Worse still, pulse area corrections defined this way do not account for the energy-dependent effect of electric-field variation on electron recombination following an interaction [51], important if there are electric-field gradients in the TPC. Specifically, recombination in low-energy ER and NR events is much less field dependent than for events with higher energies like $^{83m}$Kr or $^{131m}$Xe. Therefore, S1- or S2-pulse area corrections produced from $^{83m}$Kr or $^{131m}$Xe (which do not account for the energy dependence of recombination) inherently introduce error into the reconstructed energy calculated from them for low-energy events when an electric field gradient is present in the TPC.

Measuring $g_1$ and $g_2$ as a function of position from uncorrected S1- and S2-pulse areas results in a direct measurement of the detector response at each position, and accounts for the field and energy dependent recombination as a function of position in the TPC automatically by requiring populations of multiple energies. In this way, the geometric efficiency and electric-field effects are decoupled from each other in the overall light-collection and charge-collection efficiencies, unlike for the basic S1- or S2-pulse area corrections. Additionally, no normalization to an arbitrary location in the detector is necessary for this procedure. Measuring position-dependent $g_1$ and $g_2$ provides an alternate way to reconstruct event energies and make corrections to the measured S1 and S2 areas in LZ, while preserving the details of the physics at the interaction site. With position-dependent $g_1$ and $g_2$ measured, the quantities $S_1/g_1$ and $S_2/g_2$ for a given event are equal to the actual number of S1-photons and S2-electrons produced at the interaction site, respectively, and provide a direct probe of the local electric field.

Using the same simulated data as in section 4.2.2 which contains $^{83m}$Kr and $^{131m}$Xe injections with $\sim883k$ and $\sim28k$ events respectively, events with one S1 and one S2 (single scatter events), and with two S1s and one S2 ($^{83m}$Kr-like events) were
Figure 4.9. Histograms produced from simulated LZ TPC data. **Left:** The logarithm of S2-pulse area vs. the logarithm of S1-pulse area for single scatter and two-S1, one-S2 events. For two-S1, one-S2 events, the S1-pulse areas have been added together to create a single S1-pulse area. The $^{83m}$Kr, $^{131m}$Xe, 236 keV $^{127}$Xe, and 408 keV $^{127}$Xe peaks are selected with cuts in S2- vs. S1-pulse area, shown by overlaid red boxes. **Right:** The position of the events in the TPC which pass the peak selection cuts is shown in the negative of drift time vs. R$^2$. The division of the TPC into position bins (voxels) in which g1 and g2 are independently calculated is shown by the overlaid red lines.

selected. For events with two S1s and one S2, a single S1-pulse area is calculated by adding the two S1 areas together; This makes the $^{83m}$Kr events in which the two S1s are not merged effectively identical to the single scatter $^{83m}$Kr events in the data, allowing both topologies to be considered simultaneously. The $^{83m}$Kr and $^{131m}$Xe populations, which appear as bright peaks in a histogram of S2- versus S1-pulse area, were selected with a cut in that parameter space, shown in Fig. 4.9 (left). Additionally, 236 keV and 408 keV $^{127}$Xe peaks from simulated cosmogenic activation were present in the data, and were also selected with a cut in S2- versus S1-pulse area (Fig. 4.9, left). The TPC was divided into spatial bins (voxels) in the negative of drift time versus R$^2$, where the radius, R, is the distance from the TPC’s central axis (Fig. 4.9, right). In each spatial bin, and for the selected $^{83m}$Kr, $^{131m}$Xe, and $^{127}$Xe peaks independently, 2-D histograms of S1/E versus S2/E were filled, where E is the
Figure 4.10. The array of Doke plots produced from all of the position bins (voxels) in the simulated LZ TPC, arranged according to the bin’s position in the TPC in (negative) drift time vs. R^2.

energy of the mono-energetic decay. The histograms were fitted with gaussians in both dimensions independently, using the iterative fitting procedure described in section 4.2.2, and the 2-D mean of each population in S1/E-vs-S2/E-space was measured from the fits in each position bin (voxel). A Doke plot was created in every position bin (voxel) with a data point from the gaussian mean of each of the four mono-energetic populations. The full array of Doke plots produced this way is shown in Fig. 4.10, and an example of one of these Doke plots, from a position bin (voxel) near the simulated TPC’s center, is shown in Fig. 4.11. The Doke plots were fitted with a straight
Figure 4.11. An example Doke plot produced from simulated LZ TPC data, from a position bin (voxel) near the TPC’s geometric center. The data points are positioned at the mean S1/E vs. S2/E for the four mono-energetic peaks, and are fit with a straight line. The best fit line is shown in solid red, with dashed red lines indicating the $1\sigma$ uncertainty of the fit. The x and y intercepts multiplied by the xenon work function, $W$, give $g_1$ and $g_2$ in units of phd per photon, and per electron, propagated from the interaction site, respectively.
Figure 4.12. Maps of $g_1$ and $g_2$ as a function of position, produced from simulated LZ TPC data, in units of phd/photon ($g_1$) and phd/electron ($g_2$). The maps indicate that along the drift time ($z$) axis, light collection efficiency is highest in the bottom of the TPC while charge collection efficiency is highest near the top of the TPC, and radially, both are highest near the TPC’s center.

Line whose $x$ and $y$ intercepts provide a measurement of $g_1$ and $g_2$ in its respective position bin (voxel) when multiplied by the xenon work function, $W$ ($0.0137 \pm 0.0002$ keV/quanta [25]). The resulting maps of $g_1$ and $g_2$ as a function of position in the simulated LZ TPC are shown in Fig. 4.12.

For a given event, the $g_1$ and $g_2$ values at the position of the interaction site can be estimated by bilinear interpolation on the $g_1$ and $g_2$ maps from Fig. 4.12. With the ability to determine the unique $g_1$ and $g_2$ at any position in the TPC, the energy of a given event is reconstructed using the relationship $E = W \left( \frac{S_1}{g_1} + \frac{S_2}{g_2} \right)$ introduced in section 2.2, though with the uncorrected $S_1$- and $S_2$-pulse areas, since position-dependent effects are captured in the position dependence of $g_1$ and $g_2$. The reconstructed energy for all events which passed the initial event topology cut (single scatter and two-S1, one S2 events) in the simulated data set is shown in Fig. 4.13. The reconstructed energy spectrum from an early version of this analysis which only used peaks from $^{83m}$Kr and $^{131m}$Xe is shown in Fig. 4.14, compared to the spectrum from
Figure 4.13. A reconstructed energy spectrum from 1-S1, 1-S2 and 2-S1, 1-S2 events, produced with simulated LZ TPC data. The four mono-energetic peaks used to calculate $g_1$ and $g_2$ (red labels), as well as several other known peaks (blue labels) appear at their expected energies.
Figure 4.14. Reconstructed energy spectra from a position-dependent g1 and g2 measurement and from a traditional global g1 and g2 measurement in simulated LZ TPC data. The position-dependent g1 and g2 are seen to more accurately reconstruct the energies of the events in the data set.

an analysis of the same data with the traditional Doke analysis using corrected pulse areas. In the direct comparison, the reconstructed energy spectrum from the position-dependent Doke analysis can be seen to reconstruct event energies more accurately, with all of the identified peaks in the data appearing closer to their expected true energies than in the spectrum from the traditional Doke analysis.

S1- and S2-pulse area corrections with position-dependent g1 and g2 can be very easily defined. When S1- or S2-pulse areas are divided by the value of g1 and g2, respectively, corresponding to the position of the event in the TPC, the real numbers of (S1) photons and (S2) electrons produced at the interaction site are the result. In principle, S1/g1 and S2/g2 can be used as replacements for the traditional corrected pulse areas as is. Like with the traditional pulse area corrections, using position-dependent
g1 and g2 to correct S1- and S2-pulse areas, or to reconstruct event energies, only
accounts for time-independent systematics. One major time-dependent variable is
the LXe purity in the TPC, which affects S2 photon production since impurities can
capture free electrons on their way to the LXe surface. Measuring the time-dependent
g2 as a function of position should be possible with real LZ TPC data by combin-
ing an initial position-dependent-g2 measurement and independent measurements of
electron lifetime (xenon purity) over time.

4.2.4 Tagging $^{127}$Xe Gammas in the Xenon Skin

In $^{127}$Xe events which occur near the walls of the TPC, the associated $\gamma$-ray(s) may
escape the TPC and interact in the LXe skin. The analysis presented in this section
demonstrates the ability to identify such events, which provide mono-energetic peaks
in the TPC at low energies and mono-energetic $\gamma$-ray deposits in the skin, both of
which can be useful calibration sources in their respective detectors.

To identify escaped-$\gamma$-ray $^{127}$Xe events in the TPC, first, a cut was made selecting
only single scatter events (one S1 and one S2). A second cut was made on event
radius (distance from the TPC’s central axis) and drift time (a proxy for z position in
the TPC), selecting only events which occurred near the TPC walls and excluded the
very top and bottom of the TPC. This position selection cut is shown in Fig. 4.15. To
identify coincident pulses in the LXe skin, a cut was made to select events which had
a pulse-start time in the skin within 200 ns of the S1 pulse’s start time in the TPC.
Additionally, only skin pulses which had a PMT coincidence greater than three PMTs
were considered in the coincidence selection. Finally, a cut on the reconstructed z
position of the coincident-skin pulse (measured from the height of the TPC cathode)
was applied to exclude events with skin coincidences that had unphysical position
reconstructions (visible in Fig. 4.16).
Figure 4.15. A Histogram of the negative of drift time versus the radius from the TPC’s central axis, squared, produced with simulated LZ TPC data. The position selection used to search for escaped-γ-ray $^{127}$Xe events in the TPC is shown with overlaid red lines. With a mean free path of $\mathcal{O}(1 \text{ cm})$, the γ-ray(s) from $^{127}$Xe only escape the TPC in decays which occur near the TPC walls.
Figure 4.16. Histograms produced from simulated LZ TPC data. **Left:** Z position of the TPC scatter vs. z position of the LXe skin scatter for events near the TPC wall (passing the cut in Fig. 4.15). The strong correlation indicates that the selected scatters in the TPC and skin originate from the same source. **Right:** Angular position, theta, of the TPC scatter vs. angular position of the LXe skin scatter. As with z position, the strong correlation in angular position indicates that the selected scatters in the TPC and skin originate from the same source.

With a population of single-scatter TPC events near the wall having a coincident pulse in the skin selected, histograms comparing the z position of the TPC scatter and skin scatter, and the angular position of the TPC scatter and skin scatter, show strong position correlation for the majority of the selected events. This position correlation demonstrates the successful identification of multiple-scatters originating from the same source across the two detectors. The position correlation histograms are shown in Fig. 4.16. Using maps of $g_1$ and $g_2$ (described in section 4.2.3), the energy of the events passing the previously described cuts were reconstructed and are shown in the histogram in Fig. 4.17. The 33.2 keV K-shell and 5.2 keV L-shell Auger electron/X-ray peaks from $^{127}$Xe are clearly visible above the background in this selection, and provide the TPC with in situ calibration peaks at low energies. Additionally, identifying these populations in the TPC provides a clean selection of the associated $\gamma$-ray deposits in the LXe skin, which serve as useful calibration peaks there.
Figure 4.17. The reconstructed TPC energy of single scatter TPC events with a coincident pulse in the skin, produced with simulated LZ TPC data. The K-shell and L-shell Auger electron/X-ray peaks from $^{127}$Xe are clearly visible.

### 4.2.5 TPC Efficiency Near Threshold with $^{212}$Pb

To avoid injecting long-lived $^3$H into LZ before the first science run, $^{212}$Pb from an injection of $^{220}$Rn was used to characterize the low-energy ER band during commissioning of the LZ TPC. The analysis of simulated data performed in this section, prior to the first $^{220}$Rn injection into LZ, demonstrates the ability to study the detector efficiency near threshold, made possible by injected $^{212}$Pb.

Using NEST [51], $6 \times 10^5$ $^{212}$Pb decays in the LZ TPC (background free) were simulated using the predicted values of $g_1$ and $g_2$ from Table. 3.2. The energy of the simulated events was reconstructed using the expression $E = W (\frac{S_1}{g_1} + \frac{S_2}{g_2})$, from section 2.2, with $W$ equal to 13.7 eV/quantum [25]. The reconstructed energies of the simulated $^{212}$Pb decays were compared to the normalized ground-state $^{212}$Pb decay spectrum. The normalization was acquired by fitting the spectrum to the data in the 10-25 keVee (electron-recoil equivalent keV) range. The reconstructed energies from
Figure 4.18. Top: The reconstructed ground-state $^{212}$Pb decay energy spectrum, from decays in the LZ TPC simulated by NEST [51], compared to the theoretical spectrum [48], normalized to the data by fitting. The fitting was performed on the reconstructed-energy data between 10 and 25 keVee. Bottom: Bin-by-bin fit residuals between the simulated data and theoretical ground-state decay spectrum for $^{212}$Pb.

The ratio of the data to the theoretical $^{212}$Pb spectrum is shown in Fig. 4.19 in addition to an empirical fit to an error function, following the method used to characterize the threshold efficiency in [52]. The 50%-efficiency threshold in reconstructed energy for ER events from the simulated-$^{212}$Pb data set was found to be $1.24 \pm 0.18$ keV.

Performing this empirical error-function fit on simulated data from NEST provides a basic expectation for how the real LZ detector and analysis chain should perform with optimal pulse-finding and pulse-classification. With this expectation, end-to-end $^{212}$Pb data was simulated with BACCARAT and analyzed with LZap (section 4.2.1). The expected shape of the efficiency near threshold from the error-function fit of the NEST data was overlaid onto the reconstructed energy spectrum from the simulated BACCARAT data, and the result is shown in Fig. 4.20. The rate below $\sim 10$ keVee...
Figure 4.19. Top: Ratio of the reconstructed decay energies to the theoretical ground-state $^{212}$Pb decay spectrum for decays in the simulated LZ TPC, produced with NEST [51]. An error function is fit to the data to characterize the reconstructed energy spectrum at low energies. The 50%-efficiency threshold from the fit is $\mu = 1.24 \pm 0.18$ keVee. Bottom: Bin-by-bin fit residuals between the data and error-function best fit.
Figure 4.20. Top: Ratio of the reconstructed decay energies to the theoretical ground-state $^{212}\text{Pb}$ decay spectrum for decays in the simulated LZ TPC, produced with BACCARAT [49]. The error-function best fit to simulated data from NEST [51] is overlaid to compare the reconstructed energy spectrum with the expectation from NEST. The rate below $\sim 10$ keVee is seen to be suppressed, suggesting a possible inefficiency in the pulse-finding, pulse-classification, or analysis of the $^{212}\text{Pb}$ data produced by BACCARAT and analyzed with LZap. Bottom: Bin-by-bin fit residuals between the data and overlaid error-function fit from the NEST data, highlighting the inefficiency below 10 keVee.

for the BACCARAT data is seen to be suppressed compared to the error-function fit from NEST, suggesting a possible inefficiency in the pulse-finding, pulse-classification, or analysis of the $^{212}\text{Pb}$ data produced by BACCARAT and analyzed with LZap.

4.2.6 Tagging Radon Daughters in LUX

As described in section 3.5, radioactive decay of radon and its progeny produce some of the most problematic backgrounds for WIMP searches in liquid noble TPCs like LZ. With a wide array of decay types and energies in the radon decay chains, it is important to understand the behavior of radon daughters in LZ so that the various backgrounds produced by them can be accurately accounted for. In this section I
present an analysis of LUX data which demonstrates the ability to identify $^{220}\text{Rn}$ and $^{216}\text{Po}$ alpha decays using both time and position correlation in the TPC. Position correlation between parent and daughter atoms was not included in the simulations of LZ data.

To develop the procedure for identifying $^{220}\text{Rn}$-$^{216}\text{Po}$ pairs, calibration data taken during an injection of $^{220}\text{Rn}$ where $^{220}\text{Rn}$ and $^{216}\text{Po}$ would be the dominant alpha decay populations was chosen. Single scatter events (one S1 and one S2) were first selected, and a position cut was made to exclude all events whose reconstructed position was outside of the physical dimensions of the LUX TPC. A pulse area cut was made on S1- and S2-pulse area ($S1 > 18,000 \text{ phe}$ and $S2 < 1,200,000 \text{ phe}$) to exclude all events which are not alpha decays.

After a $^{220}\text{Rn}$ atom alpha decays to $^{216}\text{Po}$, the $^{216}\text{Po}$ promptly alpha decays into $^{212}\text{Pb}$ with a 145 ms half life. With the two alpha events occurring so closely together in time, we are able to search for $^{220}\text{Rn}$-$^{216}\text{Po}$ pairs by excluding pairs of alpha decays whose time separation is much larger than the $^{216}\text{Po}$ half life. Additionally, we can enforce a requirement that these pairs of events occur close together in position within the detector volume. To this end, a correlation parameter was defined as $ds = \sqrt{(C \cdot dx)^2 + dt^2}$, where $dt$ is the time separation between two events, $dx$ is the distance between the positions of the two events, and $C$ is a constant which correlates position separation with time separation. In this study, $C$ was chosen to be equal to the reciprocal of the approximate bulk-LXe flow velocity in the LUX TPC, 1.0 sec/cm. The bulk-flow velocity sets the length scale for how far a $^{216}\text{Po}$ atom is able to travel in the TPC after it is produced, and before it decays. For every alpha decay, $\alpha_i$, in the selected data, the correlation parameter, $ds$, was calculated for each prior alpha decay, $\alpha_j$, that occurred within the previous two seconds. The preceding alpha decay, $\alpha_j$, in this time window which had the smallest $ds$ with respect to $\alpha_i$ was selected to be $\alpha_i$’s correlated partner. This procedure selects the closest previous
Figure 4.21. Histograms of the time separation between LUX TPC events identified as correlated pairs before (left) and after (right) the correlation cut, $ds < 1$ sec, is applied. For a population composed entirely of $^{220}\text{Rn}-^{216}\text{Po}$ pairs, the time separation distribution would be a decreasing exponential with time constant equal to that of $^{216}\text{Po}$. A decreasing exponential with the $^{216}\text{Po}$ decay constant is shown on both plots as a red line. After the $ds$ cut is applied, the distribution very closely matches the expected behavior through several $^{216}\text{Po}$ half lives in $dt$, demonstrating high efficiency at finding $^{220}\text{Rn}-^{216}\text{Po}$ pairs when the decays are close together in time.

alpha decay in space and time to each alpha decay event in the selected data. With alpha-decay pairs identified this way, a cut was made on $ds$ to remove all identified pairs with $ds > 1$ sec, eliminating the majority of coincidences which don’t correspond to true $^{220}\text{Rn}-^{216}\text{Po}$ pairs. The efficacy of this cut in selecting true $^{220}\text{Rn}-^{216}\text{Po}$ pairs is demonstrated in Figures 4.21 and 4.22.

With the ability to robustly select $^{220}\text{Rn}$ events, several interesting measurements are made possible. Here, one that is of particular importance to the design of LZ calibration hardware is described briefly: a measurement of the background $^{220}\text{Rn}$ rate in LUX before and after the $^{220}\text{Rn}$ injection was performed. The primary motivation to measure the $^{220}\text{Rn}$ background rate following the injection is to check for $^{228}\text{Th}$ leakage into the detector from the $^{220}\text{Rn}$ generator hardware. While the probability of this occurring is understood to be extremely low, the result of $^{228}\text{Th}$ leakage into LZ,
Figure 4.22. Drift time vs. S1-pulse area histograms of alpha decay events in the LUX TPC, with basic volume and energy cuts (described in the text) applied. **Left:** No additional cuts applied. **Middle:** The first event (in time) of each correlated pair of alpha events passing the $ds$ cut. This selection is comprised almost entirely of $^{220}$Rn decays. **Right:** The second event (in time) of each correlated pair of alpha decay events passing the $ds$ cut. This selection is comprised almost entirely of $^{216}$Po decays. These plots demonstrate the power of the cut on the correlation parameter, $ds$, to identify and separate the $^{220}$Rn and $^{216}$Po decay populations in LUX data.

if it did occur, would be catastrophic for the backgrounds in the TPC. The measured $^{220}$Rn rate (using the $^{220}$Rn-$^{216}$Po pair selection technique outlined in this section) before and after the $^{220}$Rn injection into LUX is presented in Fig 4.23, showing no measurable change in rate between the two time periods.

The pair finding technique described in this section is applicable to background and injected $^{220}$Rn-$^{216}$Po pairs in LZ and other liquid noble TPCs generally, and may even be possible with other radon progeny such as the $^{212}$Bi-$^{212}$Po and $^{212}$Bi-$^{208}$Tl pairs belonging to the $^{222}$Rn decay chain. Analyses which identify these pairs by their unique decay characteristics promise to be extremely useful in understanding radon chain backgrounds in liquid noble TPCs.
Figure 4.23. Plot of the background $^{220}$Rn rate in the LUX TPC before and after injecting $^{220}$Rn. The start and stop of the $^{220}$Rn injection periods are shown by the colored vertical lines. Data taken during the two $^{220}$Rn injection periods is excluded from the rate measurements.

4.3 Numerical Simulation of a $^{220}$Rn Injection into LZ

To prepare for the first injection of $^{220}$Rn into LZ, a numerical simulation of the full $^{220}$Rn decay chain in the LZ TPC was created in Python, allowing for the study of the relative TPC activities of the $^{220}$Rn-chain radioisotopes following an injection. After $^{220}$Rn is injected, the number of atoms in the TPC of the $i^{th}$ isotope in the $^{220}$Rn chain at time $t$, $N_i(t)$, evolves according to the Bateman Equation:

$$\frac{dN_i(t)}{dt} = -\lambda_i N_i(t) + \lambda_{i-1} N_{i-1}(t)$$  \hspace{1cm} (4.1)

where $\lambda_i$ is the decay constant of the $i^{th}$ isotope in the $^{220}$Rn chain. For $^{220}$Rn ($i = 1$), the $i - 1$ term is equal to zero because no source of $^{220}$Rn is present. For the end of the chain, the stable isotope $^{208}$Pb ($i = 6$), $\lambda_6$ is equal to zero. The general solution to the Bateman Equation [53] for the number of atoms of the $i^{th}$ $^{220}$Rn-chain isotope at time $t$, is given by:

$$N_i(t) = \frac{1}{\lambda_i} \sum_{n=1}^{i} N_n(0) \lambda_n e^{-\lambda_n t} \cdot \prod_{j=1, j \neq n}^{i} \frac{\lambda_j}{\lambda_j - \lambda_n}. \hspace{1cm} (4.2)$$
For decay chains with more than a few radioactive daughters, computing the analytic solution to the Bateman Equation for each step in the chain quickly becomes impractical. Worse still, for injections of $^{220}\text{Rn}$ into LZ which add a mixture of $^{220}\text{Rn}$ and $^{212}\text{Pb}$ into the TPC continuously over an extended period of time, a source term must be added to the general solution of the Bateman Equation, yielding the following solution:

$$N_i(t) = \frac{1}{\lambda_i} \sum_{n=1}^{i} \lambda_n \cdot (N_n(0)e^{-\lambda_n t} + S_n(1 - e^{-\lambda_n t})) \cdot \prod_{j=1, j \neq n}^{i} \frac{\lambda_j}{\lambda_j - \lambda_n}$$  \hspace{1cm} (4.3)$$

where $S_n$ is the number of atoms of the $n^{th}$ isotope in the decay chain added to the system per unit time \[54\]. In the case of LZ, we are interested in the solution with non-zero $S_1$ and $S_3$ for injected $^{220}\text{Rn}$ and $^{212}\text{Pb}$. To approximate the solution numerically, the time-evolution of the number of atoms of each $^{220}\text{Rn}$-chain isotope in the LZ TPC is simulated using a finite difference method with discrete time steps, $dt$. For each pair of adjacent isotopes in the $^{220}\text{Rn}$ chain, the abundance of the daughter at time $t + dt$ is calculated from the activity of the parent at time $t$. The number of atoms of the $i^{th}$ isotope in the $^{220}\text{Rn}$ chain at time $t + dt$, is then given by:

$$N_i(t + dt) = (-\lambda_i N_i(t) + \lambda_{i-1} N_{i-1}(t)) \cdot dt.$$  \hspace{1cm} (4.4)$$

The discrete time step, $dt$, can be made arbitrarily small to approximate the analytic solution with arbitrarily high accuracy. The full code of the $^{220}\text{Rn}$ decay chain simulation is presented in Appendix A, and incorporates many inputs and features that are specific to LXe TPCs including: active removal by purification through a heated getter, removal of charged daughters by the TPC’s electric fields using the measured charged fractions from \[45\], and a “$^{212}\text{Pb}$-Only mode” which simulates an injection of pure $^{212}\text{Pb}$. Examples of the plots produced by the $^{220}\text{Rn}$ chain simulation are shown in Fig. 4.24 and Fig. 4.25.
Figure 4.24. The simulated activities of all of the radioisotopes in the $^{220}\text{Rn}$ chain during and after a 7-hour continuous injection of a mixture of $^{220}\text{Rn}$ and $^{212}\text{Pb}$. The activity of the $^{212}\text{Pb}$ and its daughters can be seen to build up slowly over time in the simulated TPC while the $^{220}\text{Rn}$ and $^{216}\text{Po}$ activities are constant during the injection period. Removal of the $^{220}\text{Rn}$ daughters by purification is included in this simulation with a removal time constant of 85.6 hours.
Figure 4.25. The simulated cumulative number of decays (left) and number of atoms (right) from each $^{220}$Rn chain radioisotope during and after a 7-hour continuous injection of a mixture of $^{220}$Rn and $^{212}$Pb. The number of atoms of $^{212}$Pb and its daughters can be seen to build up slowly over time in the simulated TPC as the abundance of $^{220}$Rn and $^{216}$Po are constant during the injection period. Removal of the $^{220}$Rn daughters by purification is included in this simulation with a removal time constant of 85.6 hours.
CHAPTER 5
LZ CALIBRATION PROTOTYPING

To develop new procedures for injecting calibration radio-isotopes into the LXe in LZ, a dedicated LXe detector, supporting circulation system, calibration-source generators, and a prototype source injection system (SIS) were designed and built at the University of Massachusetts (UMass) Amherst. The LXe detector and circulation system were designed to imitate the features of LZ that are relevant to the source injection procedures, most notably, the constant re-circulation and purification of the xenon through a heated getter. The full design details of the calibration-source hardware, LXe detector, and prototype SIS are detailed in this chapter, and the results from injections into the system are presented.

5.1 LZ Internal Calibration Source Hardware

The prototype LZ SIS was designed at UMass Amherst to automatically dose and inject precise activities of calibration radioisotopes into the LXe volume of LZ. The automated procedures were developed based on the injection procedures demonstrated by the LUX experiment, with several improvements made to the processes and hardware that allow for greater control and dosing precision than what was achieved by LUX. Increased dosing precision will extend the useful life of the parent isotopes and lengthen the time between source installations in LZ. The calibration radioisotopes that the SIS handles are produced in custom flow-through generators designed at UMass Amherst, or present in bottles as a gaseous mixture with carrier xenon.
5.1.1 Flow-Through Generator Housing Design

The calibration isotopes that the flow-through generators are responsible for producing for use in LZ are $^{83m}\text{Kr}$ (1.83 h half life), $^{131m}\text{Xe}$ (11.8 d half life), and $^{220}\text{Rn}$ (55.6 s half life). The flow-through source-generator hardware which contains the parents of these isotopes was fully redesigned for LZ. The basic design requirement for the flow-through generators was that the source (parent) isotope be completely trapped within the generator while allowing the calibration isotope (daughter) to be transported out with high efficiency when gaseous room temperature xenon is flowed through. The transport of calibration isotopes out of the generator is easily achievable for the LZ internal-calibration isotopes because they are noble elements and therefore do not interact with any of the metal surfaces or polytetrafluoroethylene (PTFE) valve seats in the materials used to construct the generators. Each of the noble calibration radioisotopes decays from a non-noble parent isotope, and can be conveniently stored in a solid form within its respective generator.

The LZ flow-through generators are designed to be completely interchangeable with each other in the LZ SIS, eliminating the need for unique hardware on the SIS to accommodate each. To this end, the various generators all share the same construction, described below, that is pictured in Fig. 5.1. In the flow-through generator housing design, the central volume where the source is stored is composed of a 1/2” stainless steel tee, on top of which is a 1/2” metal face-seal (VCR) cap that provides access to the source. The central volume is straddled by two sintered-nickel filters (Entegris WG3NSMJJ2 [55]) to prevent any loose source material from escaping (the source material is separately held in place, as described in the following sections). The filters used in the LZ flow-through generators have an average pore size of 3 nm, an order of magnitude smaller than the pore size of the filters used in LUX. Straddling the region enclosed by the filters are two locking diaphragm valves (Swagelok 6LVV-DPLBW4-P [56]) which have 1/4” metal face-seal (VCR) glands orbital welded
Figure 5.1. An example LZ flow-through generator for producing $^{83m}$Kr, $^{131m}$Xe, or $^{220}$Rn. The construction is symmetric with a 1/2" outer diameter stainless steel volume at the center which houses the source, accessible via a 1/2” male metal face-seal (VCR) cap (shown here with a lock installed). The central volume is straddled by two sintered-nickel filters, and two locking manual valves (shown here with padlocks installed). Two 1/4" female metal face-seal (VCR) fittings connect the generator to the source injection panel.

to them, to connect the generator to the LZ SIS. All of the generator components were purchased individually, and were orbital welded together inside of a cleanroom at the University of Wisconsin-Madison Physical Sciences Lab, where many of LZ’s subsystems were welded and assembled. The generator hardware is mounted on an aluminum panel, which makes installation onto the LZ SIS easier, and holds the installed generator more securely on the SIS.
5.1.2 $^{83m}$Kr Generator

$^{83m}$Kr is produced from the decay of $^{83}$Rb (86 day half life) through electron capture, with a branching fraction which has several different reported values in the literature including 0.750 [57] and 0.779 [58]. In the $^{83m}$Kr generator design for LZ, $^{83}$Rb is bound to radiopure activated charcoal as it was in the generators used with LUX. Unique to the LZ design, the charcoal is epoxied to a stainless steel bolt. Binding the charcoal to the threaded bolt with epoxy prevents it from moving around freely and producing charcoal dust that could be transported out of the generator, into LZ plumbing. This bound design also makes replacement of the $^{83}$Rb source much simpler. The bolt, with attached charcoal, is screwed into a metal face-seal (VCR) cap which can be installed into the 1/2” face-seal (VCR) port on an LZ flow-through generator housing. When the cap is installed on the generator housing, a helium leak tight seal is created using a silver-plated steel gasket, and the charcoal is suspended in the central generator volume. The $^{83}$Rb remains fully bound to the charcoal, while $^{83m}$Kr produced can escape and mix with carrier xenon gas which is flowed through the generator during the injection procedure. The charcoal assembly is pictured in Fig. 5.2 (left).

To prepare the source assembly, a 1” section of threads near the bolt head is filed flat on a 1.75” long 1/4”-20 threaded bolt to create space for the epoxied charcoal to fit into the generator plumbing. Using a rotary tool with a cut-off wheel attachment, a narrow vent is cut into the bolt’s end and the threads near the end of the bolt to prevent those threads from creating an isolated volume or virtual leak when installed. A corresponding 1/4”-20 threaded hole is drilled and tapped into a 1/2” metal face-seal (VCR) cap. After cleaning the bolt and cap with isopropyl alcohol to remove metal dust, the bolt is installed into the threaded hole on the cap.

The charcoal selected for use in the LZ $^{83m}$Kr generators was Calgon OVC 4x8 Coconut Granular Activated Carbon [59], chosen for its form factor and history of use.
Figure 5.2. Left: $^{83}$Rb is stored on charcoal pellets which have been epoxied to a threaded bolt. The bolt is screwed into a threaded hole machined into a 1/2” metal face-seal (VCR) cap. The cap attaches to the central volume of the flow-through generator, and makes a helium leak tight seal. Right: $^{83}$Rb aqueous solution is precisely deposited onto charcoal pellets using a micro-liter syringe.
in LUX, though Shirasagi G2x4/6 Pelletized charcoal [60] was also tested at UMass Amherst. The $^{83}$Rb was obtained from Oakridge National Laboratory as a 1 M HCl aqueous solution. Depending on the volume of the solution required to achieve the desired source activity, between one and four pieces of charcoal were selected. The $^{222}$Rn emanation rate of OVC 4x8 has been measured to be $53.6 \pm 5.6$ mBq/kg in [61], allowing us to calculate the emanation rate of each 30 ($\pm$ 10) mg pellet of charcoal used in a $^{83m}$Kr generator. For the one pellet used in the first LZ generator, the $^{222}$Rn emanation rate was $1.6 \pm 0.6$ $\mu$Bq. To prepare them for use, the selected charcoal pieces were washed with de-ionized water to remove dust, and were subsequently baked on a hot plate kept above 100 °C for an hour to remove the water from the wash process. A very thin line of Master Bond Supreme 10AOHT-LO epoxy [62] was deposited on the flat-filed surface of the threaded bolt, and the charcoal pieces were pressed into the epoxy. The epoxy was cured at 125 °C in vacuum for 75 minutes.

Once the epoxy had cured, the generator was prepared to be dosed with $^{83}$Rb. Using a syringe with 10 $\mu$L capacity and 0.1 $\mu$L graduations (Hamilton, Model 1701N [63]), the volume of $^{83}$Rb solution corresponding to the desired $^{83}$Rb activity was measured and deposited directly onto the charcoal pieces, typically a few $\mu$L. When the activity of the solution was very high and a small dose was required, dilution with deionized water was used to reduce the specific activity of the solution without any measurable loss in precision of the resulting dose. The $^{83}$Rb dosing procedure is pictured in Fig. 5.2 (right). After depositing the solution onto the charcoal, the entire assembly was baked again on a hotplate inside of a fume hood, kept above above 100 °C for 90 minutes to completely remove the water, leaving only the $^{83}$Rb bound to the charcoal. Once the water was removed and the assembly had cooled, it was installed into one of the LZ flow-through generators and pumped on with a turbo-molecular pump to a pressure below $1 \times 10^{-4}$ mBara for cleanliness (the generators were pumped on further after installation on the LZ SIS as part of the installation procedure). The
assembled $^{83m}$Kr generators were stored in this state until they were installed on the SIS for use. A $^{83m}$Kr source produced this way for LZ with an initial $^{83}$Rb activity of $\sim 100$ kBq has a useful lifetime of more than a year in the LZ SIS, given the level of control achieved on the injected $^{83m}$Kr activity, demonstrated in section 5.7.

During the $^{83}$Rb dosing procedure, the activity of the $^{83}$Rb solution, dose, and the equipment used to handle the $^{83}$Rb solution and dose were counted with a NaI(Tl) (thallium-activated sodium-iodide) crystal and PMT detector assembly (CAPTUS 3000 [64]). NaI(Tl) detectors use a single PMT to detect scintillation light produced by the NaI(Tl) when a $\gamma$-ray interacts with the crystal. The bottle containing the $^{83}$Rb solution and the prepared charcoal were counted before each time the procedure was performed to verify the remaining activity (which could also be calculated independently). The dosing syringe was counted after measuring the dose of $^{83}$Rb solution during the procedure (while still contained inside) to verify the dose activity, and was counted again after the dose had been expelled to check for residual activity in the syringe. The charcoal was counted immediately after receiving the dose, and again following the baking procedure, to verify the final activity of the source. An image of the counting setup is shown in Fig. 5.3.

5.1.3 $^{131m}$Xe Generator

$^{131m}$Xe is produced from the beta decay of $^{131}$I (8.02 day half life) with a 0.01 branching fraction [65], [66]. In the $^{131m}$Xe generator design for LZ, $^{131}$I is bound to a fine powder of NaH$_2$PO$_4$. The NaH$_2$PO$_4$ powder is contained within an Entegris sintered-metal filter gasket [55] (Gasketgard WGPM0GGT4), which consists of a sintered stainless steel cup integrated with a 1/2” metal face-seal (VCR) gasket that makes the helium leak-tight seal on the flow-through generator hardware’s source-access port. The sintered-metal filter gaskets have an average pore size of 300 nm,
Figure 5.3. The CAPTUS 3000 [64] NaI(Tl) detector probe aimed at a $^{83m}$Kr source inside of a fume hood at UMass Amherst. The detector measures the spectrum of $\gamma$-ray radiation from the various sources, and materials used to produce them, at UMass Amherst.
containing the NaH$_2$PO$_4$ while allowing for the $^{131m}$Xe produced inside to mix with the carrier xenon gas that is flowed through during an injection procedure.

The $^{131}$I is dosed onto the NaH$_2$PO$_4$ substrate and enclosed in a double-walled gelatin capsule by Jubilant DraxImage Inc. [67], and can be purchased from Cardinal Health [68], who provide calibration data for the $^{131}$I activity. The $^{131}$I solution was also available for purchase separately, allowing us to potentially produce our own sources as in the $^{83m}$Kr case, however, the short (8.02 day) $^{131}$I half life and significant health risk associated with handling an $^{131}$I solution made purchasing the capsules from Cardinal Health more convenient.

Experiments performed at UMass Amherst have shown that repeated cycling between vacuum and atmospheric pressure as part of the typical source injection procedure embrittles and weakens the gelatin layers of the capsules sold by Cardinal Health, eventually resulting in fracturing which releases the loose $^{131}$I doped NaH$_2$PO$_4$ into the plumbing. These results, which motivated the use of the sintered-metal filter gaskets, are described in detail in section 5.8. Photos of one of the $^{131}$I-doped-NaH$_2$PO$_4$ filled gelatin capsules from Cardinal Health, a sintered-metal filter gasket used to contain it, and the finished transfer of the capsule’s contents are shown in Fig. 5.4.

The procedure for transferring the $^{131}$I doped NaH$_2$PO$_4$ into the cup of the sintered-filter gasket required several safety considerations because of the slow sublimation that iodine undergoes at room temperature and pressure, and because of the dangers associated with ingesting radioactive iodine which concentrates in the thyroid gland. The $^{131}$I handling work was performed inside of a fume hood, with personal protective equipment (PPE) worn including a lab coat, safety glasses, nitrile gloves, dosimeter badge, and ring dosimeter. Additionally, the air space inside of the fume hood, and outside of the fume hood in the breathing space of the operator, was monitored by two air sampling pumps (Gilian BDX-II [69]) with in-line charcoal paper filters, designed to capture any iodine which passed through the pump. The
Figure 5.4. **Left**: A gelatin capsule from Cardinal Health, containing $^{131}$I doped NaH$_2$PO$_4$. **Center**: An Entegris sintered-stainless-steel filter gasket (WGPM0GGT4) used to contain the $^{131}$I doped NaH$_2$PO$_4$, before being inserted into the flow-through generator hardware. **Right**: The finished $^{131}$I flow-through generator assembly before the 1/2” metal face-seal (VCR) cap is attached. The $^{131}$I doped NaH$_2$PO$_4$ is suspended in the carrier xenon flow path, but contained by the sinter, and is visible in the center of the photo. $^{131m}$Xe produced from the $^{131}$I diffuses out of the sinter with high efficiency.
pumps were set to sample air at 3 l/min to approximate the average human breathing rate. The charcoal filters were counted before and after the procedure using a NaI(Tl) well detector to measure any contamination of the air spaces. A thyroid bioassay was also performed with a probe-style NaI(Tl) detector (CAPTUS 3000 [64]), where the thyroid gland of the operator was counted at a fixed distance before the the procedure was performed, and then again, 24 hours after the procedure to look for any thyroid uptake of the radioactive $^{131}$I.

The procedure began by placing a new sintered-metal filter gasket into the 1/2” metal face-seal (VCR) port of an empty LZ flow-through generator assembly. The two halves of the gelatin capsule were carefully separated, and the $^{131}$I doped NaH$_2$PO$_4$ in the capsule was dumped into a clean disposable weighing boat. If the capsule contents were stuck in one half of the gelatin capsule, the gelatin layer was either carefully crushed, or cut, to release the contents into the weighing boat. The $^{131}$I doped NaH$_2$PO$_4$ was typically comprised of a combination of a loose powdery component, and a very hard concreted component, likely formed during the $^{131}$I dosing. The concreted chunks were broken up by careful crushing, or cutting with a scalpel, to allow them to fit into the sintered-metal filter gasket more easily, and to create a more uniform consistency. Once any large pieces were broken up, the $^{131}$I doped NaH$_2$PO$_4$ was dumped into the sintered-metal filter gasket, inside the generator housing assembly, via a disposable paper funnel. The sealing surface of the sintered-metal filter gasket was ensured to be clean by wiping with a lint-free wipe, and a 1/2” metal face-seal (VCR) cap was installed, sealing the $^{131m}$Xe generator. The generator was then pumped on with a turbo-molecular pump to a pressure below $1 \times 10^{-4}$ mBara for cleanliness (the generator was pumped on further after installation on the LZ SIS as part of the installation procedure). After this initial pump-out, the source was 'conditioned' with a two-step cycle of pressurization to 1 bara with GXe and pump-out to less than $1 \times 10^{-4}$ mBara. This conditioning cycle removed any residual water.
vapor or other contaminants which might be outgassed by the NaH$_2$PO$_4$, and was necessary because the source could not be baked like the $^{83m}$Kr sources were, due to the volatility of $^{131}$I. This conditioning process was shown to be required by measurements of the emanation efficiency of $^{131m}$Xe from the source, which changed during the first few exposures of several new sources to GXe (this effect is described in detail in section 5.8). The GXe pressurization and pump-out cycle was performed five times before the $^{131m}$Xe generators were stored at vacuum prior to their final installation on the SIS for use. A typical $^{131m}$Xe source for LZ produced with an initial $^{131}$I activity of $\sim 300$ kBq has a useful lifetime of $\sim 2$ months in the LZ SIS.

5.1.4 $^{220}$Rn Generator

$^{220}$Rn is produced from the alpha decay of $^{224}$Ra (3.7 d half life), which is in turn produced from the alpha decay of $^{228}$Th (1.9 y half life). In the $^{220}$Rn generator design for LZ, $^{228}$Th is electroplated onto a platinum disk which is suspended by a threaded rod in the central generator volume. The $^{228}$Th plated disk was purchased from Eckert & Ziegler [70] with a customized ”A-2 type” disk holder which was altered by Eckert & Ziegler to have a smaller outer diameter that would fit inside of our flow-through generator housing (upper left of Fig. 5.5). The back of the holder was produced with a blind 4-40 threaded hole machined into it, allowing it to be held in place with a threaded rod.

To produce the $^{220}$Rn generator, 1/4” long slots were cut into both ends of a 4-40 threaded steel rod using a cut-off wheel attachment on a rotary tool. These slots were designed to prevent the threads near the rod’s ends from creating isolated volumes or virtual leaks when installed into a threaded hole. A 4-40 threaded hole was machined into a 1/2” metal face-seal (VCR) cap, into which the threaded rod was installed. Two 4-40 nuts were threaded onto the rod before the free end of the threaded rod was installed into the back of the $^{228}$Th-plated-disk holder. The two 4-40 nuts were
tightened against the disk holder and the 1/2” cap, respectively, preventing them from loosening on the threaded rod over time. Finally, the completed source assembly (the source attached to the 1/2” VCR cap) was inserted into the flow-through generator hardware and the 1/2” cap was tightened, sealing the $^{220}$Rn generator closed. After installation, the source is held suspended in the flow path of the carrier xenon which transports emanated $^{220}$Rn out of the generator during a typical injection procedure.

The assembled LZ $^{220}$Rn source holder is pictured in Fig. 5.5. The $^{220}$Rn generator was produced on May 1, 2020, with an initial $^{228}$Th activity of 21 kBq, giving it a useful lifetime of several years on the LZ SIS. The emanation efficiency of $^{220}$Rn from the electroplated $^{228}$Th was measured by Nicholas Chott and Richard Schnee at the South Dakota School of Mines and Technology, and was found to be $0.139 \pm 0.013$. With this emanation efficiency (fraction) known, when the $^{228}$Th activity was 21 kBq on its calibration date, the activity of free (emanated) $^{220}$Rn from the source was calculated to be $2.92 \pm 0.27$ kBq.

5.1.5 CH$_4$, CH$_3$T, and $^{14}$CH$_4$ Bottle Storage Hardware

The gaseous internal calibration isotopes which require storage in bottles include natural methane (CH$_4$), and the long-lived radioisotopes $^3$H (12.3 y half life) and $^{14}$C (5.7 ky half life), as tritiated methane (CH$_3$T) and $^{14}$C methane $^{14}$CH$_4$, respectively. The LUX bottle-source hardware design is largely preserved in the design of the LZ bottle storage hardware.

The LZ calibration source bottles are designed to be interchangeable with each other in the LZ SIS, eliminating the need for unique hardware on the SIS to accommodate each. Because the methane based radioisotopes do not decay away in the detector on a convenient timescale (or at all, in the case of CH$_4$), they must be purified out by the heated-zirconium getter in the LZ circulation system. Since these methane molecules are purified out by the getter, they must be injected into the LZ
Figure 5.5. **Upper Left:** The $^{228}\text{Th}$ electroplated platinum disk from Eckert & Ziegler inside of a custom modified A-2 type disk source holder. The circle of electroplated $^{228}\text{Th}$ is faintly visible in the center of the disk. **Lower Left:** The electroplated disk and holder are attached to the 1/2" metal face-seal (VCR) cap which seals the flow-through generator and holds the source in place inside the plumbing. **Right:** The 1/2" metal face-seal (VCR) cap positioned next to its final installation position to demonstrate the height of the source in the flow path of carrier xenon.
circulation system downstream of it, increasing the need for the bottle contents to be exceedingly pure. The bottle sources contain the calibration gas as a mixture with carrier xenon gas in 1 L stainless steel sample cylinders. One end of each cylinder is welded shut, and the other has a locking diaphragm valve (Swagelok 6LVV-DPLBW4-P [56]) welded to it, so as to be fully helium leak-tight up to the valve seat. A second manual valve in series protects the contents of the bottle from a tiny through-leak in either valve. An example of the bottle source hardware before the second valve is connected in series is pictured in Fig. 5.6. The bottles are connected to the SIS by a 1/4” metal face-seal (VCR) fitting immediately upstream of a passive methane purifier (SAES MC1-902) [71], which removes a variety of organic impurities from the methane mixtures when they are used during the injection procedures.

The natural methane was procured at ultra high purity (UHP, UN1971) from Gasco [72]. The tritiated methane (CH$_3$T) and $^{14}$C methane ($^{14}$CH$_4$) were synthesized by Moravek Biochemical [73], originally for use in LUX, and will be prepared in the
bottle hardware described above at the University of Maryland. There, the bottles will be filled with a mixture of xenon and the calibration gas, at a convenient concentration for the injection procedures. Once installed, the $\text{CH}_3\text{T}$ and $^{14}\text{CH}_4$ bottles will contain enough of each calibration gas to provide calibrations for the entire duration of LZ.

5.2 The UMass Amherst LXe Detector

The UMass LXe detector is contained within a 4.5” inner diameter (ID) vacuum-insulated stainless steel cryostat dewar from Cryofab [74], which uses a copper gasket sandwiched between stainless steel knife-edges on the cryostat dewar and lid to create a leak-tight seal. The detector inside consists of a custom machined monolithic piece of PTFE, inside of which sits 1 kg of LXe between the faces of two Hamamatsu [75] R8778 PMTs taken from the de-commissioned LUX experiment. A 3-D model of the detector is shown in Fig. 5.7, and one of the PMTs is shown in Fig. 5.8. The detector is prevented from floating in the LXe, which also surrounds the bottom of the detector, by four custom spring-loaded stainless steel threaded rods. The rods pin the detector to the bottom of the dewar when it is closed and filled with LXe, and suspend the detector from the cryostat lid when it is removed from the dewar. A 1/2” outer diameter (OD) ‘inlet’ bore which extends downwards to the height of the bottom PMT face is machined into the top of the PTFE. The bore contains the 1/4” OD PTFE inlet tube which guides newly condensed LXe into the central detector volume, where it enters onto the bottom PMT face. A weir is machined into the top of the PTFE opposite the inlet bore, at a height that is slightly above the top PMT face, imitating the relative inlet and outlet locations in LZ and setting the ultimate liquid height in the detector. As purified LXe is constantly added through the inlet, the LXe already inside the detector spills over the weir and falls down a channel machined into the side of the PTFE, into the bottom of cryostat. Once in the bottom of the cryostat, the LXe is removed from the detector through a 1/8”
Figure 5.7. **Left**: 3-D Model of the UMass LXe Detector. The PTFE is indicated in yellow. **Right**: Cross sectional drawing of the UMass LXe Detector. LXe is indicated in blue. As LXe is continuously added into the inlet bore, left of the central volume, LXe from inside the detector spills over the weir into the bottom of the cryostat. A 1/8” OD PTFE tube submerged in the LXe in the bottom of the cryostat pulls the LXe out of the detector and into the circulation system.
Figure 5.8. **Left**: One of the two Hamamatsu R8778 Photomultiplier tubes used in the UMass LXe Detector. A custom machined PTFE base protects and insulates the PMT-base pins from contact with metal surfaces. **Center**: The connections to the PMT base for the PMT signal and power cables were made by soldering pins to copper contacts on a small piece of polyimide sheet. Cables were also soldered to the contacts before the assembly was inserted into the PMT base. **Right**: The bottom PMT installed into the detector PTFE. When the copper ears are fastened to the detector PTFE, the stainless steel lip surrounding the PMT face creates a LXe-tight seal with the PTFE (LXe in the active volume is fully contained). The electronics on the base of the PMT are covered with a custom PTFE cover, held in place with PTFE screws.
OD PTFE outlet tube, contained in the weir spillover channel and submerged in the Lxe at the bottom. The constant flow of Lxe through the detector which causes the Lxe to continuously spill over the weir is driven by a metal-bellows pump as part of the xenon circulation and purification system, described in section 5.3. The weir cutout and spillover channel are visible in Fig. 5.9, which shows views of the top of the detector with and without the top PMT installed.

Capacitive liquid-level sensors are placed alongside the Lxe inlet and outlet tubes in the PTFE inlet bore and the weir spillover channel, which measure the height of the Lxe in the active detector volume and in the bottom of the cryostat, respectively. A temperature sensor in the bottom of the cryostat, under the PTFE cover which insulates the bottom PMT base (pictured in Fig. 5.8 [right]), is used along with the weir liquid level sensor to confirm the presence of Lxe in the weir-spillover channel during filling and normal operation. Spillover into the weir indicates that detector’s active volume is full during the filling process. Also under the PTFE at the bottom of the cryostat is a Kapton polyimide heater, used to speed up the evaporation of the Lxe during the recovery and detector shutdown process. Pictured in Fig. 5.10 is the weir-spillover channel, containing a liquid-level sensor, the 1/8” OD outlet tube, the Kapton heater and temperature sensor wires, and the bottom-PMT signal and power cables.

During normal operation of the detector, both PMT faces are submerged in 0.35 L (~1 kg) of Lxe contained in the detector’s active volume. A volume of approximately 3.1 L above the PTFE and PMTs is filled with GXe and is monitored by a pressure transducer. A 1/4” OD stainless steel tube extending out of the cryostat lid connects the GXe space at the top of the cryostat to the circulation system upstream of the circulation pump. Because the main circulation flow through the detector proceeds through the outlet tube submerged in the weir-spillover Lxe, the GXe space at the top of the cryostat is not efficiently circulated without this dedicated pathway. The
Figure 5.9. **Left:** The detector from above, without the top PMT installed. The bottom PMT face is visible at the bottom of the active LXe volume. The inlet bore is visible at the bottom right of the image, containing the LXe inlet tube and liquid level sensor. The weir is visible at the top left of the image, where LXe spills out of the active volume as purified LXe is added to the detector through the inlet bore. **Right:** The top PMT is pictured wrapped in Kapton polyimide film for insulation, and is attached to the PTFE with threaded stainless steel rods. The custom spring-loading hardware for the threaded rods that suspend the detector from the cryostat lid and prevent it from floating in the LXe are pictured. The threaded rods terminate above the PTFE, but are connected to it by flexible stainless steel wires which allow the detector to be suspended. If the detector moves closer to the cryostat lid, the springs contact nuts on the threaded rods and compress, preventing the detector from moving more than a few centimeters.
Figure 5.10. **Left**: The UMass LXe Detector fully assembled. The brown disc-shaped Kapton polyimide heater is visible at the bottom. **Right**: The fully assembled detector as the cryostat dewar is raised around it to be sealed. One of the custom liquid level sensors (sheathed in braided steel) and the 1/8” OD PTFE outlet tube are visible in the weir spillover channel.
flow rate of GXe out of the top of the cryostat is controlled with an inline metering valve which is set to have very high impedance so that the rate is slow compared to the main circulation speed, but still fast enough to turn over the GXe space on an \(~\) hours timescale. This slow purging of the GXe space ensures that the majority of circulated xenon comes from weir-spillover LXe from the active detector volume.

5.2.1 Insulating Vacuum and Condensing Hardware

A 16" tall and 10" diameter cylindrical vacuum vessel, positioned above the detector cryostat, contains the hardware inside which the room temperature GXe from the circulation system is cooled and condensed into LXe on its way into the detector. The vacuum vessel above the detector and the condensing hardware are pictured in Fig. 5.11, left and center, respectively. The insulating vacuum inside of the vessel is maintained by continuous pumping with a rotary-vane pump connected by a 1/2” OD copper tube to a KF40 flange on the bottom of the vessel. The pressure inside the vacuum vessel is measured with a pressure transducer which is read out by a computer in the laboratory. The lab computer reads out the pressure transducer in a custom graphical user interface (GUI), designed to monitor the detector’s many sensors. The GUI is described in detail in 5.5.

**Heat Exchanger and Condenser:** Inside the vacuum vessel, GXe on its way from circulation travels through a parallel-plate heat exchanger (Dudadiesel B3-23A 20 Plate [76]) which pre-cools it, emulating the design in [77]. In the heat exchanger, cold GXe coming from the detector’s outlet tube exchanges heat with the room temperature GXe on its way towards the detector. The pre-cooled GXe then enters the branch (parallel to the ground) of a 2.75” ConFlat (CF) tee with a custom machined copper cold-finger installed on the top end of the tee’s run (perpendicular to the ground). The copper cold-finger consists of 19 threaded copper rods installed into and protruding from a custom copper CF cap (Fig. 5.11 right).
Pulse-Tube Cryocoolers: Cooling power is supplied to the top of the copper cold-finger, in the vacuum space, by two pulse-tube cryocoolers from Superconductor Technologies Inc [78], whose cold-tips are coupled by a custom machined copper block. The cryocoolers are mounted to the outside of the vacuum vessel lid by two KF40 bulkhead clamps, and the power supplied to each cryocooler is manually controlled by two variable AC power supplies housed on a shelf next to the cryostat. The bodies of the cryocoolers extend upwards into the room, and the cold-tips extend downwards into the vacuum space. The copper block coupling the cold-tips of the two cryocoolers is tightly pressed against the top of the copper cold-finger (outside of the CF tee) using threaded rods attached to the vacuum vessel lid, which pull upwards on a platform beneath the CF tee. A 3-D model cross-sectional view of the CF tee containing the copper cold-finger, and the coupled pulse-tube cold-tips is shown in Fig. 5.11 (right). One of the pulse-tube cryocoolers was modified to be water-cooled by removing the copper heat-exhaust fins and installing a chamber through which water is continuously circulated, carrying away the heat produced by the device. The water cooling was seen to have a negligible effect on the cooling power of the cryocooler compared to cooling with a shrouded fan, the cooling method used for the other pulse-tube cryocooler.

Temperature Control and Flow into the Cryostat: The temperature of the copper cold-finger inside the xenon space is set and maintained by a proportional-integral-derivative (PID) controller which controls a heater bolted to the side of the cold-finger in the vacuum space. The setpoint temperature of the copper cold-finger is chosen to create stable LXe conditions, typically around 168 K, so that when pre-cooled GXe from the heat exchanger enters the CF tee and encounters the high surface area copper cold-finger, it condenses into liquid and falls downwards under the influence of gravity, out of the bottom of the CF tee’s run. A straight 1/4” OD stainless steel tube extends downwards out of the CF ‘condenser’ tee, and out of
Figure 5.11. Left: The detector cryostat is pictured suspended from its aluminum frame. The vacuum space containing the heat exchanger and condensing hardware rests on extensions off of an aluminum frame on the right, and sits above the cryostat. The detector cryostat is coupled to the circulation system and vacuum space only through the 12" long metal vacuum bellows that extends from the top of the cryostat to the bottom of the vacuum space, the two stainless steel lines that it contains, and a room temperature stainless steel tube that connects the GXe head at the top of the cryostat to the circulation system. Center: The heat exchanger and condensing hardware, wrapped in multi-layer insulation. The top of the copper cold-finger is visible at the top of the CF tee. Right: A 3-D model cross-sectional view of the inside of the CF tee containing the copper cold-finger. The cold-tips of the two pulse-tube cryocoolers are coupled by a custom machined copper block, visible at the top of the image, and held firmly against the copper cold-finger extending into the CF tee. The flow of xenon through the condensing hardware is shown by the arrows. When pre-cooled GXe from the heat exchanger enters the CF tee, the high surface area of cold copper threaded rods inside condense the xenon, and the LXe falls down into the detector.
the main body of the vacuum vessel, guiding the newly condensed LXe towards the detector cryostat through a 12” long KF40 metal bellows. The metal bellows extends the vacuum space downwards to the top of the cryostat, and contains two 1/4” OD stainless steel tubes: one which transports the newly condensed LXe into the cryostat as previously described (to the detector’s inlet tube), and another which transports cold GXe out of the cryostat towards the heat exchanger (from the detector’s outlet tube). The vacuum space inside the metal bellows terminates at a feedthrough which transitions the two stainless steel xenon lines from the vacuum space into the detector cryostat (xenon space). Inside the cryostat, the PTFE inlet and outlet tubes are press-fitted onto (around) the stainless steel tubes from the vacuum-space feedthrough. The relative thermal contraction of PTFE and stainless steel at cryogenic temperatures causes the fit strength to increase during cold operation, as the PTFE contracts more than the steel, gripping it more tightly. The KF40 bellows which contains the lines that deliver xenon between the vacuum vessel and cryostat is visible in Fig. 5.11 (left).

5.2.2 Liquid Level Sensor Hardware

The UMass detector contains two liquid level sensors, positioned in the PTFE’s inlet bore and in the weir-spillover channel, which measure the LXe height in the active volume and the bottom of the cryostat, respectively. These sensors were custom designed and fabricated at UMass Amherst. Each level sensor is a hollow cylindrical capacitor whose capacitance increases as the level of LXe inside it increases, due to xenon’s dielectric properties. By measuring the capacitance of the sensor relative to a reference capacitor with a fixed capacitance, positioned outside the detector, a value can be measured which has a one-to-one and isotonic mapping with the liquid level. The absolute liquid level can then be determined from the measured value after a calibration using known liquid levels is performed.
The sensors are read out by custom electronics developed at Oxford by Kathryn Boast and Hans Kraus, for use with the liquid level sensors in LZ. The custom electronics use a multi-stage feedback circuit in which amplifier gains suppress the effect of the cable capacitance from the sensor’s cabling, permitting the readout of the sensor capacitance alone. The details of the custom read-out hardware are described thoroughly in [79]. The value read out by the electronics, \( V \), is approximated by the following equation:

\[
V \approx \frac{C_S - C_R}{C_S + C_R}
\]  

where \( C_S \) is the capacitance of the sensor, and \( C_R \) is the capacitance of the reference capacitor. The reference capacitors for the level sensors at UMass Amherst were chosen to be equal to the room temperature (and empty) \( C_S \) value, such that the measured reference value once installed, \( V \), is approximately equal to zero when no LXe is present in the detector. With the reference capacitor tuned this way, the measured value increases as LXe fills the sensor (going to 1 as \( C_S \) goes to infinity). The mapping between the measured value and corresponding LXe height in the UMass detector was determined by calibration with a known LXe height in the detector, the liquid level set by the weir when full.

Photos from various stages in the construction process of the liquid level sensors are shown in Fig. 5.12. The liquid level sensors were constructed from a 12” long, 1/16” OD, brass rod held inside of a 12” long, 1/4” OD, copper tube. The brass rod and copper tube were prepared separately before being assembled. Using a cut-off wheel attachment on a rotary tool, a narrow slot was cut down the entire length of the copper tube to allow LXe to flow into the side of the sensor once assembled, ensuring that the LXe level inside and outside are always the same. A wire was soldered to one end of the tube before the tube was wrapped with PTFE heat-shrink tubing (leaving the ends open). Pinholes were poked through the shrink tubing at the location of the slot to keep the side of the tubing open without compromising the
Figure 5.12. **Left:** The unmodified 1/16” OD brass rod and 1/4” OD copper tube which make up the capacitive liquid-level sensors in the UMass detector. **Center:** An early prototype of the main level sensor component assembly, connected to the electronics interface for benchtop testing. The two ceramic reference capacitors can be seen soldered to the board above and below where the level sensor is connected. **Right:** The finished liquid-level sensor encased in its stainless steel ground sheath. When installed inside the UMass detector, the wires from the two sensors are fed out of the xenon space via a dedicated ConFlat feedthrough which allows the electronics to remain at room temperature outside of the detector cryostat.
electrical insulation that the PTFE provides. A second wire was soldered to the brass rod before it, too, was enclosed in a layer of PTFE heat-shrink tubing, insulating it from the copper tube in the final construction. Several 1/4” long rings of PTFE heat-shrink tubing were added to each end of the brass rod, increasing the diameter there to be approximately equal to the inner diameter of the copper tube so that when fitted inside the copper tube, the brass rod is held concentric with the tube at its ends. After fitting the brass rod into the insulated copper tube, the entire assembly was inserted into a 3/8” OD braided stainless steel sheath. A wire soldered to the stainless steel sheath was connected to electrical-ground in the final assembly, protecting the sensor from external interference.

5.3 The UMass Xenon Circulation System

The circulation system that continuously purifies the xenon in the UMass LXe detector was designed to include the same major features found in the LZ circulation system. A plumbing and instrumentation diagram (P&ID) of the UMass circulation system is shown in Fig. 5.13. The circulation system consists of a network of 1/4” OD stainless steel tubing which transports xenon out of the detector for purification, and delivers purified xenon into the condenser hardware before it re-enters the detector. The system’s major components are: a pump which drives the flow of xenon through the system, a mass flow controller which controls the speed of xenon circulation, a heated zirconium-getter which purifies the xenon, a xenon storage bottle, and an emergency recovery tank into which the detector xenon can vent to protect the PMTs from high pressure in the event of an over-pressure emergency.

The pump which drives xenon circulation is a metal-bellows diaphragm pump, containing all-metal wetted surfaces. The speed of the pump is controlled with a variable frequency drive which gives coarse control of the xenon circulation flow rate. A check valve connecting the pump’s outlet to its inlet is set to open at a differential
Figure 5.13. The plumbing and instrumentation diagram for the UMass detector’s circulation and purification system. The dashed line indicates the boundary of the physical panel that the hardware is mounted on. The main circulation flow path is indicated in blue. Component’s referenced in this work are shown with an additional label (e.g. PT1, MFC1, CV4, etc.).
pressure of ∼2.8 bar, slightly below the maximum allowable operating pressure for the PMTs, short circuiting the pump when the downstream pressure is high. Fine control and measurement of the circulation flow rate is achieved with a mass-flow controller (MFC) from Teledyne Hastings (HFC-D-302B) [80], located downstream of the pump and controlled by the laboratory computer through the custom GUI described in section 5.5. Typical circulation flow rates for the UMass detector range from 0.8 to 4 standard liters per minute. Downstream of the circulation pump and mass-flow controller, the xenon passes through a heated-zirconium getter (SAES PS4-MT3 [71]) which removes non-noble impurities from the xenon to a concentration below the part-per-billion (ppb) level.

The 4.6 kg of xenon in the UMass detector system was obtained from LZ collaborators at the SLAC National Accelerator Laboratory. The xenon storage bottle on the UMass circulation is a 1 gallon stainless steel sample cylinder which has an all metal face-seal (VCR) fitting welded to its open end, allowing it to be fully helium-leak tight when connected to the circulation system. A regulator near the bottle’s opening sets the pressure of the xenon supplied to the system from the storage bottle. To fill the storage bottle, a separate regulator was connected to the xenon shipping bottle, and a copper tube was used to connect the regulator to the panel’s “Initial Xe Fill Port”, indicated on the P&ID (Fig. 5.13). The xenon was transferred into the storage bottle by creating a cryogenic pump, or cryopump, using liquid nitrogen (LN₂). To perform the cryopumping procedure, a liquid-cryogen dewar was raised around the storage bottle and suspended in place. The dewar was filled with LN₂ such that roughly half of the storage bottle was submerged, lowering the temperature of the storage bottle to the LN₂ vaporization temperature, ∼77 K. As xenon was introduced slowly into the storage bottle through the shipping bottle regulator and circulation system plumbing (bypassing the storage bottle regulator), it immediately cooled to well below its freezing temperature, forming xenon ice inside the bottle.
and lowering the bottle pressure, causing additional xenon to continuously flow in. This cryopumping procedure for the xenon storage bottle can pump xenon at a rate of several standard liters per minute, and is also used to evacuate xenon from the detector between runs.

The two PMTs in the UMass detector are the most pressure sensitive components of the entire detector system, with a pressure rating of 5 atmospheres (5.07 bar). In the event of an equipment failure or power outage it is possible for the detector’s LXe to warm up unexpectedly due to a loss of cooling power or change in circulation dynamics, increasing the pressure inside the detector to a pressure well above the rating of the PMTs. Though several mitigation measures are in place to prevent such an event, including an automated alert system from the sensor GUI and a battery backup for critical equipment, an emergency recovery vessel acts as a fail-safe for detector. To protect the PMTs from this failure mode, an evacuated 28.6 gallon steel propane cylinder, the emergency recovery vessel, is connected to the circulation system, separated by a rupture disc which is engineered to break at a differential pressure of 46.8 psi (3.23 bar). The steel vessel has a metal face-seal (VCR) fitting welded to its opening, creating a connection with the circulation system plumbing which is helium-leak tight to the room air when connected. The vessel is maintained at vacuum so that if the rupture disc breaks, allowing xenon into it, the ~1 kg of xenon from the detector is contained at a safe (for the PMTs) pressure of ~2.0 bar. The xenon can then be cryopumped back into the storage bottle through the circulation system, and the rupture disc replaced. The pressure inside the emergency recovery vessel is monitored with a dedicated pressure transducer. At the time of writing, the emergency recovery vessel system has been exercised once in the lifetime of the UMass detector system, following a power outage in the lab. The rupture disc broke at the engineered differential pressure, filling the emergency recovery vessel and successfully protecting the PMTs from damage.
5.4 Prototype Source Injection System

The prototype source injection system (SIS) at UMass Amherst was designed to precisely measure and inject calibration radioisotopes from the flow-through generator and bottle source hardware detailed in section 5.1, in preparation of commissioning the LZ TPC. The design accommodates four flow-through source generators and two source bottles, though only two flow-through bays were fully commissioned for testing with the UMass detector. A plumbing and instrumentation diagram (P&ID) of the prototype SIS is shown in Fig. 5.14. Injections of radioisotopes are achieved by flowing xenon from the circulation system’s xenon storage bottle through the SIS, carrying the calibration isotopes with it into the circulation system’s main flow path.
Figure 5.15. The prototype source injection system at UMass Amherst, with the major flow paths labeled. The prototype was designed and constructed at UMass Amherst to develop and practice the procedures for injecting precise quantities of calibration radioisotopes into LXe, in preparation of commissioning the LZ TPC.

upstream of the getter (which can be bypassed for the methane-based bottle sources). The flow of xenon through the SIS’s stainless steel tubing is precisely controlled by 21 pneumatically actuated valves and two mass-flow controllers, and is monitored by three pressure transducers, all of which interface with the laboratory computer’s custom GUI, described in section 5.5. The fully constructed prototype SIS at UMass Amherst is shown in Fig. 5.15.

The pneumatically actuated solenoid valves on the prototype SIS are controlled using custom electronics assembled by Anthony Raykh at UMass Amherst, based on the design from [81]. The electronics open and close solenoids which allow compressed air into 1/8” OD polyurethane tubing connected to the pneumatic pressure ports on
the valves, opening or closing them. The pressure transducers and mass-flow controllers interface with the laboratory computer through two LabJack T4 [82] analog I/O devices.

The mass-flow controllers (labelled in Fig. 5.14 as) MFC2 and MFC3 have full-scale mass-flow rates of 250 and 50 SCCM (standard cubic centimeters per minute), respectively. The MFCs have the ability to control flow rates as low as 1% of their full-scales. MFC3, with its smaller full-scale and therefore greater ability to measure small quantities of gas precisely, controls the flow of Gxe out of the flow-through generators, simultaneously controlling and measuring the calibration-isotope dose which is subsequently flushed into the detector. MFC2 is used to control Gxe flow during the 'flush' step of the injection procedures, where Gxe is flowed through the dose volume of the SIS (bypassing the generators) and into the circulation system to flush residual calibration isotopes out of the plumbing, a procedure during which precision flow control is not required. The mass-flow controllers can be controlled from the laboratory computer, or with the integrated touchscreen on each unit.

The methane based source injection procedures use several dedicated hardware components not used during the flow-through generator injection procedures. First, a passive methane purifier (SAES MC1 [71]) removes organic impurities from the methane calibration gas on its way from source bottle to dose volume. The gas then encounters a high-impedance flow restrictor, which allows a small flow-rate (2 SCCM at 35 psid with vacuum downstream) into the closed dose volume. As the pressure slowly builds in the dose volume, it is monitored by the high precision capacitance manometer, (labelled in Fig. 5.14 as) CM2, until the desired dose is achieved. The source bottle is closed, and the dose volume is isolated, stopping flow into it. Then xenon from the circulation system storage bottle flows through MFC2 and flushes the calibration gas out of the dose volume and into the circulation system completing the source injection. The specific details of the injection procedures are unique to
each calibration source, and are therefore described independently for $^{83m}$Kr, $^{131m}$Xe, $^{220}$Rn, and the methane based sources in the following sections. The precision of the activity injected by the injection procedures is improved by controlling the initial conditions of the panel at the start of each procedure. In particular, unless otherwise noted, the panel’s initial state is such that all volumes are filled with xenon at or above the pressure in the circulation system at the location of the injection panel outlet.

5.4.1 $^{83m}$Kr Injection Procedure

In the $^{83m}$Kr injection procedure, the $^{83m}$Kr contained in the flow-through generator starts in a state of secular equilibrium with the $^{83}$Rb inside as a result of being closed for at least $\sim$10 hours prior. GXe from the circulation system’s xenon storage bottle is flowed through the $^{83m}$Kr generator, moving the desired fraction of the total $^{83m}$Kr activity into the dose volume (refer to Fig. 5.15). The flow rate into the generator plumbing is controlled by MFC2 (refer to Fig. 5.14), and the flow rate out of the generator plumbing and into the dose volume is controlled by MFC3. When the volume of gas corresponding to the desired dose has flowed through MFC3, the generator plumbing is promptly closed, and GXe from the xenon storage bottle is flowed through the dose volume to flush the dose of calibration isotopes into the circulation system. The exact steps of the procedure are presented below as a list of human-readable steps, describing the exact valve and MFC operations which perform this (automated) injection procedure, with reference to the instrument names displayed in Fig. 5.14. The $^{83m}$Kr generator is located in the generator bay enclosed by pneumatic valves IV8 and IV5 when it is used.

$^{83m}$Kr Injection Procedure:
• Close all pneumatic valves, and set all mass-flow controllers to zero to create a standardized initial state.

• Ensure that IV23, CV4, and the manual valves on the generator are open.

• Set the MFC2 & MFC3 setpoints to 0 SCCM.

• In the listed order, open CV5, IV22, IV21, IV16, IV15, IV8, IV1, IV5.

• Set the MFC2 setpoint to 50 SCCM to begin allowing xenon into the generator.

• Set the MFC3 setpoint to 20 SCCM to begin allowing the carrier xenon and calibration radioisotopes to flow out of the generator and into the dose volume.

• Wait the amount of time corresponding to the desired dose activity (calibrated from past results, detailed in section 5.7), then promptly close valve IV15.

• Set the MFC2 setpoint to 0 SCCM, and close valves IV5 and IV8.

• Set the MFC3 setpoint to 0 SCCM.

• Open valve IV6.

• Set the MFC2 setpoint to 50 SCCM to allow xenon from the storage bottle to begin flushing the calibration gas in the dose volume into the circulation system.

• After 120 seconds, close all pneumatic valves.

• Set the MFC2 setpoint to 0 SCCM.

5.4.2 $^{131m}$Xe Injection Procedure

Due to the very short (8.0 d) half-life of the $^{131}$I parent, the $^{131m}$Xe generator activity is typically orders of magnitude higher than the intended injection activity. For this reason, the $^{131m}$Xe injection procedure begins by pumping out the contents of the generator. Once the pumping on the generator has stopped, the $^{131m}$Xe generator is pressurized to 2 bara with xenon, closed, and the $^{131m}$Xe activity begins building up. After the desired dose activity has built up (anywhere from 10 minutes to 1 week), GXe from the circulation system’s xenon storage bottle is flowed through the $^{131m}$Xe generator, moving the full generator contents into the dose volume (refer to Fig. 5.15).
Flow into the generator plumbing is controlled by MFC2 (refer to Fig. 5.14), and the flow rate out of the generator plumbing and into the dose volume is controlled by MFC3. When the full generator volume has flowed through MFC3 several times, the generator plumbing is closed, and GXe from the xenon storage bottle is flowed through the dose volume to flush the dose of calibration isotopes into the circulation system. The exact steps of the procedure are presented below as a list of human-readable steps, describing the exact valve and MFC operations which perform this injection procedure, with reference to the instrument names displayed in Fig. 5.14. The $^{131m}$Xe generator is located in the generator bay enclosed by pneumatic valves IV7 and IV4 when it is used.

$^{131m}$Xe Injection Procedure:

- Close all pneumatic valves, and set all mass-flow controllers to zero to create a standardized initial state.
- Ensure that IV23, CV4, and the manual valves on the generator are open.
- Set the MFC2 & MFC3 setpoints to 0 SCCM.
- In the listed order, open CV5, IV22, IV21, IV16, IV15, IV9, IV7, IV1, IV4.
- Set the MFC2 setpoint to 125 SCCM to begin allowing xenon into the generator.
- Set the MFC3 setpoint to 50 SCCM to begin allowing the carrier xenon and calibration radioisotopes to flow out of the generator and into the dose volume.
- Wait 2 minutes for the xenon flow through the generator to move all of the generator contents into the dose volume, and close valve IV15.
- Set the MFC2 setpoint to 0 SCCM, and close valves IV4, IV9, and IV7.
- Set the MFC3 setpoint to 0 SCCM.
- Open valve IV6.
- Set the MFC2 setpoint to 50 SCCM to allow xenon from the storage bottle to begin flushing the calibration gas in the dose volume into the circulation system.
• After 120 seconds, close all pneumatic valves.
• Set the MFC2 setpoint to 0 SCCM.

5.4.3 $^{220}$Rn Injection Procedure

Due to the very short (56 sec) half-life of $^{220}$Rn, some fraction of the injected $^{220}$Rn decays on its way out of the injection panel, and any injected activity becomes undetectable after 10 minutes. To achieve a constant $^{220}$Rn activity in the detector for an extended period of time, xenon from the storage bottle is flowed continuously through the $^{220}$Rn generator and into the circulation system. The flow rate of the carrier xenon determines the transit time to the circulation system, and therefore the fraction of $^{220}$Rn which survives to the detector. The activity of $^{220}$Rn in the detector is thus controlled by adjusting the flow rate through the $^{220}$Rn generator, and because the useful flow rates are relatively large, MFC3 (refer to Fig. 5.14) is bypassed. Flow through the generator plumbing is controlled by MFC2. Once the injection is stopped, the residual $^{220}$Rn in the panel quickly decays away and doesn’t require a flush step. The exact steps of the procedure are presented below as a list of human-readable steps, describing the exact valve, and MFC operations which perform this injection procedure, with reference to the instrument names displayed in Fig. 5.14. The $^{220}$Rn generator is located in the generator bay enclosed by pneumatic valves IV7 and IV4 when it is used.

$^{220}$Rn Injection Procedure:

• Close all pneumatic valves, and set all mass-flow controllers to zero to create a standardized initial state.
• Ensure that IV23, CV4, and the manual valves on the generator are open.
• Set the MFC2 & MFC3 setpoints to 0 SCCM.
• In the listed order, open CV5, IV22, IV21, IV14, IV13, IV7, IV1, IV4.
- Set the MFC2 setpoint to the flow rate corresponding to the desired survival fraction of $^{220}$Rn (see section 5.9) to begin allowing the carrier xenon and calibration radioisotopes to flow out of the generator and into the circulation system.
- Wait desired flow time, then close all pneumatic valves.
- Set the MFC2 setpoint to 0 SCCM.

5.4.4 CH$_4$, CH$_3$T, and $^{14}$CH$_4$ Injection Procedure

The injection of the methane based sources is performed by measuring the calibration dose in the closed dose volume, and then subsequently flushing it into the circulation system. First, the dose volume is pumped out to vacuum. The bottle containing the calibration gas is opened, exposing it to the methane purifier, and the path into the dose volume is opened, beginning the flow of the calibration gas into the large (dose) volume contained between valves IV21 and IV6. The flow-restrictor allows the pressure in the dose volume to be carefully monitored by CM2 as it builds up very slowly, until the desired calibration dose is achieved. The pressure of the desired dose is calculated from the concentration of the methane mixture in the bottle. The exact steps of the procedure are presented below as a list of human-readable steps, describing the exact valve, and MFC operations which perform this injection procedure, with reference to the instrument names displayed in Fig. 5.14.

CH$_4$, CH$_3$T, and $^{14}$CH$_4$ Injection Procedure:

- Pump-out the SIS to a pressure below 1x10$^{-5}$ mBar to prepare for the methane dosing.
- Close all pneumatic valves, and set all mass-flow controllers to zero to create a standardized initial state.
- Open the getter bypass valve (the getter has integrated valves which can be used to close and bypass the purification plumbing).
• Open the manual valve on the source bottle and ensure that IV23 and CV4 are open.

• In the listed order, open IV19, IV20, and IV16 to begin flowing into the dose volume through the flow restrictor.

• When the pressure in the dose volume, read off of CM2, indicates the desired quantity of calibration gas has accumulated there, promptly close IV20 and IV19.

• Close the manual valve on the source bottle.

• Open valves IV1, IV21, IV22, and CV5.

• Set the MFC2 setpoint to 50 SCCM.

• Once the pressure downstream of MFC2 has increased such that the MFC2 setpoint flow can no longer be achieved, open IV6 to begin flushing the calibration gas into the circulation system.

• After 120 seconds, close all pneumatic valves.

• Return the getter to active purification mode, (closing the bypass valve).

5.5 The UMass Detector System GUI

Many instruments on the UMass LXe detector system are monitored or controlled using a custom graphical user interface (GUI) which was co-developed by Anthony Raykh, using the Tkinter library in Python. The pressure transducers, liquid-level and temperature sensors, mass-flow controllers, and pneumatic valves are all integrated into the GUI, allowing for fully automated procedures, alarm notifications, and real-time plotting.

Twenty-two pneumatically actuated valves are controllable via a dedicated valve-interface screen of the GUI, pictured in Fig. 5.16. In addition to individual control of each valve, a "close all" button changes the state of all valves to closed, simultaneously, and changes the setpoints of the mass-flow controllers to zero, closing them as well.
Figure 5.16. The valve control screen of the UMass LXe detector system’s GUI. The buttons controlling the state of the pneumatically-actuated valves are overlaid onto an image of the prototype Source Injection System P&ID, with each button positioned at the location of the valve that represents it in the diagram. A ”Close All” button simultaneously closes all of the pneumatic valves controlled by the interface, and changes the mass-flow controller setpoints to zero.
The main screen of the UMass LXe detector system GUI is pictured in Fig. 5.17. The main screen displays the read-out from all of the digital sensors in the UMass detector system as live-updating plots, with adjustable time ranges to display data as far back as desired. In addition to the real-time plots, the most recent sampled value of each sensor is displayed separately in dedicated display boxes. Input fields allow the user to send setpoint change commands to the three mass-flow controllers on the circulation and injection systems, to change the display parameters of the live plots, and to set alarm thresholds on the detector pressure. If an alarm threshold is crossed, the GUI automatically sends an SMS (text) message and email to the user with details of the specific alarm that was triggered. Alarms on the detector pressure have changeable thresholds in the GUI, while alarms on the emergency recovery vessel and insulating vacuum vessel pressures are hardcoded to trigger if either measured pressure deviates significantly from vacuum, indicating a hardware issue.

Six input fields allow the user to set the parameters of the automated flow-through-generator source injection procedures, described in section 5.4. The procedures are initiated by two additional buttons, also on the main GUI screen. Automating the procedures with tunable parameters contributes to both ease of use, and high precision of the achieved dose. The adjustable control parameters for the injection procedures are: 1.) The GXe mass-flow rate through the generator. 2.) The amount of time GXe is flowed through the generator. 3.) The GXe mass-flow rate through the flush path (refer to Fig. 5.15) of the panel (to move residual activity into circulation). 4.) The amount of time GXe is flowed through the flush path. 5.) The number which is multiplied by the MFC3 setpoint to give the setpoint for MFC2 during dosing (The MFC2 setpoint is set higher than the MFC3 setpoint to allow the generator to gradually pressurize during the injection procedure, necessary for precision because of the high impedance of the generator filters). 6.) The amount of time between setting
Figure 5.17. The main screen of the UMass LXe detector system’s GUI. All of the sensors are read out in fully customizable live-updating plots, and dedicated buttons set plot and injection procedure parameters in addition to executing the automated injection procedures carried out by the source injection system. The most recent value measured from each sensor is displayed in the array of text-boxes in the top right.
MFC2 and MFC3 in the injection procedure (a 1-2 second delay allows pressure to build briefly in the generator, resulting in a more constant flow through MFC3).

5.6 Data Acquisition

The two PMTs in the UMass LXe detector are read out by a SkuTek DDC-10 [83]. The DDC-10 is a Field-Programable Gate Array (FPGA) based ten-channel digitizer, featuring Embedded Linux, that constitutes a complete Data Acquisition system (DAQ). The DDC-10 interfaces with a computer running Scientific Linux 7 via ethernet, and is fully programmable there. The two PMTs are biased with a bench-top high voltage power supply at a voltage that depends on the energy of the decay being studied, typically between 700-1250 Volts. During data-taking, when the PMT signal voltage in either channel exceeds a programmed threshold and rate-of-rise setting on the DDC-10, a 1 $\mu$s window containing the signal-voltage waveforms from both PMTs are recorded as an event. The trigger threshold for the PMTs are set independently based on each PMT’s respective gain, so that their signal amplitudes are approximately equal when exposed to the same number of photons. The 1 $\mu$s event window is recorded as 100 bins, each with 10 ns width, and with the trigger positioned at the 25$^{th}$ bin in the event window.

Unlike in LZ, no applied electric is field present in the UMass LXe detector. The PMTs are therefore sensitive only to the scintillation light (S1) produced after a scattering event in the LXe. The secondary scintillation signal (S2), produced by drifting ionized electrons through GXe with an applied electric field, is not necessary to achieve the primary goal of the UMass LXe detector: measuring activities of injected calibration isotopes.

To increase sensitivity to small changes in event rate (small injected activities), the background rate of the detector is reduced by surrounding the detector cryostat on its sides and bottom with lead bricks, shielding it from external particles and
radiation. For PMT voltage and trigger settings that result in a sensitivity threshold of $\sim 10$ keV, the addition of lead shielding was found to reduce the background event rate by roughly a factor of five, down to $\sim 20$ Hz. The lead surrounded cryostat is pictured in Fig. 5.18, where the DDC-10 and high-voltage power supply can also be seen resting on the detector frame and on the shelf inside of the frame, respectively.

5.6.1 Dead Time Correction

When the signal voltage on one of the detector PMTs crosses the set trigger threshold, a 1 $\mu$s event window is recorded. While event information is being saved to disk following a trigger (before the trigger is rearmed by the FPGA) new events in the detector are not recorded. Time when the trigger is unarmed and new events cannot be recorded is called "dead time". The 1 $\mu$s event window is also part of the dead time because during the event window no new triggers can be accepted. Time when the FPGA trigger is armed and prepared to record a new event is called "live time". For each new event, the DDC-10 records the total dead time and live time since the previous event.

When the event rate in the detector becomes high, the amount of dead time can become large enough that a significant fraction of events in the detector fall within dead-time periods and are not recorded. Large event rates in the UMass LXe detector are produced by large injections of radioisotopes, whose decays are Poisson distributed in time. A measurement of the event rate can therefore be corrected, accounting for the events lost during the dead time, by multiplying by a correction factor. For a given time interval with dead time, $d$, and live time, $l$, the true (corrected) event rate, $\lambda_c$, is given by:

$$\lambda_c = \frac{\lambda_m}{1 - \frac{d}{d+l}} = \frac{\lambda_m}{1 - D_F}$$

(5.2)

where $\lambda_m$ is the measured rate of the DAQ, and $D_F$ is the fraction of the time interval which is dead time.
Figure 5.18. A photo of the fully shielded UMass LXe detector. Lead bricks surrounding the detector cryostat are stacked to a height above the LXe level, on top of a cinder block foundation below the cryostat. The DDC-10 rests on a platform at the top left of the aluminum frame from which the detector cryostat is suspended. Directly below the DDC-10, on top of the shelf inside of the detector frame, the high-voltage power supply which biases the PMTs is pictured supplying 1250 volts to the PMTs. Three AC power supplies which provide variable AC voltage to the pulse-tube cryocoolers (one power supply for each, and a spare) are pictured at the bottom left.
Figure 5.19. Example waveforms from the two PMTs in the UMass LXe detector. 
**Top:** Example waveforms from a single scatter interaction in the detector’s LXe. 
**Bottom:** Example waveforms from a two-scatter event in the detector’s LXe, likely an $^{83m}$Kr decay.

### 5.6.2 Pulse Finder and Reduced Quantities

The pulse finder for the UMass LXe detector’s PMT signal data was developed to identify and characterize pulses in the raw PMT waveforms to provide a set of useful reduced quantities from each event for analysis. The pulse-finding algorithm was specifically designed to identify up to two pulses in a given event, to be maximally useful for studying the two-step $^{83m}$Kr decay. Example waveforms from the two PMTs in the UMass detector are shown in Fig. 5.19. The basic method used by the pulse finder is to search for the maximum sample in the waveform, which typically corresponds to the triggering pulse. Next, the algorithm defines the edges of the
pulse (in time) relative to its peak using hard coded (asymmetric) offsets which were determined by hand-scanning waveforms to identify the values that encompass the full pulse in the highest energy events. The pulse finder then scans the pulse between the defined edges to determine at which sample (in time) the waveform of the pulse-integral exceeds 10% and 90% of its total area. The time between the 10% area sample and the 90% area sample is used to define a pulse width parameter. After a few other characteristics of the first pulse are measured, the algorithm looks for a second pulse in the fraction of the event window after the end of the first pulse. There, a second maximum sample is found and defines the peak of a second pulse. The algorithm proceeds to calculate characteristics of the second pulse the same way it did for the first pulse. If no true second pulse exists in the event window, the second-pulse area will be extremely small, and can easily be removed with a data quality cut, or ignored in an analysis.

The pulse-finding algorithm code, written in Python, is presented in full in Appendix B. The reduced quantities which are calculated by the pulse-finding algorithm from the raw PMT-signal waveforms are listed and described below, named as they appear in the code:

- **baseline_0, baseline_1**: The mean value of the first 15 samples in the event window (before the trigger) from the top and bottom PMT waveforms, respectively.

- **bl_stddev_0, bl_stddev_1**: The standard deviation of the first 15 samples in the event window (before the trigger) from the top and bottom PMT waveforms, respectively.

- **amp_0a, amp_0b**: The amplitudes of first and second pulse, respectively, in the top PMT waveform.

- **amp_1a, amp_1b**: The amplitudes of the first and second pulse, respectively, in the bottom PMT waveform.
• **amp\_Sa, amp\_Sb**: The amplitudes of the first and second pulse, respectively, in the summed top and bottom PMT waveforms.

• **area\_0a, area\_0b**: The areas under the first and second pulse, respectively, in the top PMT waveform.

• **area\_1a, area\_1b**: The areas under the first and second pulse, respectively, in the bottom PMT waveform.

• **area\_Sa, area\_Sb**: The areas under the first and second pulse, respectively, in the summed top and bottom PMT waveforms.

• **indx\_0a, indx\_0b**: Sample number where the maximum amplitude occurs in the first and second pulse, respectively, in the top PMT waveform.

• **indx\_1a, indx\_1b**: Sample number where the maximum amplitude occurs in the first and second pulse, respectively, in the bottom PMT waveform.

• **indx\_Sa, indx\_Sb**: Sample number where the maximum amplitude occurs in the first and second pulse, respectively, in the summed top and bottom PMT waveforms.

• **separation\_0, separation\_1, separation\_S**: The number of samples between the peaks of the first and second pulses in the top, bottom, and summed PMT waveforms, respectively.

• **tba**: The top-bottom light-collection asymmetry, a proxy for Z position in the detector. This is defined as:

\[
\frac{\text{area\_0a} - \text{area\_1a}}{\text{area\_0a} + \text{area\_1a}} \quad (5.3)
\]

• **pre\_peak\_frac\_0a, post\_peak\_frac\_0a**: Fraction of total pulse area located before and after the peak, respectively, in the top PMT waveform.

• **pre\_peak\_frac\_1a, post\_peak\_frac\_1a**: Fraction of total pulse area located before and after the peak, respectively, in the bottom PMT waveform.
• **pre_peak_frac_Sa, post_peak_frac_Sa**: Fraction of total pulse area located before and after the peak, respectively, in the summed top and bottom PMT waveform.

• **pulse_width_0a, pulse_width_1a, pulse_width_Sa**: The number of 10 ns samples between where the pulse reaches 10% of its total area and 90% of its total area in the top and bottom PMT waveforms, respectively.

### 5.7 $^{83m}$Kr Injection Results from the UMass Detector

$^{83m}$Kr injection data from the UMass LXe detector was taken with a PMT bias voltage of 1250 V. At the time of writing, a total of five $^{83m}$Kr generators have been used to perform injections into the UMass LXe detector with the prototype SIS. The first three generators used Shirasagi G2x4/6 Pelletized charcoal [60], and the final two, including the first $^{83m}$Kr generator for LZ, used the coconut-based Calgon OVC 4x8 granular activated carbon [59] to hold the parent $^{83}$Rb. When $^{83m}$Kr is injected into the UMass LXe detector following the procedure in section 5.4.1, it appears as two bright bands, 33 and 42 (33+9) keV, in a histogram of bottom-PMT versus top-PMT pulse area for the first pulse of the events in the data set (see section 4.1.1 for details on the $^{83m}$Kr decay). An example is shown in Fig. 5.20 (upper left). Though carefully selecting the $^{83m}$Kr events is not required to measure the activity injected, the simple cut shown in Fig. 5.20 (upper right) was performed to increase the ratio of $^{83m}$Kr to background events, extending the time window in which an exponential can be fit to the decaying event rate following an injection. Also shown in Fig. 5.20 are histograms of the first-pulse versus second-pulse area for the events in the data set.

Early $^{83m}$Kr injections into the UMass LXe detector revealed a possible limitation of the system’s hardware: only a tiny fraction of the injected $^{83m}$Kr activity was reaching and dissolving into the bulk LXe. Further, the constant circulation of xenon
Figure 5.20. Histograms of data taken by the UMass LXe detector following the injection of $^{83m}$Kr. **Upper Left:** A histogram of the logarithm of the pulse area in the bottom PMT vs. the top PMT for the first pulse in the events. In this parameter space, mono-energetic decays form populations along lines of anti-correlation, with their precise location along those lines depending on the position of the event in the detector. When the two decays of $^{83m}$Kr appear as separate pulses in the event window, the first (33 keV) decay populates this plot. When the two decays occur close together in time and are merged into one (33+9 keV) pulse, a second, 42 keV, population is formed. **Upper Right:** A simple cut selecting $^{83m}$Kr events is applied to the events in the histogram in the top left. Reducing the rate of background with this selection cut allows for a larger useful time range in which the decaying $^{83m}$Kr event rate in the detector can be fitted (appears above background). **Lower Left:** The first-pulse vs. second-pulse areas for the summed top and bottom PMT waveforms. **Lower Right:** The first-pulse vs. second-pulse areas for the summed top and bottom PMT waveforms with the $^{83m}$Kr selection cut (from the top right histogram) applied. The events where the two decays from the $^{83m}$Kr event are merged appear as a separate population than those where the decay is separable.
removal of $^{83\text{m}}$Kr from the bulk LXe through the outlet at a faster rate than $^{83\text{m}}$Kr was being introduced into the LXe at the detector's inlet. An example of a $^{83\text{m}}$Kr-injection data set during which this issue was observed is shown in Fig. 5.21. The issue was found to be resolved by increasing the circulation flow rate from 1.5 SLPM to $\sim 3$ SLPM. We speculate that the issue is caused by $^{83\text{m}}$Kr dissolving into LXe trapped in the condenser hardware's ConFlat tee (see section 5.2.1). At higher flow rates, trapped LXe in the condenser tee is either pushed into the detector or evaporated, where it then re-condenses inside the detector cryostat or is bubbled through the bulk LXe at the end of the inlet tube as cold GXe. A histogram showing the event rate during a high-circulation-speed $^{83\text{m}}$Kr-injection data set is shown in Fig. 5.22.

The way that the injected activity following a $^{83\text{m}}$Kr injection is measured (also demonstrated in Fig. 5.22) is as follows: First the location (in time) of the rising edge produced in the event rate by the injected activity is identified by searching for where the data first exceeds a pre-determined rate-of-rise threshold. The background rate
Figure 5.22. A histogram showing the event rate in UMass-LXe-detector data containing an injection of $^{83m}$Kr, during which the circulation flow rate was set to 3.0 SLPM. The rate of $^{83m}$Kr events observed by the PMTs decays with the expected half-life. The injected activity is calculated by extrapolating the exponential fit shown in blue (with the decay constant as a free parameter) backwards in time to the beginning of the injection, indicated by the grey line on the rising edge of the injected $^{83m}$Kr event rate. The $^{83m}$Kr rate from before the start of the rising edge is subtracted from the extrapolated peak value to determine the measured injected activity. With reference to the quantities shown in the figure, the Injected Activity is equal to the Free Decay Amp minus the Background Kr$^{83m}$ Rate. A second exponential fit is also performed with the $^{83m}$Kr half life fixed, and the residuals from both exponential fits are shown in the bottom plot.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Background Bin</td>
<td>127.8 min</td>
</tr>
<tr>
<td>Injection Start</td>
<td>137.8 min</td>
</tr>
<tr>
<td>Fixed Decay Amp</td>
<td>677.65 +/- 3.06 Bq</td>
</tr>
<tr>
<td>Free Decay Amp</td>
<td>692.72 +/- 10.76 Bq</td>
</tr>
<tr>
<td>Free Decay Tau</td>
<td>153.03 +/- 0.6 min (Half-life = 106.1 +/- 0.4 min)</td>
</tr>
<tr>
<td>Peak Measured Activity</td>
<td>687.88 +/- 1.95 Bq</td>
</tr>
<tr>
<td>Background Kr$^{83m}$ Rate</td>
<td>2.0 +/- 0.11 Bq</td>
</tr>
<tr>
<td>Injected Activity</td>
<td>699.72 +/- 10.76 Bq</td>
</tr>
</tbody>
</table>
in the detector immediately before the time of the rising edge is recorded. A time range following the injection is then chosen for fitting an exponential to the decaying event rate, typically several hours (and longer than the $^{83\text{m}}\text{Kr}$ half life). The fit range begins at least 30 minutes after the time of the rising edge to allow sufficient time for the $^{83\text{m}}\text{Kr}$ to mix into the detector’s LXe and become homogenous. The exponential fit is performed two ways: with the half-life as a free parameter and with the half life fixed to the $^{83\text{m}}\text{Kr}$ half life. Comparing the two fits allows us to look for evidence of trapping or systematic removal of $^{83\text{m}}\text{Kr}$, like what was previously observed at low circulation flow rates. Provided the fits are in relative agreement, the fit with the half-life as a free parameter is used to infer the total $^{83\text{m}}\text{Kr}$ activity present in the detector immediately following the injection, by extrapolating the fit backwards to the time of the rising edge. The injected activity is then measured by subtracting the recorded background rate from the inferred total $^{83\text{m}}\text{Kr}$ rate. The fraction of the total xenon in the detector that is active (visible by the PMTs) is used to scale the measured rates when the results are analyzed.

The injection campaign for the first $^{83\text{m}}\text{Kr}$ source was performed prior to the inclusion of the dead time correction in the data analysis chain (see section 5.6.1), so the measured injected activities suffered from systematic error, affecting the largest injected activities the most. Though these results are not useful for estimating injected activities from future sources, they provided the first demonstration of the level of precision which can be achieved with the prototype source injection system. The results from injections with the first $^{83\text{m}}\text{Kr}$ source are shown in Fig. 5.23. After implementing the dead time correction in the analysis of $^{83\text{m}}\text{Kr}$ injection data, the emanation efficiency of $^{83\text{m}}\text{Kr}$ from the $^{83}\text{Rb}$-doped charcoal (Shirasagi G2x4/6) was found to be approximately 13%.

Calgon OVC 4x8 charcoal was obtained to measure whether its $^{83\text{m}}\text{Kr}$ emanation efficiency would be significantly different from the Shirasagi G2x4/6 $^{83\text{m}}\text{Kr}$ emanation
Figure 5.23. A plot of the results from $^{83m}$Kr injections into the UMass LXe detector with the prototype SIS, from the first $^{83m}$Kr source. The measured activities shown have large systematic errors from not accounting for the DAQ’s dead time in this data (see section 5.6.1). This error particularly affects the highest activity injections by suppressing the measured rate proportionally to the real rate. Despite the rate suppression, these results demonstrate the ability to precisely control the injected $^{83m}$Kr activity across more than 3 orders of magnitude, thus also demonstrating the success of the prototype SIS hardware.
efficiency. Calgon OVC 4x8 was specifically chosen because of its history of use in LUX, and much lower surface area than that of the Shirasagi G2x4/6. A generator (the first LZ $^{83m}$Kr generator) was produced with $^{83}$Rb bound to Calgon OVC 4x8 charcoal, and injections were performed across the full range of control demonstrated (in Fig. 5.23) with the first source. The complete results from the Calgon-charcoal $^{83m}$Kr source are shown in Fig. 5.24. A comparison of the maximum possible injected activity with the Calgon-charcoal $^{83m}$Kr source and a Shirasagi-charcoal source is shown in Fig. 5.25.

A continuous-flow injection was also demonstrated using the first LZ $^{83m}$Kr source in the UMass LXe detector with the prototype SIS. In this injection, GXe from the xenon storage bottle was flowed continuously through the $^{83m}$Kr generator, at a small flow rate ($\sim$1 SCCM) such that a significant fraction of the $^{83m}$Kr produced by the generator decayed on its way to the circulation system. Injecting this way, a constant activity of $^{83m}$Kr can be maintained in the detector for as long as the system can supply the flow through the generator. The results of the injection performed this way with the prototype SIS into the UMass LXe detector are shown in Fig. 5.26.

### 5.8 $^{131m}$Xe Injection Results from the UMass Detector

$^{131m}$Xe injection data in the UMass LXe detector was taken with a PMT bias voltage of 1250 V. When $^{131m}$Xe is injected into the UMass LXe detector following the procedure in section 5.4.2, it appears as a single bright band (164 keV) in a histogram of bottom-PMT versus top-PMT pulse area for the first pulse from the events in the data set. An example histogram is shown in Fig. 5.27, as well as a cut selecting the $^{131m}$Xe population. This selection cut reduces the background rate and random error in the measurements of the injected $^{131m}$Xe activity.

The way that the injected activity following a $^{131m}$Xe injection is measured (also demonstrated in Fig. 5.28) is as follows: First, the start time of the injection proce-
Figure 5.24. A plot of the results from injections performed with the prototype SIS into the UMass LXe detector with the first $^{83m}$Kr source produced using Calgon OVC 4x8 charcoal (also the first $^{83m}$Kr source used in LZ). Injected activities with the source spanned 3 orders of magnitude, and saw a maximum injectable activity of $\sim$10% of the parent $^{83}$Rb activity (equal to an emanation fraction of 0.13 for a $^{83}$Rb branching fraction to $^{83m}$Kr of 0.78).
Figure 5.25. A plot of the results from $^{83m}$Kr injections performed with the prototype SIS into the UMass LXe detector. Injections with $^{83m}$Kr sources containing Shirasagi G2x4/6 Pelletized charcoal [60] are shown in purple, and Calgon OVC 4x8 charcoal [59] are shown in blue. The two charcoals showed comparable $^{83m}$Kr emanation efficiencies. The observed systematic difference in injected activity between the sources is possibly due to a $\sim 2.0$ K temperature difference in the LXe between these data sets, or to minor differences in the detector hardware between the data sets.

Figure 5.26. A histogram showing the event rate in UMass-LXe-detector data taken during a continuous injection of $^{83m}$Kr. The flow rate of GXe through the $^{83m}$Kr generator during the injection was $\sim 1$ SCCM. Injecting $^{83m}$Kr slowly and continuously allows a constant $^{83m}$Kr activity to be maintained in the detector for extended periods of time despite the relatively short $^{83m}$Kr half life.
Figure 5.27. Histograms of data taken by the UMass LXe detector following the injection of $^{131m}$Xe. **Left:** A histogram of the logarithm of the pulse area in the bottom PMT vs. the top PMT for the first pulse in the events. In this parameter space, mono-energetic decays form populations along lines of anti-correlation, with their precise location along those lines depending on the position of the event in the detector. **Right:** A simple cut selecting $^{131m}$Xe events is applied to the events in the histogram on the left. This cut reduces the background rate and random error in the measurement of the injected activity.
Figure 5.28. A histogram showing the rate of events passing the $^{131m}$Xe selection cut in the UMass LXe detector following an injection of $^{131m}$Xe. The injected activity is calculated by subtracting the average rate before the start of the injection from the average rate, after some amount of "mixing time", following the injection. The time when the injection procedure was started is shown by the vertical grey line, and the time periods over which the background rate and total rate following the injection were measured are shown by the horizontal black lines, positioned at a height corresponding to the average rate that they measured.

dure is input by the user. A time window before the start of the injection is selected, typically 300 minutes, and the average event rate for the events passing the $^{131m}$Xe selection cut in the time window is measured to determine the background rate at the time of the injection. A time window after the start of the injection is selected, typically 300 minutes, and the average event rate for events passing the $^{131m}$Xe selection cut is measured in the time window. The start of the time window after the injection is offset by a "mixing time" (typically 60 minutes), which allows the injected $^{131m}$Xe to become homogenous in the detector before the rate measurement starts. The injected activity is measured by subtracting the background rate from the total event rate measured after the injection.
At the time of writing, a total of five $^{131}$I capsules have been purchased and tested in the prototype source injection system, following the standardized injection procedure described in section 5.4.2. The first three capsules were installed in the generator plumbing without modifying their form-factor, leaving the $^{131}$I-doped NaH$_2$PO$_4$ inside of the double-walled gelatin capsule that they were delivered in.

Fifty-eight injections were performed with the first two (gelatin enclosed) $^{131m}$Xe sources, during which the pattern of injected activities revealed consistent changes in the relative injected activity over time. This change indicated that some property of these sources was evolving over time with repeated exposure to GXe and vacuum pressure. The plot in Fig. 5.29 shows the injected activities increasing to values much larger than expected early in the lifetime of the first two capsules, before eventually producing consistent results closer to the expectation later in the capsule lifetimes. The third source (not pictured) showed a similar evolution in time. When these capsules were removed from the generators at the end of their useful life times, it was discovered that the gelatin capsules had become embrittled and ruptured from the repeated cycle of GXe pressure and vacuum that the injection procedure requires. We speculate that this repeated cycling is likely responsible for the evolution of the injected activities in Fig. 5.29, by removing water vapor or some other impurity from the sources over time. The broken gelatin capsules are pictured in Fig. 5.30. In an effort to better understand the issue of inconsistent initial injections, and to better contain the source, the sintered-metal filter-gasket hardware, described in section 5.1.3, was adopted.

Ten injections performed with the first sintered-metal filter-gasket source showed a similar trend in the ratio of expected to measured injection activity over the source's lifetime, plotted in Fig. 5.31. With the gelatin capsule breakage removed as a contributing factor, we observe that the repeated cycle of GXe pressure and vacuum from the injection procedure changes the physical properties of the $^{131}$I-doped NaH$_2$PO$_4$, 

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Figure 5.29. A plot of the results from $^{131m}$Xe injections performed with the prototype SIS into the UMass LXe detector, with the first two (gelatin enclosed) $^{131m}$Xe sources. Strong inconsistency was observed during the first several injections, before both sources eventually became much more predictable. We speculate that this is likely related to the removal of water vapor or some other impurity in the source, from repeated GXe pressure and vacuum cycling. The timescale for this change is complicated by the fact that the gelatin capsules broke during the testing campaign of both sources.

Figure 5.30. Photos of the first two $^{131m}$Xe sources tested at UMass Amherst in the LXe detector. During the injection campaigns with these gelatin enclosed sources, the repeated cycle of exposure to vacuum and GXe pressure caused the gelatin to become brittle, and eventually fracture. The two halves of the first source are shown in the photos on the left, and the second source is shown on the right, still inside the spring which was used to contain the gelatin capsules in the original hardware design.
Figure 5.31. Plots showing the results from $^{131m}$Xe injections performed with the prototype SIS into the UMass LXe detector, using the third $^{131m}$Xe source (and first source with the sintered-metal filter-gasket hardware). The injection campaign with this source showed similar time-evolution to the gelatin enclosed sources, with higher-than-expected initial injections converging to lower-than-expected (for a branching fraction of 1%) injection activities that remained consistent for the remainder of the source’s useful lifetime. This “conditioning” period is shown as a function of the age of the source in the left plot, and is shown to be independent of the absolute injected activity by plotting against a proxy for the source activity in the right plot. The expected injection activity is shown as a red line in both plots.
resulting in a change in the emanation efficiency of $^{131m}$Xe from the source. We call this change over time "conditioning", generically.

With all of the "pre-conditioning" results removed from the final compilation of $^{131m}$Xe injection results, a measurement of the product of the $^{131}$I branching fraction and the $^{131m}$Xe emanation efficiency from the source, for the two source form factors, respectively, can be made. Aggregating all of the results from all of the sources tested in the UMass LXe detector, the $(^{131}$I branching fraction)$\times$($^{131m}$Xe Emanation Efficiency) was found to be 0.00355 ± 0.00013 for the gelatin enclosed sources, and 0.00898 ± 0.00020 for the metal-sinter enclosed sources. A histogram demonstrating this measurement is shown in Fig. 5.32, and the complete set of $^{131m}$Xe injections performed with the prototype SIS in the UMass LXe detector is shown in the plot in Fig. 5.33.

5.9 $^{220}$Rn Injection Results from the UMass Detector

To reduce the rate of background events and increase the sensitivity of the UMass LXe detector to (higher-energy) alpha decays, the PMT bias voltage was decreased to 750 V for the $^{220}$Rn data taking. The $^{220}$Rn injection campaign at UMass Amherst consisted of two phases performed with a single source: Injections into LXe, and a single injection into room temperature GXe. In LXe, the prompt $^{220}$Rn (55 s half life) and $^{216}$Po (145 ms half life) $\alpha$-decays (6,405 and 6,907 keV, respectively) appear as bright bands in a histogram of bottom-PMT versus top-PMT pulse area for the first pulse from the events in the data set. An example of a bottom-PMT versus top-PMT pulse area histogram is shown in Fig. 5.34, with a faint band visible from the $\alpha$-decay of $^{212}$Po (8,954 keV). Due to the very short (145 ms) half life of $^{216}$Po, the activity measured in the UMass LXe detector following an injection of $^{220}$Rn is the $^{220}$Rn+$^{216}$Po activity, which is equal to twice the $^{220}$Rn activity. The presence
Figure 5.32. A histogram of all of the measured $^{131m}$Xe injection activities, from every source tested in the UMass LXe detector, normalized by the $^{131}$I activity in the generator at the time of the injection. The result is two normally distributed populations corresponding to the gelatin enclosed and sintered-metal enclosed sources, respectively. The mean of these distributions is equal to the product of the $^{131}$I branching fraction and $^{131m}$Xe emanation efficiency for the two form factors, respectively.
Figure 5.33. A plot of the results from $^{131m}$Xe injections performed with the prototype SIS into the UMass LXe detector for all $^{131m}$Xe sources tested at UMass, excluding data from each source’s "conditioning" period. A model for the equilibrium $^{131m}$Xe activity in the generator at the time of injection is shown for each source form factor as a dashed line. The measurements of the product of the $^{131m}$Xe emanation efficiency and $^{131}$I branching fraction for each form factor (from Fig. 5.32) are used as an inputs in the models.
Figure 5.34. Histograms of data taken with the UMass LXe detector following the injection of $^{220}\text{Rn}$. **Left:** A histogram of the logarithm of the pulse area in the bottom PMT vs. the top PMT for the first pulse in the events. In this parameter space, mono-energetic decays form populations along lines of anti-correlation, with their precise location along those lines depending on the position of the event in the detector. The mono-energetic populations of $^{220}\text{Rn}$, $^{212}\text{Bi}$, $^{216}\text{Po}$, and $^{212}\text{Po}\alpha$-decay events are visible. **Right:** A simple cut selecting $^{220}\text{Rn}$ and $^{216}\text{Po}$ events is applied to the events in the histogram on the left. This cut reduces the background rate and random error in the measurement of the injected activity.
of $^{212}$Po $\alpha$-decays implies the presence of $\alpha$-decays from its parent, $^{212}$Bi (6207 keV), which overlaps with $^{220}$Rn in this parameter space.

Over the course of back-to-back $^{220}$Rn injections, $^{212}$Bi and $^{212}$Po in the detector are in secular equilibrium with their $^{212}$Pb parent, decaying with the 10.6 hour $^{212}$Pb half life. However, the decay of $^{212}$Pb and its daughters is offset by the production of $^{212}$Pb from the decay of the injected $^{220}$Rn, resulting in $^{212}$Bi and $^{212}$Po decay rates that are approximately constant over the short (~30 min) time scales of the injected $^{220}$Rn+$^{216}$Po measurements. The simple selection cut shown in Fig. 5.34 (right) is used to slightly reduce the number of background events in the $^{220}$Rn+$^{216}$Po rate measurement. The inclusion of decays from $^{212}$Bi and $^{212}$Po in the selection is permissible because of the approximately constant rate of $^{212}$Bi and $^{212}$Po over the time scale of the injections.

The $^{220}$Rn injection proceeds (as described in section 5.4.3) by flowing GXe through the $^{220}$Rn generator and into circulation continuously, for an extended period of time, during which the equilibrium $^{220}$Rn activity in the detector depends on the GXe flow rate through the generator (survival rate of $^{220}$Rn to the circulation system). Injections were performed into the UMass LXe detector across a range of GXe flow-rates through the $^{220}$Rn generator, and the steady-state detector activity was measured for each. Results from an example injection and measurement of the injected $^{220}$Rn+$^{216}$Po activity are shown in Fig. 5.35. Following a short 'mixing' period which allows the $^{220}$Rn rate to equilibrate in the detector after the start of the injection flow, the average rate of the selected events is measured. The background rate of the selected events (measured prior to the start of flow) is subtracted from the equilibrium rate to obtain a measurement of the injected $^{220}$Rn+$^{216}$Po activity. The periodic dips in event rate seen in Fig. 5.35 are a result of uncounted dead time that occurs when the DAQ finishes collecting events for one of its 100k-event acquisitions, and prepares to begin a new one. These dips are ignored in the measurement of the average event
Figure 5.35. A histogram showing the rate of events passing the $^{220}$Rn+$^{216}$Po selection cut in the UMass LXe detector during an injection of $^{220}$Rn. The injected $^{220}$Rn+$^{216}$Po activity is measured by calculating the difference between the average rate of the selected $^{220}$Rn+$^{216}$Po before and during the injection. The periods of time used to measure both rates are shown by black lines in the plot, at a height corresponding to the average value that they measured. Dips seen in the rate are due to short breaks in the DAQ’s data taking during the transition between 100k-event acquisitions, and are ignored by the rate-measuring algorithm.
Figure 5.36. A plot showing the complete set of results from $^{220}\text{Rn}$ injections into the UMass LXe detector with the prototype SIS. A model (equation 5.4) for the fraction of $^{220}\text{Rn}$ which survives the transit from the generator to the detector as a function of the carrier GXe flow-rate is fitted to the data, providing a measurement of the $^{220}\text{Rn}$ transport efficiency, $T_e = 0.163 \pm 0.015$. The residuals from the fit are shown below the results plot.

The activity of $^{220}\text{Rn} + ^{216}\text{Po}$ that survives the transit to the detector without decaying can be modeled by:

$$A = (T_e) \cdot 2A_{\text{Rn}}E_e \cdot 2^{-\frac{T_0}{T_{1/2}}}$$  \hspace{1cm} (5.4)
where $T_e$ is a generic $^{220}$Rn "transport efficiency" and is the only free parameter in the fit to the data, $A_{Rn}$ is the activity of the $^{220}$Rn source, $E_e$ is the emanation efficiency of $^{220}$Rn from the source, $T_{1/2}$ is the $^{220}$Rn half life, and $T_t$ is the transit time of the carrier xenon from the $^{220}$Rn generator to the circulation system. The emanation efficiency of $^{220}$Rn from the $^{228}$Th-plated source was measured by Nicholas Chott and Richard Schnee at the South Dakota School of Mines and Technology, and was found to be $E_e = 0.139 \pm 0.013$. The transit time of the carrier GXe from the $^{220}$Rn generator to the circulation system can be calculated by:

$$T_t = \frac{P \cdot V}{F}$$

where $P$ and $V$ are the pressure (measured from a pressure transducer) and volume (calculated from plumbing dimensions) of the SIS outlet plumbing, downstream of the $^{220}$Rn generator, and $F$ is the mass-flow rate of the carrier GXe (controlled and measured by the mass-flow controllers on the prototype SIS). The time spent in the circulation system by the injected $^{220}$Rn is not accounted for in $T_t$ because it is relatively difficult to predict, and is expected to be very short compared to the time spent in the SIS. Additionally, the transit through the circulation system involves large and irregularly shaped volumes in the heat exchanger and condenser tee, temperature and pressure gradients, and high surface areas of copper and steel at LXe temperatures. Instead, because the circulation system conditions were constant across the range of injection flow-rates, the fraction of $^{220}$Rn which decays in the circulation system is captured by the generic transport efficiency, $T_e$, in equation 5.4. In total, $T_e$ accounts for $^{220}$Rn decay during transit in the circulation system, possible sticking of $^{220}$Rn to cold metal surfaces, and a possible difference between the flow speed of the $^{220}$Rn and its carrier GXe. The best fit of the model in equation 5.4 to the injection data results in a measured transport efficiency of $T_e = 0.163 \pm 0.015$ for $^{220}$Rn in the prototype SIS and circulation system of the UMass LXe detector (with a circulation system mass-
flow rate of 1.5 SLPM). A version of this model with the efficiency factor multiplied by the transit time was fitted to the data and found to perform significantly worse than the linear scaling of the efficiency factor, $T_e$, in the present model. This result suggests that the transport (in)efficiency is not a function of the injection flow-rate, but rather, is constant for constant circulation system and detector conditions.

Following the injection campaign into LXe, a single injection was performed into room temperature GXe in the UMass detector. The PMT bias voltage was increased to 1000 V to observe the smaller amount of scintillation light produced from scattering events in GXe. Because adding GXe to the detector in this mode causes the detector pressure to increase over the course of an injection, the injection was kept shorter than those performed during the LXe injection campaign. GXe was flowed continuously through the $^{220}$Rn generator for 10 minutes for this one-off injection. The circulation flow rate was not controlled by the circulation mass-flow controller, rather, the mass-flow controller was set to be maximally open to achieve a high turnover rate of the GXe in the detector (flow rate $\sim$6 SLPM) allowing the injected $^{220}$Rn to quickly become evenly mixed. GXe was flowed through the $^{220}$Rn generator and into circulation at a rate of 100 SCCM for 5 minutes, followed immediately by 200 SCCM for 5 minutes. The total event rate in the detector during the injection into GXe is shown in Fig. 5.37. The measured $^{220}$Rn+$^{216}$Po activity in the detector 15 minutes after the start of the injection was approximately 325 Bq. The volume of 'active' GXe between the PMTs in the UMass detector is 303 cc, and the total volume of the detector and circulation system are 3500 cc, giving an active xenon fraction (in GXe operation mode) of 0.087. The total injected $^{220}$Rn+$^{216}$Po can then be calculated to be approximately $325/0.087 = 3,736$ Bq. For an injection flow rate of 200 SCCM through the generator, the carrier-GXe transit time out of the SIS is calculated from equation 5.5 to be $\sim$19 seconds ($\rho = 1.46$ bara, $V = 43$ cc). From equation 5.4 we can calculate the transport efficiency in the room-temperature GXe mode to be
Figure 5.37. A histogram showing the event rate in the UMass LXe detector while at room temperature, filled with GXe, during a continuous injection of $^{220}$Rn. The flow rate of GXe through the $^{220}$Rn generator was increased from 100 SCCM to 200 SCCM five minutes after the start of the injection.

$0.90 \pm 0.17$ including a 10% uncertainty in the detector+circulation system volume. The room-temperature GXe transport efficiency being significantly higher than the cold LXe transport efficiency is not surprising considering the much higher circulation flow-rate during the former. However, we speculate that $^{220}$Rn’s stickiness to cold metal surfaces, the speed of $^{220}$Rn dissolution at the LXe-GXe interface, and the time taken for the $^{220}$Rn to travel into the active fraction of the LXe (between the two PMT faces) all contribute to the much lower transport efficiency observed in the cold LXe mode as well.
CHAPTER 6
FIRST RESULTS AND ASSOCIATED ANALYSES FROM THE LZ SOURCE INJECTION SYSTEM

At the time of writing, the LZ Source Injection System (SIS) is installed underground at SURF in service of the LZ detector, and many of the calibration procedures for which the system was designed have been tested as part of the commissioning process for LZ. This chapter describes some of the key differences between the prototype SIS built and tested at UMass Amherst and the LZ SIS, and presents the results from the first calibrations performed in LZ using the LZ SIS.

Note: The LZ detector data presented in this chapter was collected as part of the experiment’s first early commissioning phase. The detector and circulation conditions and settings were changing frequently, and are not the final settings chosen for LZ’s first dedicated science run. The data processing framework was also under frequent revision and improvement. All the results here should be taken as first demonstrations of calibration capabilities and calibration methods, rather than as describing the final detector conditions and sensitivities of the eventual first science run.

6.1 The LZ Source Injection System Hardware

The LZ SIS was assembled in clean room conditions at the University of Wisconsin-Madison Physical Sciences Lab. The system was designed to be functionally identical to the prototype SIS at UMass Amherst, and to approximate the same relative volumes as it despite the LZ SIS’s unique physical layout, which is necessitated by space
Figure 6.1. The plumbing and instrumentation diagram for the LZ source injection system.

constraints in the Davis cavern at SURF. The LZ SIS is contained within the same connected cabinets that house the LZ circulation system and can be continuously purged with nitrogen to mitigate the risk of an air leak into LZ plumbing. A plumbing and instrumentation diagram of the LZ SIS is shown in Fig. 6.1.

Several hardware differences between the prototype SIS at UMass Amherst and the LZ SIS are notable. First, the LZ SIS features four flow-through calibration-source generator bays and two bottle-source bays (compared to the two flow-through source, and one bottle source bays on the UMass prototype SIS). In the LZ SIS, the bottle sources are mounted on the wall of the cabinet containing the system and are connected with flexible jacketed-metal bellows, rather than being mounted on the panel itself and connected with rigid plumbing as was done on the prototype SIS. An additional xenon bottle, 1706VES, is connected to the LZ SIS into which any pump-out containing radioisotopes is performed by cryopumping (at UMass Amherst, radioisotopes are pumped-out directly into a laboratory fume hood). An additional
Figure 6.2. A photo of the LZ source injection system. A bottle containing natural methane (CH$_4$) can be seen at the left edge of the photo, and three flow-through calibration sources ($^{83m}$Kr, $^{131m}$Xe, and $^{220}$Rn) can be seen installed on the system near the center of the photo. The calibration-source plumbing is indicated with a red overlay, while the plumbing which is used to flush the calibration isotopes into the circulation system after they are dosed into the dose volume (and which goes through the dose volume), is indicated with a blue overlay. The dose volume is indicated with a green overlay.

A photo of the LZ SIS is shown in Fig. 6.2, and a second photo picturing the first $^{83m}$Kr, $^{131m}$Xe, and $^{220}$Rn generators installed on the LZ SIS is shown in Fig. 6.3.
Figure 6.3. A photo of the first $^{83m}$Kr, $^{131m}$Xe, and $^{220}$Rn generators installed onto the LZ source injection system.
6.2 The LZ Source Injection System Procedures

During operation of the LZ SIS, the injection procedures developed with the prototype SIS at UMass Amherst (sections 5.4.1, 5.4.2, 5.4.3, and 5.4.4) can be executed as-is with a single simple change. To account for the higher pressure of the LZ circulation system (∼6 bara) compared to the UMass detector’s circulation system (∼2 bara), all flow rate (MFC) setpoints in the injection procedures for the flow-through calibration sources are multiplied by a factor of 3 in the procedures for the LZ SIS (unless the factor of three exceeds the maximum MFC setpoint, in which case the maximum setpoint is used). Increasing the flow rate setpoints by the same factor as the pressure difference maintains a constant carrier-GXe flow speed between the procedures in the two systems, therefore, the timing of each step in the procedures remains the same. The flow rates only need to be adjusted in the procedures which flow carrier GXe directly into the circulation system, where the flow from the SIS must overcome the circulation-system pressure to flow into it.

The modified procedures for injecting each of the calibration sources into LZ, using the LZ SIS, are written explicitly in this section for completeness, with reference to the instrument names in the LZ plumbing and instrumentation diagram in Fig. 6.1.

6.2.1 $^{83m}$Kr Injection Procedure for LZ

- Close all pneumatic valves, and set all mass-flow controllers to 0 SCCM on the LZ SIS to create a standardized initial state.
- Ensure that the manual valves 1772MDV and 1703MDV are open.
- If the $^{83m}$Kr source is in:
  - Bay 1: Open 1741MDV and 1744MDV.
  - Bay 2: Open 1735MDV and 1738MDV.
  - Bay 3: Open 1729MDV and 1732MDV.
  - Bay 4: Open 1723MDV and 1726MDV.
- Open 1704PDV, 1752PDV, 1755PDV, 1768PDV, and 1776PDV.
• If the $^{83}\text{mKr}$ source is in:
  – Bay 1: Open 1740PDV and 1745PDV.
  – Bay 2: Open 1734PDV, 1739PDV, and 1749PDV.
  – Bay 3: Open 1728PDV, 1733PDV, 1748PDV, and 1749PDV.
  – Bay 4: Open 1722PDV, 1727PDV, 1747PDV, 1748PDV, 1749PDV.

• Set 1751MFC setpoint to 50 SCCM and 1713MFC setpoint to 150 SCCM.

• Open 1711PDV to begin flowing GXe through the generator.

• Wait the amount of time that achieves the GXe flow volume corresponding to 
  the desired dose activity (based on past results detailed in section 5.7 [need $\sim 3x$
  the UMass SIS GXe flow volume for the equivalent activity with the LZ SIS]),
  then promptly close valves 1752PDV and 1711PDV.

• Set the 1751MFC and 1713MFC setpoints to 0 SCCM.

• If the $^{83}\text{mKr}$ source is in:
  – Bay 1: Close 1740PDV and 1745PDV.
  – Bay 2: Close 1734PDV, 1739PDV, and 1749PDV.
  – Bay 3: Close 1728PDV, 1733PDV, 1748PDV, and 1749PDV.
  – Bay 4: Close 1722PDV, 1727PDV, 1747PDV, 1748PDV, 1749PDV.

• Open valves 1779PDV and 1755PDV.

• Set the 1713MFC setpoint to 500 SCCM.

• Open 1711PDV to begin flowing GXe to flush residual $^{83}\text{mKr}$ activity into the 
  circulation system.

• After 6 minutes, close all pneumatic valves (1704PDV, 1711PDV, 1755PDV, 
  1768PDV, 1779PDV and 1776PDV) and set the 1713MFC setpoint to 0 SCCM.

### 6.2.2 $^{131}\text{mXe Injection Procedure for LZ}$

• Close all pneumatic valves, and set all mass-flow controllers to 0 SCCM on the 
  LZ SIS to create a standardized initial state.

• Ensure that the manual valves 1772MDV and 1703MDV are open:
• If the $^{131m}$Xe source is in:
  
  – Bay 1: Open 1741MDV and 1744MDV.
  – Bay 2: Open 1735MDV and 1738MDV.
  – Bay 3: Open 1729MDV and 1732MDV.
  – Bay 4: Open 1723MDV and 1726MDV.

• Open 1704PDV, 1752PDV, 1755PDV, 1768PDV, and 1776PDV.

• If the $^{131m}$Xe source is in:
  
  – Bay 1: Open 1740PDV and 1745PDV.
  – Bay 2: Open 1734PDV, 1739PDV, and 1749PDV.
  – Bay 3: Open 1728PDV, 1733PDV, 1748PDV, and 1749PDV.
  – Bay 4: Open 1722PDV, 1727PDV, 1747PDV, 1748PDV, 1749PDV.

• Set 1751MFC setpoint to 50 SCCM and 1713MFC setpoint to 150 SCCM.

• Open 1711PDV to begin flowing GXe through the generator.

• Wait 6 minutes to thoroughly flush the $^{131m}$Xe generator contents into the SIS outlet plumbing, then close valves 1752PDV and 1711PDV.

• Set the 1751MFC and 1713MFC setpoints to 0 SCCM.

• If the $^{131m}$Xe source is in:
  
  – Bay 1: Close 1740PDV and 1745PDV.
  – Bay 2: Close 1734PDV, 1739PDV, and 1749PDV.
  – Bay 3: Close 1728PDV, 1733PDV, 1748PDV, and 1749PDV.
  – Bay 4: Close 1722PDV, 1727PDV, 1747PDV, 1748PDV, 1749PDV.

• Open valves 1779PDV and 1755PDV.

• Set the 1713MFC setpoint to 500 SCCM.

• Open 1711PDV to begin flowing GXe to flush residual $^{131m}$Xe activity into the circulation system.

• After 6 minutes, close all pneumatic valves (1704PDV, 1711PDV, 1755PDV, 1768PDV, 1779PDV and 1776PDV) and set the 1713MFC setpoint to 0 SCCM.
6.2.3 $^{220}$Rn Injection Procedure for LZ

- Close all pneumatic valves, and set all mass-flow controllers to 0 SCCM on the LZ SIS to create a standardized initial state.
- Ensure that the manual valves 1772MDV and 1703MDV are open.
- If the $^{220}$Rn source is in:
  - Bay 1: Open 1741MDV and 1744MDV.
  - Bay 2: Open 1735MDV and 1738MDV.
  - Bay 3: Open 1729MDV and 1732MDV.
  - Bay 4: Open 1723MDV and 1726MDV.
- Open 1753PDV, 1754PDV, 1768PDV, and 1776PDV.
- If the $^{220}$Rn source is in:
  - Bay 1: Open 1740PDV, 1745PDV, and 1749PDV.
  - Bay 2: Open 1734PDV, and 1739PDV.
  - Bay 3: Open 1728PDV, 1733PDV, and 1748PDV.
  - Bay 4: Open 1722PDV, 1727PDV, 1747PDV, and 1748PDV.
- Set 1713MFC to 500 SCCM.
- Open 1704PDV and 1711PDV to begin flowing GXe through the $^{220}$Rn generator into the LZ circulation system.
- After flowing continuously for as long as desired, close all pneumatic valves (1704PDV, 1711PDV, 1753PDV, 1754PDV, 1768PDV, 1776PDV, and 1722PDV, 1727PDV, 1728PDV, 1733PDV, 1740PDV, 1745PDV, 1747PDV, 1748PDV, and 1749PDV depending on which Bay the $^{220}$Rn generator was in) and set the 1713MFC setpoint to 0 SCCM.

6.2.4 $\text{CH}_4$, $\text{CH}_3\text{T}$, and $^{14}\text{CH}_4$ Injection Procedure for LZ

- Pump-out the SIS to a pressure below $1\times10^{-5}$ mBar to prepare for the methane dosing.
• Close all pneumatic valves, and set all mass-flow controllers to 0 SCCM on the LZ SIS to create a standardized initial state.
• Ensure that the manual valves 1772MDV and 1703MDV, and the manual valve on the bottle source, are open (1757MDV for Bay 1 or 1759 MDV for Bay 2).
• Open 1765PDV, 1767PDV, and 1755PDV.
• If the source bottle is in:
  – Bay 1: Open 1758PDV.
  – Bay 2: Open 1760PDV.
• The methane mixture from the source bottle will now be flowing into and slowly filling the dose volume on the LZ SIS. Once the desired pressure is reached on 1766PT (desired dose quantity), close valves 1767PDV, 1765PDV, and 1758PDV or 1760PDV depending on the bottle bay (both should be in the closed state after this step).
• Close 1757MDV or 1759MDV depending on which bay the source bottle is installed in (both should be closed and locked at this step if there are two bottles installed).
• Open valves 1777PDV (post-getter outlet), 1768PDV, 1704PDV, and 1711PDV.
• Set the 1713MFC setpoint to 500 SCCM.
• Open 1779PDV to begin flushing the dosed methane mixture into the LZ circulation system.
• After 6 minutes, close all pneumatic valves (1704PDV, 1711PDV, 1768PDV, 1779PDV and 1777PDV).

6.3 Results from the first $^{220}$Rn Injection into Cold GXe in LZ

Prior to filling the LZ TPC with LXe, TPC data was taken while filled with cold GXe ($\sim$180 K, $\sim$2 bara). During this time, the very first injection using the LZ
SIS was performed following the procedure in section 6.2.3. $^{220}$Rn was continuously injected into the TPC using a range of GXe flow rates through the $^{220}$Rn generator. During the injections, the LZ circulation flow rate was 240 SLPM. The injection flow-rate and durations are shown in Fig. 6.4, along with the raw trigger rate in the TPC during the injection period. During the periods of higher injection flow rate, $^{220}$Rn was transported to the circulation system faster, resulting in a larger surviving $^{220}$Rn fraction and a higher activity measured in the detector. The surviving fraction of $^{220}$Rn to the LZ TPC can be modeled, as in section 5.9, using the $^{220}$Rn generator activity, $A_{Rn}$, the emanation efficiency of $^{220}$Rn from the generator, $E_e$, the $^{220}$Rn half life, $T_{1/2}$, and the transit times in the source injection system and circulation system, $T_i$ and $T_c$, respectively. Due to the short (145 ms) half life of $^{216}$Po, the decays from $^{220}$Rn and $^{216}$Po occur in approximately the same position in the detector, and the
combined $^{220}\text{Rn}+^{216}\text{Po}$ activity, equal to twice the $^{220}\text{Rn}$ activity, is what is measured in the GXe-filled TPC. The expected $^{220}\text{Rn}+^{216}\text{Po}$ activity surviving the transit from the generator to the TPC in LZ is given by:

$$A = (2A_{Rn}E_e) \cdot 2^{\frac{(T_i+T_c)}{T_{1/2}}}.$$  (6.1)

The transit times, $T_i$ and $T_c$, are equal to:

$$T_i = \frac{P_i \cdot V_i}{F_i} \text{ and } T_c = \frac{P_c \cdot V_c}{F_c}.$$  (6.2)

where $P$, $V$, and $F$ are the pressure, volume, and xenon flow rate in the source injection system (subscript i) and the circulation system (subscript c), respectively. The pressures are directly measured with pressure transducers, the volumes are calculated from the plumbing dimensions, and the mass-flow rates are directly measured by mass-flow controllers. The summarized results from the $^{220}\text{Rn}$ injections into the cold-GXe-filled LZ TPC are shown in Fig. 6.5 along with the model (blue curve) for the injected $^{220}\text{Rn}$ activity. Several fits of the model to the data were tried, including a simple scaling factor applied to the result of equation 6.1 as a free-parameter, as in the model in section 5.9, equation 5.4. Somewhat surprisingly, the resulting best fit was found to model the data very poorly, despite its success modeling the physics of the UMass circulation system. A much better fit to the data was obtained with a scaling factor on the total transit time as a free parameter, suggesting that the transport efficiency is proportional to the injection and circulation flow rates. This more successful fit model is given by:

$$A = (2A_{Rn}E_e) \cdot 2^{\frac{(T_i+T_c)}{T_{1/2}}}C_T.$$  (6.3)

where the free parameter, $C_T$, is the 'correction' factor for the total transit time of the $^{220}\text{Rn}$ in the source injection and circulation systems. The fit of equation 6.3 to
Figure 6.5. A plot summarizing the results of the measured $^{220}$Rn activity injected into the GXe-filled LZ TPC as a function of carrier-GXe flow rate through the $^{220}$Rn generator. The expected activity delivered to the detector is shown by the blue curve, and is seen to model the measured data very poorly. A model with the total transit time as a free parameter is fitted to the data and indicated by the red curve.
the data is shown by the red curve in Fig. 6.5. The transit time correction measured from the fit is $C_T = 2.20 \pm 0.22$. One possible interpretation of this result is that the $^{220}\text{Rn}$ moves more slowly through the source injection and circulation systems than the carrier GXe, at approximately 0.45 ($= \frac{1}{C_T}$) times the carrier-GXe speed. We speculate that one possible reason for the apparent qualitative difference in the $^{220}\text{Rn}$ behavior between the UMass and LZ results is that the carrier-GXe flow in the LZ circulation system is significantly more turbulent, with flow rates two orders of magnitude higher than in the UMass circulation system despite plumbing diameters of the same order of magnitude. Other important differences such as the fact that the injections were performed into LXe at UMass Amherst, and GXe in LZ may, however, contribute more significantly to the differences in the data than the flow characteristics.

During the $^{220}\text{Rn}$ injections into GXe no electric field was present in the TPC, so only prompt scintillation light, $S_1$, was collected. Without drifting the freed electrons to produce an $S_2$ signal following an interaction, 3-D position reconstruction was not possible. However, the top-bottom asymmetry was used as a proxy for the z position of the interactions in the TPC in this data. The top-bottom asymmetry (TBA) is defined from the $S_1$ light collected by the top and bottom PMT arrays as:

$$
\text{TBA} = \frac{S_{1T} - S_{1B}}{S_{1T} + S_{1B}} \quad (6.4)
$$

where $S_{1T}$ and $S_{1B}$ are the total $S_1$ light (phd) collected by the top and bottom PMT arrays, respectively. TBA ranges from -1 for events near the bottom array, to 1 for events near the top array, and is approximately symmetric in z about the TPC center for a uniformly distributed population in the GXe-filled LZ TPC. Histograms of TBA versus total pulse area are shown in Fig. 6.6, from time periods during (left) and after (right) the $^{220}\text{Rn}$ injection. The $^{220}\text{Rn}$ and $^{216}\text{Po}$ $\alpha$-decays appear as a single bright population which is distinct from the predominantly low-energy background in
Figure 6.6. Histograms of TBA versus total pulse area for data taken during the $^{220}$Rn injection into the GXe-filled LZ TPC (left) and on the following day (right). The real time of the data in each histogram is indicated by the black text. The prompt $^{220}$Rn and $^{216}$Po $\alpha$-decays appear as a single bright band during the $^{220}$Rn injection, distinct from the lower-energy background. On the following day, $\alpha$-decays from $^{212}$Bi and $^{212}$Po (stuck to surfaces in the TPC) appear combined with the background $^{222}$Rn-chain alphas. Asymmetries in TBA for the alpha populations are predominantly a reflection of asymmetries in the TPC and PMT-array geometries.
the cold-GXe TPC. The $\alpha$-decay population on the day following the $^{220}$Rn injection is a combination of background $^{222}$Rn-chain $\alpha$-decays, and residual $^{212}$Bi and $^{212}$Po from the $^{220}$Rn injection, stuck to surfaces in the TPC. The purification time constant when circulating the GXe at a flow rate of 240 SLPM through the heated getter, with $\sim$90 kg of GXe in the TPC, is estimated to be approximately 1 hour. Therefore, on the day following the $^{220}$Rn injection date, any $^{220}$Rn-daughters which were not stuck to surfaces in the TPC would be expected to have been purified out by circulation.

## 6.4 $^{127}$Xe K-Shell Calibration from Gammas Tagged in the Xenon Skin

The earliest calibration peaks available for the LXe-filled LZ TPC were the mono-energetic peaks from the naturally present xenon activation products $^{131m}$Xe, $^{127}$Xe, and $^{129m}$Xe. For $^{127}$Xe events which occur near the walls of the TPC, the associated $\gamma$-ray radiation escapes the TPC and deposits its energy in the LXe skin some fraction of the time. In addition to being easily tagged by their unique topology, these events leave behind Auger electrons and/or X-rays in the TPC which provide mono-energetic calibration peaks whose energy depends on which $^{127}$Xe orbital the electron was captured from (see section 4.1.5 for details of the $^{127}$Xe decay). The analysis in this section describes a measurement of the escaped-$\gamma$-ray $^{127}$Xe-decay tagging efficiency for $^{127}$Xe decays with K-shell electron captures. With the ability to tag escaped-$\gamma$-ray $^{127}$Xe events already demonstrated with simulated LZ data (section 4.2.4), applying a similar tagging prescription to real data in LZ was straightforward. The data used for this analysis was taken before the LZ grids were biased, meaning no electric field was present in the TPC and only prompt scintillation light (S1) was measured.

First, a basic S1-pulse area correction was developed to account for the position-dependent light collection efficiency. A histogram of top-bottom asymmetry (TBA) versus pulse area including every S1 pulse from all of the events in the data set is
Figure 6.7. Histograms of top-bottom asymmetry vs. uncorrected (left) and corrected (right) S1-pulse area in the LZ TPC just after being filled with LXe. The naturally present activation peaks from $^{131m}\text{Xe}$, $^{127}\text{Xe}$, and $^{129m}\text{Xe}$ appear as bright bands in the histogram. The uncorrected S1-pulse areas show strong position dependence in each mono-energetic population. An S1-pulse area correction, normalized to the S1-pulse areas at TBA= 0, is applied to the data in the histogram on the right. The TBA in this data is not symmetric about TBA = 0 because of the high reflectivity of the LXe-GXe interface, which results in the majority of photons being collected by the bottom PMT array.

shown in Fig. 6.7 (left), and demonstrates the need for an S1 area correction. Three populations from the xenon activation products can be seen as bright bands, with significantly higher S1-pulse areas at low TBAs. TBA, a proxy for z position in the TPC, is defined in equation 6.4 in the previous section. To correct the S1-pulse areas, the mean S1 area of the $^{131m}\text{Xe}$ population (furthest left) was measured at several values of TBA, and a histogram of the mean S1 areas as a function of TBA was constructed to be the ”correction map”. For every raw S1-pulse area in the data set, the corrected pulse area was found by interpolating on the correction map to find the mean $^{131m}\text{Xe}$ S1 area at the TBA of the event in question. The raw S1-pulse area was then divided by the result of the interpolation, and multiplied by a normalization constant, the mean $^{131m}\text{Xe}$ S1-pulse area at TBA = 0 in this case. The S1-pulse areas with the correction applied are shown in Fig. 6.7 (right).
Figure 6.8. Histograms of the positions of coincident events in the LZ TPC and LXe skin, during a period of data taking in which $^{127}\text{Xe}$ was naturally present from activation. **Left:** The top-bottom asymmetry in the TPC versus in the LXe Skin. **Right:** The angular position (theta) in the TPC versus in the LXe skin. The artificial population at Skin Theta = 45 degrees is the result of setting it equal to 45 degrees in events with light distributions that cannot be used to properly calculate an angular position. Both histograms demonstrate the coincidence requirement’s ability to select events which have strongly correlated positions, most likely escaped-$\gamma$-ray $^{127}\text{Xe}$-decays.

In each event and for each S1 pulse, coincident pulses in the LXe skin were identified as those which occurred within ±100 ns of the TPC pulse and were detected by >3 skin-PMTs. For events with a coincident pulse in the LXe skin, strong position correlation between the skin and TPC pulses was observed without any additional cuts. Histograms of TPC versus skin TBA and angular position (theta), showing the position correlation of the coincident events, are shown in Fig. 6.8. With the S1-pulse area correction applied, the 33 keV K-shell Auger electron/X-ray peak from escaped-$\gamma$-ray $^{127}\text{Xe}$ decays is visible above the background in a histogram of S1-pulse area. The number of these events is measured by fitting the S1-pulse area spectrum with a model that is the sum of independent gaussian, exponential, and constant components. The exponential+constant components model the background, while the gaussian component models the 33 keV peak from $^{127}\text{Xe}$, allowing it to be independently measured from the parameters of the gaussian component of the fit.
The three-component fit is performed on the S1-pulse area spectrum in the region of S1-pulse area that corresponds to the 33 keV peak in histograms with and without the skin-coincidence requirement. Examples of these histograms including the three-component fits are shown in Fig. 6.9. The ratio of the gaussian integral when the coincidence is required to when no coincidence is required provides a measurement of the LXe-skin tagging efficiency for escaped-\(\gamma\)-ray K-shell \(^{127}\text{Xe}\) decays. Using this method to measure the efficiency, the TPC was divided into bins in TBA to study the efficiency as a function of \(z\) position. The division into TBA bins is shown in Fig. 6.10 and the measured efficiencies at the various positions in TBA are shown in Fig. 6.11, along with the result of a measurement over the entire range of TBA.

As expected, the efficiency of tagging escaped-\(\gamma\)-ray K-shell \(^{127}\text{Xe}\) events with the LXe skin is highest near the bottom of the TPC where the corresponding LXe skin is the thickest, and lowest near the top of the TPC where the LXe skin is the thinnest and the associated \(\gamma\)-rays can escape into the GXe. In dedicated simulations of \(^{127}\text{Xe}\) events near the TPC walls, produced by Sally Shaw and analyzed by Alissa Monte, it was found that in \(^{127}\text{Xe}\) events where the \(\gamma\)-ray radiation is not deposited in the TPC or LXe Skin, the \(\gamma\)-ray radiation is most commonly deposited (in order of decreasing probability): below the cathode grid in the reverse field region, in the PTFE walls of the TPC, in the liquid scintillator of the outer detector, in the GXe at the top of the TPC, or in the titanium that composes the ICV.

### 6.5 Results from the first CH\(_4\) Injection into LXe in LZ

The ability to remove CH\(_3\)T and \(^{14}\text{CH}_4\) from the LXe bulk in the LZ TPC, by circulation through the heated getter, was tested with an injection of natural (non-radioactive) methane, CH\(_4\), during the commissioning phase of LZ. The methane injection followed the example set by the LUX experiment, and was prepared by LZ collaborators at the University of Maryland. A bottle containing equal volumes
Figure 6.9. Histograms of the corrected S1-pulse area in the LZ TPC over the range of corrected S1-pulse area containing the 33 keV Auger electron/X-ray peak from escaped-γ-ray K-shell $^{127}$Xe decays. A model is fit to the data which is the sum of a constant, an exponential, and a gaussian component. The constant+exponential components model the background, while the gaussian component models the 33 keV peak. The fit parameters from the gaussian component are used to measure the number of events in the 33 keV peak. The efficiency of tagging the escaped-γ-ray K-shell $^{127}$Xe decays is measured by calculating the ratio of the gaussian-component integral from the fit with a skin coincidence required (right histogram) to the gaussian-component integral from the fit with no skin coincidence required (left histogram). The measured activities of the gaussian populations are reported on each histogram in black text, including the percent of total $^{127}$Xe decays which contribute to each population. To determine the contributing percentage, the total $^{127}$Xe activity was calculated by integrating a gaussian fit of the 403 keV $^{127}$Xe peak in a histogram of corrected-S1-pulse area, and dividing the integral by the total live time of the data, and the fraction of $^{127}$Xe decays that are expected to fall into the 403 keV peak (47.6%).
Figure 6.10. A histogram of the top-bottom asymmetry versus the logarithm of the TBA-corrected S1-pulse area in the LZ TPC for events which have coincident pulses in the LXe skin. The 33 keV Auger electron/X-ray peak from escaped-γ-ray K-shell $^{127}$Xe decays is distinct above the background after the coincidence requirement is applied.
Figure 6.11. A plot showing the results of measurements of the LXe skin tagging efficiency for escaped-$\gamma$-ray K-shell $^{127}$Xe decays in the LZ TPC. The measured efficiency from the aggregated data across all TBA values is shown as the solid blue line, with the one sigma uncertainties shown by the dashed blue lines. The measured efficiencies from the selected TBA ranges are shown in black.
(at standard pressure) of xenon and natural methane was shipped to SURF and installed on the LZ SIS. Approximately 200 standard cc of the methane mixture was flowed through the methane purifier on the SIS, measured in the dose volume, and injected into the LZ circulation system downstream of the heated-getter following the procedure in section 6.2.4.

The removal timescale of the injected methane was determined by measuring its concentration in samples of GXe drawn from the circulation system periodically, following the injection. The methane concentration of the xenon samples was measured by John Armstrong, of the University of Maryland, using a coldtrap/mass-spectrometry method originally developed for LUX and EXO-200 [84], [85]. The measured concentration of methane over time was then fitted with an exponential to measure the time constant for methane removal from the LZ xenon. The results of the concentration measurements from the xenon sampling, and best fit (work and analysis performed by John Armstrong) are shown in Fig. 6.12. The removal time constant measured from this preliminary analysis is $\tau = 85.8 \pm 2.0$ hours. During the time over which this data was taken, the circulation (purification) flow rate changed once, from 500 to 600 SLPM, and was not accounted for in the analysis. The average flow rate through the heated getter over the time period corresponding to the fitted data was $\sim 567$ SLPM. Performing this measurement enables the injection of long-lived methane-based calibration sources, CH$_3$T and $^{14}$CH$_4$, to proceed (as in LUX [52]) without the fear of residual activity remaining in the detector, contaminating the WIMP search ROI. This preliminary result is reassuring, but will likely be repeated more carefully under more stable operating conditions in the future.

### 6.6 Results from the first $^{83m}$Kr Injection into LXe in LZ

The LXe flow pattern inside of any TPC is typically complex, and is driven primarily by the location and intensity of small heat-loads on the vacuum-insulated
Figure 6.12. The natural methane concentration measured from samples of xenon taken from the LZ circulation system, following the injection of approximately 100 standard cc of natural methane into the LZ circulation system. The measurements and fit to the data were performed by John Armstrong, from the University of Maryland. The last two data points are not included in the fit and are adjusted by subtracting off time during which the getter was turned off, following the first nine samples. The preliminary methane-removal time constant for the LZ circulation system was measured to be $\tau = 85.8 \pm 2.0$ hours.
cryostat containing the TPC and cryogenic liquid. The first $^{83m}$Kr injection into the LZ TPC was performed with the primary goal of studying the timescale over which the $^{83m}$Kr becomes uniformly mixed in the LXe. Understanding the mixing timescale is important for informing the usefulness of $^{83m}$Kr as a calibration source in LZ due to its relatively short (1.83 hour) half life, and for planning future injections.

Approximately 50 Bq of $^{83m}$Kr was injected into the LZ TPC from the LZ SIS following the standard $^{83m}$Kr injection procedure in section 6.2.1. To select $^{83m}$Kr events in the analysis of the $^{83m}$Kr injection data, events with either one or two S1 pulses and with one S2 pulse were selected. In events with two S1 pulses, the two S1-pulse areas were added together to form a single S1 pulse. In this preliminary LZ data, taken during the commissioning of the LZ TPC, the details of the pulse-classifier were actively being tuned, and several PMTs were known to have their IDs swapped in the position reconstruction code. The quality of the data taken during this injection is not representative of the quality of any future LZ data. A basic quality cut selecting events with correlated drift time and top-bottom asymmetry, shown in Fig. 6.13 (upper left), was applied to the $^{83m}$Kr injection data. The $^{83m}$Kr events appear as a clear peak in a histogram of the logarithm of S2-pulse area versus the logarithm of S1-pulse area, making it easy to select them there with the cut shown in Fig. 6.13 (upper right).

With $^{83m}$Kr selected, the mixing timescale was studied by projecting a histogram of the event drift times, in time, using each event’s unique timestamp. The time-projected drift time histogram is shown in Fig. 6.13. The injected $^{83m}$Kr enters the bottom of the TPC (drift time = -950 $\mu$s) near TimeStamps = 0, and can be seen to slowly mix into the TPC with a well defined front, reaching drift time = -425 $\mu$s (~halfway) after approximately 3.75 hours, and drift time = -250 $\mu$s (~75% of the TPC height) after approximately 5.5 hours. In Fig. 6.13, the $^{83m}$Kr events seem to never mix into the top $\sim$100 $\mu$s of drift time in the TPC. We speculate that this
Figure 6.13. Histograms of data taken by the LZ TPC following the injection of $^{83m}$Kr. **Upper Left:** A histogram of top-bottom asymmetry versus the negative of the drift time for single-scatter (and two-S1, one-S2 events where the S1-pulse areas have been combined). A cut is shown selecting the events between the solid red lines, to remove accidental or otherwise unphysical S1-S2 pairs from the data. **Upper Right:** A histogram of the logarithm of S2-pulse area versus the logarithm of S1-pulse area for single-scatter events (and two-S1, one-S2 events where the S1-pulse areas have been combined). A cut selecting the $^{83m}$Kr events is shown by the solid red lines. **Bottom:** A histogram of the event time stamps versus the negative of the drift time for the $^{83m}$Kr events selected by the cuts in the first two histograms. The $^{83m}$Kr atoms are seen to enter the TPC at the bottom (large negative drift time) and slowly mix into the bulk. The gaps in the data are from periods of time when the DAQ was disabled.
apparent barrier at drift time = 100 $\mu$s is an artifact of the event selection. Near the top of the TPC (and extraction field) the width of S2 pulses is narrower because the S2 electrons travel a shorter distance and are subjected to less gaussian diffusion before being extracted. The narrower S2 pulses near the top of the TPC allow the two step decay of $^{83m}$Kr to be resolvable into two distinct S2s, such that some fraction of events near the top are not captured by the single-S2 (single scatters) selection cut in the above figures. More investigation is required to confirm that the data conforms to these ideas.

6.7 S1 Area Correction with $^{131m}$Xe and Injected $^{83m}$Kr in LZ

For events of a given energy and type, the pulse area of the measured S1 and S2 signals vary systematically as a function of position in the LZ TPC, as described in section 4.2.2, because of the position dependence of light and charge collection efficiency. In this section I present a correction to the S1-pulse areas in the LZ TPC as a function of 3-D position, demonstrated using the naturally present $^{131m}$Xe and an injection of $^{83m}$Kr. For the data in this analysis, the grids in the LZ TPC were biased at the 'Commissioning Voltages' reported in table 3.1.

6.7.1 $^{131m}$Xe-based S1 Area Correction in LZ

In-between testing and tuning of the grid voltages during the commissioning phase of LZ, approximately 19 hours of data containing $\sim$0.7 Bq of uniformly distributed $^{131m}$Xe from cosmogenic activation was used to produce the first S1-pulse area correction in the LZ TPC, presented here. First, all events with one S1 and one S2 (single scatter events) were selected. Within this data, the $^{131m}$Xe population ($\sim$44,000 $^{131m}$Xe events) appeared as a bright peak in a histogram of the logarithm of S2-pulse area versus the logarithm of S1-pulse area. The $^{131m}$Xe population was selected with a cut in this space (upper left of Fig 6.14). The TPC volume was then divided into
1,000 bins of equal volume (10×10×10) in x position versus y position versus the negative of the drift time, where the negative of the drift time is a proxy for the z position of an event in the TPC. The division of the TPC into position bins is shown in a set of three 2-D histograms in Fig. 6.14.

In each of the 1,000 position bins (voxels), the S1-pulse areas from events in the selected $^{131m}$Xe population were histogrammed and fit with a gaussian using the iterative fitting procedure described in section 4.2.2, if the histogram contained more than 25 events. The mean from the resulting gaussian fit in each position-bin (voxel) provides a measurement of the mean $^{131m}$Xe S1-pulse area at that position in the TPC. Example fits to the S1-pulse area histograms from four different TPC position bins (voxels) are shown in Fig 6.15. The mean from the gaussian fit in each position bin was used to fill a 3-D histogram of the negative of drift time versus x position versus y position, shown in Fig. 6.16. The 3-D histogram was normalized by dividing each bin (voxel) value by the average value of the eight bins (voxels) closest (and equidistant) to the TPC’s geometric center. This new map of the (mean) S1-pulse area relative to the TPC center constitutes the S1 area ‘response map’, and provides the value by which the S1-pulse area of any event in the TPC is divided to correct for position-dependent light-collection efficiency.

Because interpolation on this map is performed between bin-centers, events with reconstructed positions at high radius or extreme drift time can fall outside of the interpolatable boundaries of the map. To address this issue, a ‘map-extension algorithm’ was developed to fill the position bins (voxels) in the map where no data was present for fitting (or there were too few events [less than 25]), extending the boundaries of the map to beyond the positions corresponding to the physical TPC boundaries. The algorithm works by filling each empty bin in the response map with the distance-weighted average, with weight $p$, of the nearest $N$ bins which do have values from the gaussian fitting procedure. The distance weighted average used to fill
Figure 6.14. Histograms produced from LZ TPC data containing $^{131m}$Xe, with single-scatter events selected. **Top Left:** A histogram of the logarithm of S2-pulse area versus the logarithm of S1-pulse area. A cut selecting $^{131m}$Xe events is shown with solid red lines, and is applied to the other three histograms. **Top Right:** A histogram of the x position versus y position for the selected $^{131m}$Xe events in the LZ TPC. The division of the TPC into position bins (voxels) in this space is shown by the solid red lines. The apparent holes in the distribution are due to PMTs which were off during this preliminary data-taking period. **Bottom Left:** A histogram of the negative of the drift time versus x position for the selected $^{131m}$Xe events in the LZ TPC. The division of the TPC into position bins (voxels) in this space is shown by the solid red lines. **Bottom Right:** A histogram of the negative of the drift time versus y position for the selected $^{131m}$Xe events in the LZ TPC. The division of the TPC into position bins (voxels) in this space is shown by the solid red lines.
Figure 6.15. Histograms of the $^{131m}$Xe S1-pulse areas in four different position bins (voxels) in the LZ TPC. The resulting fit from the iterative gaussian fitting procedure is shown on each histogram in red. The position details of each bin, as well as a description of the bin’s relative position, are included.
Figure 6.16. A 3-D histogram mapping the mean $^{131}\text{Xe}$ S1-pulse area in the LZ TPC, in the negative of the drift time versus x position, versus y position, of the bin-centers of the position bins (voxels) used to divide the data. The same histogram is shown from two different views. The light-collection efficiency (mean $^{131}\text{Xe}$ S1-pulse area) appears highest at the bottom of the TPC, near the radial center.

Each empty bin is given by:

$$M_{\text{ext}} = \sum_{i=0}^{N} \frac{M_i \cdot d_{i-p}^{-p}}{d_{i-p}^p}.$$  \hspace{1cm} (6.5)

where $M_i$ is the value of, and $d_i$ is the distance to, the $i^{th}$ closest bin containing a value from gaussian fitting. The distance in 3-D is calculated with a scaling factor on the drift-time dimension, which converts the drift time to the same units as the x and y positions, centimeters. With the scaling factor applied, the distance between any two bins is given by:

$$d_i = \sqrt{\Delta X^2 + \Delta Y^2 + (\Delta t \cdot C)^2}.$$  \hspace{1cm} (6.6)

where the drift-time scaling factor, $C$, is equal to the height of the TPC (150 cm) divided by the maximum drift time for the present detector conditions (950 $\mu$s), $C = \frac{150 \text{ cm}}{950 \mu\text{s}} = 0.1579 \frac{\text{cm}}{\mu\text{s}}$. 

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Figure 6.17. A 3-D histogram mapping the mean $^{131}$Xe S1-pulse area in the LZ TPC, in the negative of the drift time versus x position, versus y position, of the bin-centers of the position bins (voxels) used to divide the data. **Left:** In this map, the previously empty bins have been filled by the extension algorithm in equation 6.5. The normalized values in this 'response map' are equal to the S1-light collection efficiency relative to the efficiency at the TPC's geometric center. **Right:** The same 'response map' is shown with the planes of constant drift time filled in by interpolation to better visualize the variation in x and y position.

The results of the normalization to the TPC center, and the filling of the empty position bins (voxels) using the extension algorithm with $N = 9$ and $p = 4$, are shown in the final response map, in Fig. 6.17. For a given event in the LZ TPC, the corrected S1-pulse area is obtained by performing trilinear interpolation on the response map (Fig. 6.17) at the position of the event in consideration. The raw S1-pulse area is divided by the result of the interpolation to produce the corrected S1-pulse area. Histograms of the initial data with only the single-scatter selection cut applied are shown with uncorrected and corrected S1-pulse areas in Fig. 6.18.

### 6.7.2 $^{83m}$Kr-based S1 Area Correction in LZ

Following the success of the first $^{83m}$Kr injection into LZ, a second, much larger, $^{83m}$Kr injection was performed to overcome the previously observed hours-long mixing.
Figure 6.18. Histograms produced from single-scatter events in the LZ TPC. Top Row: Histograms of the uncorrected S1-pulse area, the negative of the drift time versus the uncorrected S1-pulse area, and the uncorrected S1-pulse area versus x position, for all single-scatter events in the data set containing the $^{131m}$Xe population. Bottom Row: The same histograms appearing in the top row are reproduced with the S1-pulse area correction applied to all of the events. The various populations present in the data become more clearly resolved in each of the histogrammed parameter spaces.
timescale in the LZ TPC. The goal of the injection was to inject an activity of $^{83m}Kr$ which was large enough that the total activity would still be high ($\sim 100$ Bq) by the time that it became roughly uniform in the TPC, approximately 6 hours after the end of the injection. An injection of $\sim 1.6$ kBq of $^{83m}Kr$ was performed with the LZ SIS following the standard $^{83m}Kr$ injection procedure in section 6.2.1, and provided more than one million useful, and approximately uniformly distributed, $^{83m}Kr$ events. The large and uniform $^{83m}Kr$ population allowed for the development of an S1-pulse area correction with much higher resolution than the one developed from the population of $^{131m}Xe$ events in the previous section.

Following the injection, events with either one or two S1 pulses, and one S2 pulse, were selected. In events with two S1 pulses, the two pulse areas were added together to construct a single S1-pulse area for the event. A simple quality cut, shown in Fig. 6.19 (upper left), was applied to the selected events which further selected those which had a correlated top-bottom asymmetry (defined in equation 6.4) and drift time. With the quality cut applied, the $^{83m}Kr$ population was selected with a cut on the S1- and S2-pulse areas in the same way that the $^{131m}Xe$ was in the previous section (shown in Fig. 6.19 [upper right]). With many more $^{83m}Kr$ events than in the $^{131m}Xe$-based correction, the TPC was divided more finely, into 27,000 equally sized position bins (voxels) $(30\times30\times30)$ in x position versus y position versus the negative of the drift time. The results of the map produced by the iterative gaussian fitting of the S1-pulse area histograms in each bin, and the final normalized map produced by the extension algorithm with $N = 9$ and $p = 4$ (equation 6.5) are shown in Fig. 6.20.

Histograms of the initial data with only the single-scatter selection cut applied are shown with uncorrected and corrected S1-pulse areas in Fig. 6.21, demonstrating the success of the correction. The position binning in three orthogonal coordinates, and with high resolution, provides a more comprehensive correction of position-dependent effects than the S1 area corrections produced with simulated data, detailed in section.
Figure 6.19. Histograms produced from LZ TPC data following an injection of $^{83m}$Kr, with single-scatter events (and two-S1, one-S2 events where the S1-pulse areas have been combined) selected. **Upper Left:** A histogram of top-bottom asymmetry versus the negative of the drift time for all of the selected events. A cut selecting the events between the solid red lines, which removes accidental or otherwise unphysical S1-S2 pairs, is shown. **Upper Right:** A histogram of the logarithm of S2-pulse area versus the logarithm of S1-pulse area with the quality cut from the histogram in the upper left applied. A cut selecting the $^{83m}$Kr events is shown by the solid red lines. **Bottom Row:** Histograms showing the division of the TPC into position bins (voxels) in y position versus x position, the negative of the drift time versus y position, and the negative of drift time versus x position. The binning is shown by the overlaid red lines. In this preliminary LZ data, several PMT positions are known to be swapped in the position reconstruction algorithm, and several PMTs are off, resulting in non-uniformities in the reconstructed position distributions. The apparent non-uniformities at drift times near zero are likely an artifact of the selection cuts, since $^{83m}$Kr may produce events with two S2 pulses for decays very near the top of the TPC drift field (see section 6.7 for a more detailed discussion of the non-uniformity at drift times near zero).
Figure 6.20. 3-D histograms produced from selected $^{83m}$Kr events in the LZ TPC, in the negative of the drift time versus x position, versus y position, of the bin-centers of the position bins (voxels) used to divide the data. **Left:** A 3-D histogram of the $^{83m}$Kr S1-area means from iterative gaussian fits of the raw S1-pulse areas. **Right:** The 3-D LZ TPC response map, containing the normalized (to the TPC center) $^{83m}$Kr S1-area means. The bins without values from the iterative gaussian fitting were filled by the extension algorithm in equation 6.5 with $N = 9$ and $p = 4$. The normalized values in this response map are equal to the S1-light collection efficiency relative to the efficiency at the TPC’s geometric center.
Figure 6.21. Histograms produced from single-scatter events (and two-S1, one-S2 events where the S1-pulse areas have been combined) in the LZ TPC, in data following an injection of $^{83m}$Kr. **Top Row:** Histograms of the uncorrected S1-pulse area, the negative of the drift time versus the uncorrected S1-pulse area, and the uncorrected S1-pulse area versus x position. **Bottom Row:** The same histograms that appear in the top row are reproduced with the S1-pulse area correction from the map in Fig. 6.20 applied to all of the events. The various populations present in the data become more clearly resolved in each of the histogrammed parameter spaces.
4.2.2, or with the $^{131m}$Xe present in LZ from activation, presented in the previous section. The 30×30 binning in x and y position (900 bins in each plane of constant drift time) is significant because it exceeds a resolution of one x-y bin per-PMT, and is therefore sensitive to position-dependent effects below the length-scale of a single PMT in the LZ TPC.

6.8 Results from the first two $^{220}$Rn Injections into LXe in LZ

Prior to the first dedicated science run in LZ, $^{220}$Rn was injected continuously into the LXe in the LZ TPC on two separate dates, 19 days apart, following the injection procedure in section 6.2.3. The detector conditions were similar during the two injections, allowing the data from both injections to be combined for the analysis presented in this section. The grids in the LZ TPC were biased at the 'Commissioning Voltages' reported in table 3.1 during the two $^{220}$Rn injections. Both injections were performed by flowing carrier GXe through the $^{220}$Rn generator at 500 SCCM. The first injection consisted of 7 hours of flow through the generator punctuated by separate breaks of 20 minutes and 1 hour. The second injection consisted of 6 hours of continuous flow with no breaks.

The first surprising result from the two injections was that $^{220}$Rn atoms injected into the LZ circulation system were seen to survive the transit to the TPC, despite the expected >5 minute transit time for the carrier GXe. The $\alpha$-decays from $^{220}$Rn and $^{216}$Po appeared approximately 4.5 minutes after the start of flow through the $^{220}$Rn generator, and were identified by a sudden increase in the trigger rate in the TPC, as well as by their position distribution in the TPC. The alphas were seen to decay promptly upon entering the TPC, as bright spots in histograms of event y position versus x position, and of the negative of drift time versus radius from the TPC’s central axis, squared. Both histograms, for single scatter (one-S1, one-S2) events, are
Figure 6.22. Histograms produced from single-scatter events in the LZ TPC during, and immediately following, two injections of $^{220}$Rn (the data from the two injections is combined in the histograms). **Left:** A histogram of the y position versus the x position for the events in the selected data. The prompt α-decays from $^{220}$Rn and $^{216}$Po are seen to be concentrated at the location of the seven TPC inlet tubes from the LZ circulation system. One inlet tube is located at the radial center, and the others are located at the vertices of a hexagon, concentric with the TPC. Four additional high density populations are visible at the location of known grid 'hot-spots', where electrons are spontaneous emitted from the biased grids in this preliminary LZ TPC data. Events from the grid hot-spots will be vetoed in the future with data-quality cuts, or mitigated with changes to the grids themselves. **Right:** A histogram of the negative of the drift time versus the radius from the TPC’s central axis, squared, for the events in the selected data. The prompt α-decays from $^{220}$Rn and $^{216}$Po are seen to be concentrated at the bottom of the TPC, at the radii of the TPC inlet tubes from the LZ circulation system.

shown in Fig. 6.22 with the data taken during and immediately after both injections combined.

The primary goal of these $^{220}$Rn injections was to identify and characterize the low-energy ER band using ground-state decays from $^{212}$Pb, which decays with β-energies all the way down to the energy threshold of LZ. During this data, the LZ analysis chain was continually improving its ability to identify and classify low-energy pulses, though many issues were present at the time that this data was analyzed, both understood and not. Of particular note, several PMT tag-names were swapped in the
position-reconstruction code, and have since been fixed. Additionally, the pulse-classifier had not been fully tuned yet, and used the $^{220}$Rn injection data presented here to inform further adjustments. At the time of this analysis, none of the data-quality cuts presented in the following paragraphs had been standardized.

To understand whether we had succeeded in injecting enough $^{212}$Pb to characterize the low-energy ER band, a series of basic data-quality cuts were developed to remove mis-classified and accidental, or coincidence, background events in the low-energy single-scatter data. First, a fiducial volume cut was applied to select single-scatter events whose reconstructed positions were not near the walls of the TPC, where signal loss is most severe. With the fiducial cut applied, quantities called ”Good Area” and ”Bad Area” were defined for each event. Good Area was defined as the sum of the S1 and S2 pulse area, and Bad Area was defined as the sum of all other identified pulses in the event (which were not S1 or S2 pulses), which include single electrons emitted by the LXe surface, single or multiple photo-electrons spontaneously emitted from the PMT photo-cathodes, or any other sources of PMT noise. The fiducial volume cut, as well as a cut on Bad Area are shown in the histograms in Fig. 6.23 (top).

Also shown in Fig. 6.23 are two histograms which illustrate another data-quality cut that was applied. First, a straight line was fitted to the peak of the correlated population in the histogram of the negative of the drift time versus the top-bottom asymmetry (TBA) for the single-scatter events which passed the fiducial volume cut. This best fit constitutes the ”TBA-prediction” from the drift time of a given event. The TBA-prediction model can be used to predict the TBA of low-energy events with S1-pulse areas too small to define an accurate TBA. A second histogram was made, demonstrating the failure of TBA for small S1-pulse areas, of the difference between the TBA and the drift-time-predicted TBA from the fit, versus the S1-pulse area of the event. Accounting for the fact that the strength of the correlation between
Figure 6.23. Histograms produced from single scatter events in the LZ TPC during and after two $^{220}$Rn injections (combined data), illustrating data quality cuts for the low-energy ER-band analysis with injected $^{212}$Pb. The histogram in the top left has no additional cuts applied, and the other three histograms have only the fiducial volume cut (shown in the top left) applied. Upper left: A histogram of the negative of drift time versus the radius from the TPC’s central axis, squared, for the selected events. Events inside of the overlaid red box (fiducial volume) were selected to remove events near the TPC walls and grids from the data. Upper right: A histogram of the logarithm of the constructed "Good Area" quantity versus the logarithm of the constructed "Bad Area" quantity (defined in the text). Events below the red line were selected in the low-energy ER-band analysis to remove events with a high fraction of PMT noise and accidental coincidences. Lower left: Histogram of the negative of drift time versus top-bottom asymmetry (TBA) for the selected events. The dashed black line was fitted to the peak of the correlated population in this parameter space. The dashed black line is used to predict the TBA from the known drift time, when the S1-pulse area is too small to define an accurate TBA. Lower right: A histogram of the difference between the TBA and the drift-time-predicted TBA of the event versus the event’s S1-pulse area. A cut is applied selecting events which don’t deviate strongly from the "TBA-prediction" model, between the solid red lines overlaid in the histogram. In total, this cut selects events which have correlated TBA and drift time, but allows the correlation to be weaker for small S1-pulse areas.
drift time and TBA is dependent on S1-pulse area, the selection cut was made in the second parameter space, and is shown in Fig. 6.23 (lower right).

Four more data-quality cuts, designed to eliminate events with mis-classified pulses, coincidental S1 and S2 pairings, and other unphysical backgrounds, were applied and are shown in Fig. 6.24. First, events with a small root-mean-square S1-pulse width were selected, rejecting events whose S1 pulses were un-physically wide (or were mis-classified) (Fig. 6.24, upper left). The root-mean-square width of a given S2 pulse is a function of drift time, since in events where the electrons produced must drift further through the TPC before being extracted, the electrons naturally become more diffuse. A cut selecting the anti-correlated population in a histogram of the negative of the drift time versus the root-mean-square S2-pulse width was also applied (Fig. 6.24, upper right). The maximum S1-pulse area measured by a single PMT channel divided by the total S1-pulse area from all PMT channels is a quantity which increases sharply for small S1 pulses, where a larger fraction of the S1 photons are detected by fewer PMTs. A histogram of this ratio versus the total S1-pulse area was used to define a cut which selects events with statistically physical PMT pulse-area distributions in the TPC (Fig. 6.24, lower left). The last data-quality cut applied to the $^{220}$Rn injection data was on a pulse-shape quantity defined as the ratio of the time from the start of the S2 pulse in which the pulse reached 5% of its total pulse area, to the time from the start of the S2 pulse in which the pulse reached 50% of its total pulse area. S2 pulses with a very sharp rising edge have a ratio close to 1, while S2 pulses with a very gradual rising edge have a ratio closer to 0. Real S2 pulses are seen to have a characteristic ratio between approximately 0.2 and 0.7, the range that the cut was chosen to select (Fig. 6.24, lower right).

With all of these cuts applied, the ratio of ‘real’ interactions in the TPC to coincidence and accidental background events is significantly increased in the low-energy ER region. The ER band produced from decays of the $^{212}$Pb population in the TPC
Figure 6.24. Histograms of single scatter events during and after the two $^{220}$Rn injections into the LZ TPC (combined data), illustrating data quality cuts for the low-energy ER-band analysis with injected $^{212}$Pb. All four histograms shown have the fiducial volume cut from Fig. 6.23 applied. **Upper Left:** Histogram of the root-mean-square S1-pulse width versus the logarithm of the S1-pulse area. Events below the solid red line overlaid onto the histogram were selected to remove events with mis-classified S1 pulses (unphysical S1 pulse widths). **Upper Right:** Histogram of the negative of the drift time versus the root-mean-square S2-pulse width. Events between the solid red lines overlaid onto the histogram were selected to remove events with mis-identified or coincident S2 pulses (unphysical S2 pulse widths). **Lower Left:** Histogram of the maximum S1-pulse area measured by a single PMT channel divided by the total S1-pulse area from all PMT channels, versus the total S1-pulse area. Events below the overlaid red line were selected to remove events with unphysical PMT pulse-area distributions. **Lower Right:** Histogram of the ratio of the time from the start of the S2 pulse in which the pulse reached 5\% of its total pulse area to the time from the start of the S2 pulse in which the pulse reached 50\% of its total pulse area, versus the logarithm of the S2-pulse area. Events between the overlaid red lines are selected to remove events with uncharacteristic S2-pulse shapes.
Figure 6.25. Histograms produced from low-energy single-scatter events in the LZ TPC during and immediately following two $^{220}$Rn injections (combined data). **Upper Left:** Histogram of the logarithm of the S2-pulse area versus the logarithm of the S1-pulse area. **Upper Right:** The same histogram of the logarithm of the S2-pulse area versus the logarithm of the S1-pulse area after applying the fiducial volume cut, and the six data-quality cuts described previously in this section. The series of cuts reveal the ER-band from the injected $^{212}$Pb.

during and after the two $^{220}$Rn injections is shown in Fig. 6.25, before and after the selection cuts described in this analysis were applied.

The NEST-simulated threshold response of the LZ TPC that was detailed in section 4.2.5 can be used to analyze the efficiency of the analysis chain which produced the low-energy ER band detailed in this section. The same empirical error-function best fit to the reconstructed energy spectrum of $6 \times 10^5$ NEST-simulated $^{212}$Pb events is shown in Fig. 6.26, overlaid onto the reconstructed energy spectrum of the low-energy ER events in the LZ TPC, selected by data-quality cuts detailed in this section. The 50%-efficiency threshold from the error-function fit to the NEST data is $\mu = 1.24 \pm 0.18$ keVee. The g1 and g2 values used to reconstruct the energies of the LZ ER-band events (following equation 2.1) were measured separately. The (lower-than-expected) shape of the reconstructed energy spectrum for the ER-band events below $\sim 10$ keVee in Fig. 6.26 appears to indicate an inefficiency at identifying or selecting the lowest energy events in the LZ TPC. This inefficiency could be introduced by some combination of the pulse identification and pulse-classification algorithms, or
Figure 6.26. Top: The ratio of the reconstructed energy spectrum of the $^{212}$Pb ER-band events in the LZ TPC to the theoretical ground-state $^{212}$Pb decay spectrum. An empirical error-function best fit to the ratio of the simulated (with NEST) reconstructed energy spectrum to the theoretical ground-state $^{212}$Pb decay spectrum is overlaid onto the plot as a red line. The discrepancy between the data and the model in the number events below 10 keVee hints at a possible inefficiency in some part(s) of the analysis chain. The higher-than-expected number of events in the 1 keVee bin suggests that accidental or mis-classified background events are still present after the data-quality cuts isolating the ER-band were applied. **Bottom:** Bin-by-bin fit residuals between the data and overlaid error-function fit from the NEST simulation, highlighting the inefficiency below 10 keVee.
the data-quality cuts described in this analysis. With a detailed study, adjustments
to any of these could potentially be made to recover some of this lost efficiency near
threshold. All of the data-quality cuts described in the ER-band analysis presented
in this section were adjusted to be relatively conservative, cutting as few real low-
energy ER-band events from the selection as possible at the expense of background
rejection. Because of this, some un-physical events remain in the selected population
in figures 6.25 and 6.26. In particular, the higher-than-expected number of events in
the 1 keVee bin in Fig. 6.26 suggests that a significant amount of accidental or mis-
classified background events are still present after the application of the data-quality
cuts developed for the ER-band selection. New data-quality cuts will be developed
in the future (and refinements will be made to the existing ones) which improve the
efficiency of the low-energy ER-band selection in the LZ TPC.

6.9 Position-Dependent g1 and g2 Analysis in LZ

Traditionally, the detector gains, g1 and g2 (the average number of detected pho-
tons [phd] per interaction-site photon and electron, respectively), are calculated after
position corrections are applied to the S1- and S2-pulse areas. This traditional Doke
analysis results in single g1 and g2 values which describe the entire detector volume.
In this section, we present a novel alternative approach in which the position correc-
tion step is omitted, and the position dependence of S1- and S2-pulse areas is folded
into the definition of g1 and g2, turning g1 and g2 into position-dependent quantities
(as was shown with simulated LZ data in section 4.2.3). Measuring g1 and g2 as
a function of position, from uncorrected S1- and S2-pulse areas, results in a direct
measurement of the detector response at each position, and accounts for the field and
energy dependent recombination as a function of position in the TPC automatically.
In this way, this alternative position-dependent Doke analysis supplies a substan-
tial refinement over the traditional approach, by naturally separating the two main sources of position dependence in the TPC’s measured light and charge signals:

- position dependence from gain/efficiency effects (g1 and g2), including those from the geometry of the TPC materials.
- position dependence of the true number of photons and electrons produced at the interaction site, including as a result of electric field variations.

The position-dependent Doke analysis measures the gains directly, ‘orthogonalizing’ the problem naturally by distinguishing position dependence in gains from position dependence in electron-ion recombination. Any additional variation in signal amplitudes, unaccounted for by the position-dependent gains, must then be attributed to variation in the initial number of photons and electrons produced by the interaction. As in the traditional approach, the position-dependent g1 and g2 can still be used for event energy reconstruction as well.

The data from the second (1.6 kBq) $^{83m}$Kr injection into LZ was used for the analysis in this section because of the naturally present $^{131m}$Xe, $^{129m}$Xe, and $^{127}$Xe populations from activation, in addition to the very large number of $^{83m}$Kr events. The $^{129m}$Xe and (202 keV-\(\gamma\) + K-Shell EC) $^{127}$Xe populations appear at the same energy, as one overlapping peak in the data at 236 keV. First, events with one S1 and one S2 (single scatter events), and with two S1s and one S2 (\(83m\)Kr-like events) were selected. For events with two S1s and one S2, a single S1-pulse area was calculated by adding the two S1-pulse areas together. A cut on the data in top-bottom asymmetry (TBA) versus the negative of the drift time, shown in Fig. 6.27, was made to remove accidentals or otherwise unphysical S1-S2 pairs. Next, the $^{83m}$Kr, $^{131m}$Xe, and 236 keV populations, which appear as bright peaks in a histogram of S2- versus S1-pulse area, were selected with a simple cut in that parameter space, also shown in Fig. 6.27. The TPC was then divided into 252 spatial bins (voxels) in the negative of drift time versus x position versus y position (7×6×6). The division of the TPC is
Figure 6.27. Histograms produced from LZ TPC data following an injection of $^{83m}$Kr, with single-scatter events (and two-S1, one-S2 events where the S1-pulse areas have been combined) selected. **Left:** A histogram of top-bottom asymmetry versus the negative of the drift time for all of the selected events. A cut selecting the events between the solid red lines, which removes accidental or otherwise unphysical S1-S2 pairs, is shown. **Upper Right:** A histogram of the logarithm of the corrected S2-pulse area versus the logarithm of corrected S1-pulse area with the cut defined in the histogram on the left applied. Despite using the uncorrected pulse areas for the remainder of the Doke analysis, the corrected pulse areas are used for the simple task of selecting the populations at the beginning of the analysis.
Figure 6.28. Histograms showing the division of the TPC into position bins (voxels) in y position versus x position (left), the negative of the drift time versus x position (center), and the negative of drift time versus y position (right). The binning is shown by the overlaid red lines. In this preliminary LZ data, several PMT positions are known to be swapped in the position reconstruction algorithm, and several PMTs are off, resulting in non-uniformities in the reconstructed position distributions.

illustrated in Fig. 6.28, which shows the position distribution of the combined $^{83m}$Kr, $^{131m}$Xe, and $^{129m}$Xe + (202 keV-γ + K-Shell EC) $^{127}$Xe populations from the selection cuts. In each spatial bin, and for each of the selected populations independently, 2-D histograms of S1/E versus S2/E were filled, where E is the energy of the given population’s (mono-energetic) decay. The histograms were fitted with gaussians in both dimensions independently, using the iterative gaussian fitting procedure described in section 4.2.2, and the 2-D mean in S1/E-vs-S2/E-space was measured from the fits for each population, and for each position bin (voxel). A Doke plot was created in every position bin (voxel) with a data point from the gaussian mean of each of the three mono-energetic populations. Four of these Doke plots are shown in Fig. 6.29 as examples. The Doke plots were fitted with a straight line whose x and y intercepts provide a measurement of g1 and g2 in each respective position bin (voxel) when multiplied by the xenon work function, W ($0.0137 \pm 0.0002$ keV/quanta [25]). The resulting maps of the LZ TPC g1 and g2 as a function of position are shown in Fig. 6.30. Filling in the maps by interpolation in the planes of constant drift time
Figure 6.29. Example Doke plots produced from iterative gaussian fits to the uncorrected S1- and S2-pulse area distributions of selected $^{83m}$Kr, $^{131m}$Xe, and $^{129m}$Xe + (202 keV-$\gamma$ + K-Shell EC) $^{127}$Xe populations in the LZ TPC. The position of the bin-center is displayed for each Doke plot’s corresponding position bin (voxel), and the relative position of the bin (voxel) in the TPC is described.
Figure 6.30. Maps of the LZ TPC g1 and g2, in units of phd/photon (g1) and phd/electron (g2), as a function of position, produced from data containing $^{83m}$Kr, $^{131m}$Xe, and $^{129m}$Xe + (202 keV-γ + K-Shell EC) $^{127}$Xe populations.

makes the variation in g1 and g2 as a function of position much easier to visualize, and is shown in Fig. 6.31. As is expected, the light-collection efficiency (g1) is highest near the bottom of the TPC and bottom PMT array (the LXe-GXe interface at the top of the TPC is highly reflective, resulting in the majority of S1 photons being observed by the bottom PMT array). Also expected, the charge-collection efficiency (g2) is highest near the radial center of the TPC, furthest from the TPC walls (where signal loss is the most prevalent).

For a given event, the g1 and g2 values at the position of the interaction site can be estimated by trilinear interpolation on the g1 and g2 maps from Fig. 6.30. With the ability to estimate the unique g1 and g2 at any position in the TPC, the energy of a given event is again reconstructed using the relationship $E = W(\frac{S_1}{g_1} + \frac{S_2}{g_2})$, introduced in section 2.2, though with the uncorrected S1- and S2-pulse areas, since position-dependent effects are captured in the position dependence of g1 and g2. The reconstructed energy spectrum of the events which passed the initial event topology cut (single scatter and two-S1, one-S2 events) is shown in Fig. 6.32, in addition to the reconstructed energy spectrum calculated from global g1 and g2 values. The global g1
Figure 6.31. The maps of the LZ TPC $g_1$ and $g_2$ as a function of position from Fig. 6.30 with the planes of constant drift time filled in by interpolation to better visualize the position-dependence. The light-collection efficiency ($g_1$) is highest near the bottom of the TPC, while the charge-collection efficiency ($g_2$) is highest near the radial center of the TPC, furthest from the TPC walls.

and $g_2$ values were obtained from the best fit to the Doke plot produced by fitting the selected $^{83m}$Kr, $^{131m}$Xe, and 236 keV populations with the $^{83m}$Kr S1-area correction from section 6.7.2 applied (with no position binning). In the direct comparison of the reconstructed energy spectra from the traditional (global) $g_1$ and $g_2$, and from the position-dependent $g_1$ and $g_2$, the two spectra are extremely similar despite the relatively coarse division of the TPC in the position dependent $g_1$ and $g_2$ analysis, demonstrating the power of this novel approach.

S1- and S2-pulse area corrections can be very easily defined from the position-dependent $g_1$ and $g_2$ maps. When an S1- or S2-pulse area is divided by the value of $g_1$ or $g_2$, respectively, at the position where the event occurred in the TPC, the result is the real number of (S1) photons or (S2) electrons produced at the interaction site. For the selected $^{83m}$Kr population, maps of $S_1/g_1$ (interaction site photons produced) and $S_2/g_2$ (interaction site electrons produced) were created and are shown in Fig. 6.33,
Figure 6.32. Reconstructed energy spectra from the position-dependent g1 and g2 measurement in the LZ TPC detailed in this section (blue), and from a traditional global g1 and g2 measurement (red), performed separately with the same data. The position-dependent g1 and g2 produce an extremely similar energy spectrum to the global g1 and g2, despite having a relatively crude (7×6×6) interpolation-map resolution.
Figure 6.33. Maps of $S1/g1$ (interaction-site photons produced) and $S2/g2$ (interaction-site electrons produced) as a function of position for $^{83m}\text{Kr}$ in the LZ TPC. The planes of constant drift time are filled in by interpolation to better visualize the position-dependence. The observed variation in the number of photons and electrons produced as a function of position is consistent with there being no electric-field variation in the fiducial volume. Slight variation is observed however, near the very top and bottom of the TPC, consistent with the expected shape of the electric-field variation near the grids.

with the planes of constant drift time filled in by interpolation to better visualize the variation with position.

The ability of the position-dependent Doke analysis to produce comparable results to the standard global analysis with a relatively low resolution ($7 \times 6 \times 6$) division of the TPC is promising for the future of this analysis, when a much finer binning may be achieved. The resolution of the position-binning was limited in this analysis by the activity of the $^{131m}\text{Xe}$, $^{129m}\text{Xe}$, and $^{127}\text{Xe}$ in the LZ TPC, but could be greatly improved if both $^{83m}\text{Kr}$ and $^{131m}\text{Xe}$ were injected into the TPC before the analysis, and if the $^{129m}\text{Xe}$ and $^{127}\text{Xe}$ activity was slightly enhanced, perhaps as the result of a recent DD or AmLi neutron calibration. In addition to the accurate energy reconstruction, the production of $S1/g1$ and $S2/g2$ maps were made possible by the
position-dependent $g_1$ and $g_2$ maps, and provided direct insight into the interaction-site micro-physics of each event. These maps can be used in the future to study electric field variation in the LZ TPC by searching for variation in the relative number of photons and electrons produced in interactions.
CHAPTER 7
CONCLUSION

The unique calibration challenges presented by tonne-scale LXe detectors have been shown in this work to be successfully addressed by calibration hardware designed, constructed, and tested in a dedicated LXe detector at UMass Amherst, built explicitly for this purpose. The prototype source injection system (SIS) and accompanying calibration source hardware, developed at UMass Amherst, have demonstrated the ability to precisely measure and inject calibration radio-isotopes directly into the LXe targets of the UMass LXe detector and the LZ experiment. The calibration hardware for LZ has demonstrated over three-orders of magnitude of control of the injected activity for the flow-through calibration sources tested with the UMass LXe detector. This precision in the injected activity has saved valuable time in the commissioning schedule of the LZ experiment, allowing calibrations to be planned efficiently, and with the ability to reliably estimate the activity of each calibration radio-isotope in the TPC at all times. Additionally, the successful injections of $^{83m}$Kr, $^{131m}$Xe, $^{220}$Rn, and CH$_4$ into LZ, using procedures developed and tested at UMass Amherst, have facilitated the variety of critical calibrations of the LZ TPC and LXe skin presented in this work.

A preliminary measurement of the methane removal timescale from the LZ TPC by purification in the circulation system was made possible by the successful injection of CH$_4$ (natural methane) with the LZ SIS. This measurement paves the way for an injection of CH$_3$T into LZ, to produce a high-stats calibration of the low-energy ER-band following the first dedicated WIMP-search run. In situ $^{127}$Xe present in early LZ
data from cosmogenic activation of the xenon was used to make the first measurement of the tagging efficiency of the LXe skin for $\mathcal{O}(100\text{ keV})$ $\gamma$-rays produced by $^{127}\text{Xe}$ decays near the TPC walls.

The analyses in this thesis which were developed and practiced on simulated LZ data have contributed to the success of the analogous analyses of real LZ data. Critical to the success of LZ, a correction for position-dependent effects on S1-pulse area was developed with injected $^{83\text{m}}\text{Kr}$ in the LZ TPC, with high enough resolution to be sensitive to effects at sub-single-PMT length scales. A novel method for measuring the detector gains, $g_1$ and $g_2$, as a function of position was developed, achieving a more accurate event-energy reconstruction than achieved with the traditional $g_1$ and $g_2$ procedure, in simulated data. The measurement of position-dependent $g_1$ and $g_2$ was demonstrated using $^{83\text{m}}\text{Kr}$, $^{131\text{m}}\text{Xe}$, $^{129\text{m}}\text{Xe}$, and $^{127}\text{Xe}$ in real LZ data, and achieved event-energy reconstruction that was as accurate as with the global $g_1$ and $g_2$ analysis, despite its low-resolution ($7 \times 6 \times 6$) division of the TPC into position bins, leaving significant room for future improvement. The successful measurement of position-dependent $g_1$ and $g_2$ in LZ opens up promising new analyses too, particularly regarding electric-field variation, using the direct measurements of interaction-site photon ($S_1/g_1$) and electron ($S_2/g_2$) production demonstrated in this thesis.

The LZ internal calibration hardware, developed for LZ and extensively tested at UMass Amherst, represents the cutting edge in precision for calibrating LXe TPCs. The results achieved in the UMass LXe detector, and the early success of the first calibration injections into LZ, have prepared the LZ experiment to be highly sensitive in its WIMP-search data-taking. The LZ calibration-source and injection-system hardware presented in this work, and the lessons learned from using them, will be valuable contributions to calibration source hardware in next-generation LXe TPCs, and future liquid-noble particle detectors of all types.
APPENDIX A
NUMERICAL $^{220}$Rn DECAY CHAIN SIMULATION

The code of the numerical $^{220}$Rn-decay-chain simulation, described in section 4.3, is presented below. The simulation was written with Python 3.8:

```python
import numpy as np
import matplotlib.pyplot as plt
import math
import time as stopwatch

#--------------------------- Settings ----------------------------#
Rn_0 = 4.0  # Rn220 Specific Activity Entering the Detector (Initial rate if Continuous == False, Steady-State rate if Continuous == True)
Pb_a = 10.0  # Pb212 Atoms Entering the Detector Independent of Rn_0 per second

time = 17.0  # Total time to simulate (hours)
dt = 0.2  # Time step - seconds. Small for better approximation
inj_L = 7.0  # Length of injection in hours (only used when Continuous is True)

ER_Background = 19.06  # Events/keV in 60d between 1.5-6.5 keV
pur_tau = 3.57  # Purification by re-circulation 'half-life' (10,000 kg LXe at 550 SLPM) (used if Purification == True)

#pur_tau = 0.0424  # Purification by re-circulation 'half-life' (90 kg Gx at 250 SLPM) (used if Purification == True)
pur_dt = 1.0  # Purification time step in seconds (if Purification = True)

Pb212_only_mode = False  # If True, Rn220 and Po216 are not shown (don't make it into the TPC)

Purification = True  # If True, isotopes are removed according to LZ
Continuous = True  # If True, the Rn220 rate will stay fixed at the injection value
Cryopumping = False  # If True, performs additional injection 24 hours after the first one, to account for a cryopumping period
Gas_only_mode = False  # If True, only alpha decays are shown in the plots
```

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Time_Units_plt = 'hours'  # Minutes or Hours or Days

#-------------------------- Constants -----------------------------#

#-- Decay Constants --#
Rn220_C = math.log(2)/55.6  # Halflife = 55.6 sec
Po216_C = math.log(2)/0.145  # Halflife = 145.0 ms
Pb212_C = math.log(2)/(10.64*60.0*60.0)  # Halflife = 10.64 h
Bi212_C = math.log(2)/(60.55*60.0)  # Halflife = 60.55 min
Po212_C = math.log(2)/(0.000000299)  # Halflife = 0.299 us
Tl208_C = math.log(2)/(3.053*60.0)  # Halflife = 3.053 min

alpha_ion_frac = 0.503  # Charged frac of alpha daughters from EXO-200
beta_ion_frac = 0.764  # Charged frac of beta daughters from EXO-200

Bi_Po = 0.6406  # Bi212->Po212 Branching Fraction
Bi_Tl = 0.3594  # Bi212->Tl208 Branching Fraction

#----------------- Defining Convenient Variables -----------------#
alpha_neutral_frac = 1.0-alpha_ion_frac  # Neutral frac of alpha daughters
beta_neutral_frac = 1.0-beta_ion_frac  # Neutral frac of beta daughters

secs = int(60.0*60.0*time)  # Run time in seconds
steps = int(secs/dt)  # Number of dt steps
pur_frac = pur_dt/(pur_tau*24.0*60.0*60.0)  # fraction of isotopes removed each pur_dt

#---------------------- Initializing Arrays -----------------------#
t = np.zeros(steps)  # time array

#- Number of Atoms # #-- Decayed Atoms # #-- Cumulative Events #-
Rn220=np.zeros(steps); dRn220=np.zeros(steps); Rn220C=np.zeros(steps);
Po216=np.zeros(steps); dPo216=np.zeros(steps); Po216C=np.zeros(steps);
Pb212=np.zeros(steps); dB212=np.zeros(steps); Pb212C=np.zeros(steps);
Bi212=np.zeros(steps); dB212=np.zeros(steps); Bi212C=np.zeros(steps);
Po212=np.zeros(steps); dPo212=np.zeros(steps); Po212C=np.zeros(steps);
Tl208=np.zeros(steps); dTl208=np.zeros(steps); Tl208C=np.zeros(steps);
Pb208=np.zeros(steps);

Rn220[0] = Rn_0/Rn220_C  # Number of atoms
dRn220[0] = Rn_0  # Initial dN/dt

#------------------------ Main Loop ---------------------------#
for i in range(1,steps):
    t[i] = dt*i

    #---------- Rn220 ----------
dRn220_tmp = (Rn220_C*Rn220[i-1]*dt)  # Number of decays in dt
    if(dRn220_tmp > Rn220[i-1]):  # If the # decayed > # remaining
        Rn220[i] = 0  # Then the # remaining is 0 (not negative)
        dRn220[i] = Rn220[i-1]  # The # decayed = current # of atoms
    else:
        Rn220[i] = Rn220[i-1]-dRn220_tmp
        dRn220[i] = dRn220_tmp

    Rn220C[i] = Rn220C[i-1]+dRn220[i]

if Continuous==True:
    if Cryopumping==True:
        full = (t[i]<3600.0*inj_L) | \
        (t[i]>3600.0*24.0) & (t[i]<3600.0*(24.0+inj_L))
if(full == True):
    Rn220[i] = Rn220[i]+(Rn_0*dt)

elif(t[i]<3600.0*inj_L):
    Rn220[i] = Rn_0/Rn220_C

#------------- Po216 --------------#

dPo216_tmp = (Po216_C*Po216[i-1]*dt)
if(dPo216_tmp > Po216[i-1]):
    Po216[i] = 0
dPo216[i] = Po216[i-1]
else:
    Po216[i] = Po216[i-1]+dRn220[i]-dPo216_tmp
dPo216[i] = dPo216_tmp

Po216C[i] = Po216C[i-1]+dPo216[i]

#------------- Pb212 --------------#

dPb212_tmp = (Pb212_C*Pb212[i-1]*dt)
if(dPb212_tmp > Pb212[i-1]):
    Pb212[i] = 0
dPb212[i] = Pb212[i-1]
else:
    Pb212[i] = Pb212[i-1]+dPo216[i]-dPb212_tmp
dPb212[i] = dPb212_tmp

Pb212C[i] = Pb212C[i-1]+dPb212[i]

if Continuous==True:
    if Cryopumping==True:
        full = ((t[i]<3600.0*inj_L)) | ((t[i]>3600.0*24.0) & (t[i]<3600.0*(24.0+inj_L)))
        if(full == True):
            Pb212[i] = Pb212[i]+(Pb_a*dt)
        elif(t[i]<3600.0*inj_L):
            Pb212[i] = Pb212[i]+(Pb_a*dt)

#------------- Bi212 --------------#

dBi212_tmp = (Bi212_C*Bi212[i-1]*dt)
if(dBi212_tmp > Bi212[i-1]):
    Bi212[i] = 0
dBi212[i] = Bi212[i-1]
else:
    Bi212[i] = Bi212[i-1]+dPb212[i]-dBi212_tmp
dBi212[i] = dBi212_tmp

Bi212C[i] = Bi212C[i-1]+dBi212[i]

#------------- Po212 --------------#
# These decay instantly in the time-steps of this sim, so never accumulate
dPo212[i] = dBi212[i]*Bi_Po
Po212[i] = 0
Po212C[i] = Po212C[i-1]+dPo212[i]

#------------- Tl208 --------------#

dTl208_tmp = (Tl208_C*Tl208[i-1]*dt)
if(dTl208_tmp > Tl208[i-1]):
    Tl208[i] = 0
\[dTl208[i] = Tl208[i-1]\]

else:
\[Tl208[i] = Tl208[i-1]+(dBi212[i]*Bi_Tl)-dTl208\_tmp\]
\[dTl208[i] = dTl208\_tmp\]
\[Tl208C[i] = Tl208C[i-1]+dTl208[i]\]

#---------------------- Final Analysis ---------------------------#

# Total Activities
Total = (dRn220[0::2]/dt)+(dPo216[0::2]/dt)+(dPb212[0::2]/dt)
\[\rightarrow +(dBi212[0::2]/dt)+(dPo212[1::2]/dt)+(dTl208[0::2]/dt)\]
\[Pb212Total = (dBp212[0::2]/dt)+(dBi212[0::2]/dt)+(dPo212[1::2]/dt)\]
\[\rightarrow +(dTl208[0::2]/dt)\]
Gas_Total = (dRn220[0::2]/dt)+(dPo216[0::2]/dt)
\[\rightarrow +(dBi212[0::2]/dt)*Bi_Tl)+(dPo212[1::2]/dt)\]

# Total Cumulative Events
TotalC = Rn220C[0::2]+Po216C[0::2]+Pb212C[0::2]+Bi212C[0::2]
\[\rightarrow +Po212C[1::2]+Tl208C[0::2]\]
\[Pb212TotalC = Pb212C[0::2]+Bi212C[0::2]+Po212C[1::2]+Tl208C[0::2]\]
\[\rightarrow \] Cumulative events w/o Rn220, Po216

# Total Atoms
TotalA = Rn220[0::2]+Po216[0::2]+Pb212[0::2]+Bi212[0::2]
\[\rightarrow +Po212[1::2]+Tl208[0::2]+Pb208[0::2]\]
\[Pb212TotalA = Pb212[0::2]+Bi212[0::2]+Po212[1::2]+Tl208[0::2]+Pb208[0::2]\]
\[\rightarrow \] Total Atoms w/o Rn220, Po216

print("Computation Time = "+str(round(stopwatch.time()-t0,1))\+" sec")

# Only show 1 of every X timesteps on plots, reduce memory usage
X = 20 # must be even
T_X = int(X/2.0)

if Time_Units_plt == 'days':
    t=t/(60.0*60.0*24.0) # Days
cryoline = (24.0+inj_L)/24.0 # Days
injline = inj_L/24.0 # Days
simtime = time/24.0 # Days

if Time_Units_plt == 'hours':
    t=t/(60.0*60.0) # Hours
cryoline = 24.0+inj_L # Hours
injline = inj_L # Hours
simtime = time # Hours

if Time_Units_plt == 'min':
    t=t/(60.0) # Minutes
cryoline = (24.0+inj_L)*60.0 # Minutes
injline = inj_L*60.0 # Minutes

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simtime = time*60.0  # Minutes

BG = (ER_Background/(60.0*24.0*60.0*60.0*0.002))*1.25  # Pb212 Equivalent BG

BG_Counts = (ER_Background*5*1.25)/0.002

# ----------------------- Plotting -------------------------#

# ---------------- Activity Plot -----------------#

plt.figure(1)

if (Pb212_only_mode==True):
    plt.plot(t[0::X], Pb212Total[0::T_X], 'grey', label='Total (No Rn220, Po216)')
    plt.plot(t[0::X], dPb212[0::X]/dt,'k',label='Pb212 (beta Q=569.1 keV)', linewidth=4)
    plt.plot(t[0::X], dBi212[0::X]/dt,'c',label='Bi212 (beta[64%] Q=2.3 MeV; alpha[36%] 6.2 MeV)')
    plt.plot(t[0::X], (dPo212[0::X]/dt),'b',label='Po212 (alpha 9.0 MeV)')
    plt.plot(t[0::X], dTl208[0::X]/dt,'y',label='Tl208 (beta Q=5.0 MeV)')

elif (Gas_only_mode==True):
    plt.plot(t[0::X], Gas_Total[0::T_X], 'grey', label='Total (Alphas Only)')
    plt.plot(t[0::X], dRn220[0::X]/dt,'k',label='Rn220 (alpha 6.4 MeV)', linewidth=3)
    plt.plot(t[0::X], (dPo216[0::X]/dt),'g',label='Po216 (alpha 6.9 MeV)')
    plt.plot(t[0::X], (dBi212[0::X]/dt)*Bi_Tl,'c',label='Bi212 (alpha[36%] 6.2 MeV)')
    plt.plot(t[0::X], (dPo212[0::X]/dt),'b',label='Po212 (alpha 9.0 MeV)')

else:
    plt.plot(t[0::X], Total[0::T_X], 'grey', label='Total')
    plt.plot(t[0::X], dRn220[0::X]/dt,'r',label='Rn220 (alpha 6.4 MeV)', linewidth=3)
    plt.plot(t[0::X], (dPo216[0::X]/dt),'g',label='Po216 (alpha 6.9 MeV)')
    plt.plot(t[0::X], dPb212[0::X]/dt,'k',label='Pb212 (beta Q=569.1 keV)', linewidth=4)
    plt.plot(t[0::X], dBi212[0::X]/dt,'c',label='Bi212 (beta[64%] Q=2.3 MeV; alpha[36%] 6.2 MeV)')
    plt.plot(t[0::X], (dPo212[0::X]/dt),'b',label='Po212 (alpha 9.0 MeV)')
    plt.plot(t[0::X], dTl208[0::X]/dt,'y',label='Tl208 (beta Q=5.0 MeV)')

plt.plot([injline, injline], [0, 100], color='r', linestyle='--', label="End of Injection")

if Cryopumping==True:
    plt.plot([1, 1], [0, 100], color='g')
    plt.plot([cryoline, cryoline], [0, 100], color='r')

plt.legend(loc="upper right")
plt.ylabel("Activities (Bq)")
plt.xlabel("Time (+Time_Units_plt")
plt.grid()  
plt.xlim(0,math.ceil(max(t)))

if Continuous==True:
    plt.title("Rn220 Chain Activities")
else:
    plt.title("Rn220 Chain Activities ("+str(Rn_0)+" Bq Rn220 Injection")

# ----------------- Cumulative Events Plot ------------------#

plt.figure(2)

if(Pb212_only_mode==False):
    #...
plt.plot(t[0::X], Rn220C[0::X], 'r', label='Rn220 (alpha 6.4 MeV)', linewidth="3")
plt.plot(t[0::X], Po216C[0::X], 'g', label='Po216 (alpha 6.9 MeV)', linewidth="2")
plt.plot(t[0::X], Pb212C[0::X], 'k', label='Pb212 (beta Q=569.1 keV)', linewidth=4)
plt.plot(t[0::X], Bi212C[0::X], 'c', label='Bi212 (beta[64\%] Q=2.3 MeV; alpha[36\%] Q=6.2 MeV)')
plt.plot(t[0::X], Po212C[0::X], 'b', label='Po212 (alpha 9.0 MeV)')
plt.plot(t[0::X], Tl208C[0::X], 'y', label='Tl208 (beta Q=5.0 MeV)')

plt.plot([injline, injline], [0.1, 1200000], color='r', linestyle='--', label="End of Injection")
if Cryopumping==True:
    plt.plot([1, 1], [0, 12000000], color='g')
else:
    plt.plot([cryoline, cryoline], [0, 0], color='g')
plt.legend(loc="lower right")
plt.ylabel("Number of Events")
plt.xlabel("Time ("+Time_Units_plt+")")
plt.ylim(0.02, 10000000)
plt.yscale('log')
plt.grid()
plt.xlim(0,math.ceil(max(t)))
if Continuous==True:
    plt.title("Rn220 Chain Cumulative Events")
else:
    plt.title("Rn220 Chain Cumulative Events")

#---------- Number of Atoms Plot -----------#
plt.figure(3)
if(Pb212_only_mode==False):
    plt.plot(t[0::X],Rn220[0::X], 'r', label='Rn220')
    plt.plot(t[1::X],Po216[1::X], 'g', label='Po216')
    plt.plot(t[0::X],Pb212TotalA[0::T_X], 'grey', label='Total')
    plt.plot(t[0::X],Pb212[0::X], 'k', label='Pb212')
    plt.plot(t[0::X],Bi212[0::X], 'c', label='Bi212')
    plt.plot(t[0::X],Po212[0::X], 'b', label='Po212')
    plt.plot(t[0::X],Tl208[0::X], 'y', label='Tl208')
    plt.plot(t[0::X],Pb208[0::X], 'm', label='Pb208')
    plt.plot([injline, injline], [0, 1000000000], color='r', linestyle='--', label="End of Injection")
if Cryopumping==True:
    plt.plot([(2*inj_L)/24.0, (2*inj_L)/24.0], [0, 1000000000], color='g')
    plt.plot([(3*inj_L)/24.0, (3*inj_L)/24.0], [0, 1000000000], color='r')
plt.legend(loc='lower right')
plt.ylabel("Number of Atoms")
plt.xlabel("Time ("+Time_Units_plt+")")
plt.yscale('log')
plt.grid()
plt.ylim(0.1, max([max(Rn220), max(Po216), max(Bi212), max(Po212),
    max(Pb212), max(Tl208), max(Pb208)])*1.5)
plt.xlim(0,math.ceil(max(t)))
if Continuous==True:
    plt.title("# of Rn220 chain atoms")
else:
plt.title("# of Rn220 chain atoms")
plt.show()
APPENDIX B
UMASS LXE DETECTOR PULSE FINDING ALGORITHM

The UMass-LXe-Detector Pulse-Finding Algorithm takes the raw PMT-signal waveforms from events recorded by the DAQ, identifies pulses in the waveforms, and measures a variety of useful features of the pulses for use in analysis. The complete list of the measured Reduced Quantities is presented in section 5.6.2. Other variables which appear in the pulse-finding code below are described here for completeness. Quantities which are directly recorded by the DAQ are:

- **eventnum**: A unique identification number assigned to each event in a single acquisition file from the DAQ.
- **livetime**: The time between when the FPGA rearmed the trigger following the previous event and when the trigger for the current event occurred in units of number of (600 MHz) CPU clock cycles.
- **deadtime**: The time since the beginning of the previous event trigger during which the trigger was not armed, including the previous event window and time during which the previous event was being saved to disk, in units of number of (600 MHz) CPU clock cycles.
- **timestamp**: The time of the trigger for the current event in units of number of (600 MHz) CPU clock cycles since the processor was powered on.
- **waveArr**: The raw PMT waveforms. For our 100 sample event windows, this is the PMT signal voltage (mV) of each sample, stored in an array.

Variables used as inputs in the pulse-finding algorithm code:
• **areawindow_low, areawindow_high**: The number of samples before and after a pulse, respectively, which are used to define the pulse boundaries.

• **baseline_samples**: The number of samples before the trigger used for measuring the PMT signal baseline characteristics.

• **gain_correct**: The correction factor by which the top PMT voltage samples are multiplied to account for the difference in the gains of the two PMTs. This is chosen to make the top-bottom light-collection asymmetry histogram symmetric. With a properly chosen value for gain_correct, an event which produces an equal number of photons incident on the top and bottom PMT faces will have identical pulses in the two PMT waveforms.

• **eventwindow**: The number of samples chosen to define the event window, 100 for the work presented in this thesis.

The pulse-finding algorithm code was written using Python 2, and is presented in full below:

```python
areawindow_low = 5  # samples below peak max for area measurement
areawindow_high = 13 # samples above peak max for area measurement
baseline_samples = 12 # samples at beginning of event, before pulse
gain_correct = 7.0    # Top PMT area multiplier to normalize gains
eventwindow = 100    # samples in the event window

# Load/save data from/to local machine
path_name = "/home/*********/********/

# import statements
import time
t0 = time.time()
import numpy as np
import matplotlib.pyplot as plt
import csv
import math
from matplotlib.colors import LogNorm
from pylab import rcParams
from os import path

def bitfield(n):
    tmp = [1 if digit=='1' else 0 for digit in bin(n)[2:]]
    return tmp[::-1]

def Read_DDC10_BinWaveCap_ChSel(fName):
    waveInfo = {}
    fp = open(fName,"rb")
    numEvents = int(np.fromfile(fp,dtype=np.uint32,count=1))
    waveInfo['numEvents'] = numEvents
    numSamples = int(np.fromfile(fp,dtype=np.uint32,count=1))
```

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waveInfo['numSamples'] = numSamples
chSelMask = int(np.fromfile(fp,dtype=np.uint32,count=1))
chMap = np.where(bitfield(chSelMask))[0]
waveInfo['chMap'] = chMap
numChannels = len(chMap)
waveInfo['numChannels'] = numChannels
byteOrderPattern = hex(int(np.fromfile(fp,dtype=np.uint32,count=1)))
waveArr = np.zeros((numChannels,numEvents,numSamples),dtype=np.int16)
for ievt in range(numEvents):
for ich in range(numChannels):
dummy = np.fromfile(fp,dtype=np.uint32,count=2)
waveTmp = np.fromfile(fp,dtype=np.int16,count=numSamples)
waveArr[ich,ievt,:] = waveTmp
dummy = np.fromfile(fp,dtype=np.uint32,count=1)
fp.close()
return (waveArr,waveInfo)
CPUdt = 1000000000.0/600000000.0 # 600 MHz time steps in ns
for filename in files:
if (path.exists(path_name+filename+"/"+filename+".npz") &
,→
(reprocess!=True)):
print(filename+" has already been processed")
else:
areawindow
eventnum =
deadtime =
datalen =

= areawindow_high+areawindow_low
[]; timestamp = []; livetime
= [];
[]; baseline_0 = []; baseline_1 = [];
[];

waveArr, waveInfo = Read_DDC10_BinWaveCap_ChSel(path_name
,→
+filename+"/"+filename+".bin")
with open(path_name+filename+"/"+filename+".txt","rU") as data:
csvReader = csv.reader(data)
for row in csvReader:
if len(row) > 2:
eventnum.extend([int(row[0])-1])
timestamp.extend([round((int(row[1])*CPUdt)/1000.0)])
livetime.extend([round((int(row[2])*CPUdt)/1000.0)])
deadtime.extend([round((int(row[3])*CPUdt)/1000.0)])
for i in range(0, len(waveArr[0])):
baseline_0.extend([np.mean(waveArr[0,i,0:baseline_samples])])
baseline_1.extend([np.mean(waveArr[1,i,0:baseline_samples])])
waveArr[0,i] = waveArr[0,i]-baseline_0[i]
waveArr[1,i] = waveArr[1,i]-baseline_1[i]
waveArrSum = np.array(np.sum((gain_correct*waveArr[0,:,:],
,→
waveArr[1,:,:]), axis=0))
eventnum = np.array(eventnum)
timestamp = np.array(timestamp)
livetime = np.array(livetime)
deadtime = np.array(deadtime)
ts = timestamp - timestamp[0]
runtime = ts[len(ts)-1]/1000000.0
tba
amp_0a
amp_1b
area_0a

=
=
=
=

[];
[]; amp_0b = []; amp_1a = [];
[]; amp_Sa = []; amp_Sb = [];
[]; area_0b = []; area_1a = [];

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area_1b = []; area_Sa = []; area_Sb = [];
indx_0a = []; indx_0b = []; indx_1a = [];
indx_1b = []; indx_Sa = []; indx_Sb = [];
post_peak_frac_0a = []; pre_peak_frac_0a = [];
pulse_width_0a = []; pulse_width_Sa = [];
post_peak_frac_1a = []; pre_peak_frac_1a = [];
pulse_width_Sa = [];
pre_peak_frac_Sa = [];
pulse_width_1a = []; pulse_width_Sa = [];
bl_stddev_0 = []; bl_stddev_1 = [];
for i in range(0, len(waveArr[0])):
    bl_stddev_0.extend([np.std(waveArr[0,i,0:baseline_samples])])
    bl_stddev_1.extend([np.std(waveArr[1,i,0:baseline_samples])])

# Primary Pulse Finder
mx0, indx0 = max((waveArr[0,i,k], k) for k in range(0,
    len(waveArr[0,i])))
mx1, indx1 = max((waveArr[1,i,k], k) for k in range(0,
    len(waveArr[1,i])))
mx00, indx00 = max((waveArrSum[i,k], k) for k in range(0,
    len(waveArrSum[i])))
indx_0a.extend([indx0])
indx_1a.extend([indx1])
indx_Sa.extend([indx00])
amp_0a.extend([mx0])
amp_1a.extend([mx1])
amp_Sa.extend([mx00])
area_0a.extend([sum(waveArr[0, i, 
    indx0-areawindow_low:indx0+areawindow_high])*10]) # 10 ns
    sample width
area_1a.extend([sum(waveArr[1, i, 
    indx1-areawindow_low:indx1+areawindow_high])*10]) # 10 ns
    sample width
area_Sa.extend([sum(waveArrSum[i, 
    indx00-areawindow_low:indx00+areawindow_high])*10])

# Calculate Pulse Shape Parameters for Top PMT
if area_0a[i]>0:
    post_peak_frac_0a.extend([float(sum(waveArr[0, i, 
            indx0:indx0+areawindow_high])*10) / float(area_0a[i])])
    pre_peak_frac_0a.extend([float(sum(waveArr[0, i, 
            indx0-areawindow_low:indx0])*10) / float(area_0a[i])])
    S1_0 = float(area_0a[i])
    tmp_area = 0
    counter = 0
    for z in range(indx0-areawindow_low,indx0+areawindow_high):
        tmp_area = tmp_area + (waveArr[0, i, z]*10)
        if ((tmp_area >= 0.10*S1_0) & (counter == 0)):  
            tenpercent = z
            counter = counter + 1
        if tmp_area >= 0.90*S1_0:
            ninetypercent = z
            break
    pulse_width_0a.extend([ninetypercent - tenpercent])
else:
    post_peak_frac_0a.extend([-1])
    pre_peak_frac_0a.extend([-1])
    pulse_width_0a.extend([-1])

print('--- Job Finished ---')
# Calculate Pulse Shape Parameters for Bottom PMT

```python
if area_1a[i] > 0:
    post_peak_frac_1a.extend([float(sum(waveArr[1, i, indx0: indx0 + areawindow_high]) * 10) / float(area_1a[i])])
    pre_peak_frac_1a.extend([float(sum(waveArr[1, i, indx0 - areawindow_low: indx0]) * 10) / float(area_1a[i])])

    S1_1 = float(area_1a[i])
    tmp_area = 0
    counter = 0

    for z in range(indx1 - areawindow_low, indx1 + areawindow_high):
        tmp_area = tmp_area + (waveArr[1, i, z] * 10)
        if (tmp_area >= 0.10*S1_1) & (counter == 0):
            tenpercent = z
            counter = counter + 1
        if tmp_area >= 0.90*S1_1:
            ninetypercent = z
            break

    pulse_width_1a.extend([ninetypercent - tenpercent])
else:
    post_peak_frac_1a.extend([-1])
    pre_peak_frac_1a.extend([-1])
    pulse_width_1a.extend([-1])
```

# Calculate Pulse Shape Parameters for Summed PMT Waveforms

```python
if area_Sa[i] > 0:
    post_peak_frac_Sa.extend([float(sum(waveArrSum[i, indx00: indx00 + areawindow_high]) * 10) / float(area_Sa[i])])
    pre_peak_frac_Sa.extend([float(sum(waveArrSum[i, indx00 - areawindow_low: indx00]) * 10) / float(area_Sa[i])])

    S1_S = float(area_Sa[i])
    tmp_area = 0
    counter = 0

    for z in range(indx00 - areawindow_low, indx00 + areawindow_high):
        tmp_area = tmp_area + (waveArrSum[i, z] * 10)
        if (tmp_area >= 0.10*S1_S) & (counter == 0):
            tenpercent = z
            counter = counter + 1
        if tmp_area >= 0.90*S1_S:
            ninetypercent = z
            break

    pulse_width_Sa.extend([ninetypercent - tenpercent])
else:
    post_peak_frac_Sa.extend([-1])
    pre_peak_frac_Sa.extend([-1])
    pulse_width_Sa.extend([-1])
```

# Second Pulse Finder

```python
if (indx0 < (eventwindow - areawindow_high)):
    mx2, indx2 = max((waveArr[0, i, l], l) for l in range(indx0 + areawindow_high, len(waveArr[0, i])))
    indx_0b.extend([indx2]); amp_0b.extend([mx2])

    if (indx2 < (eventwindow - areawindow_high)):
area_0b.extend([sum(waveArr[0, i, indx2-areawindow_low:
    indx2+areawindow_high])*10])
else:
    area_0b.extend([sum(waveArr[0, i, indx2-areawindow_low:
    len(waveArr[1,i])])*10])
else:
    area_0b.extend([0]); indx_0b.extend([0]);
    amp_0b.extend([0]);

if (indx1 < (eventwindow - areawindow_high)):
    mx3, indx3 = max((waveArr[1,i,l], l) for l in
    range(indx1+areawindow_high, len(waveArr[1,i])))
    indx_1b.extend([indx3])
    amp_1b.extend([mx3]);
if (indx3 < (eventwindow - areawindow_high)):
    area_1b.extend([sum(waveArr[0, i, indx3-areawindow_low:
    indx3+areawindow_high])*10])
else:
    area_1b.extend([sum(waveArr[1, i, indx3-areawindow_low:
    indx3+areawindow_high])*10])
else:
    area_1b.extend([0]); indx_1b.extend([0]);
    amp_1b.extend([0]);

if (indx00 < (eventwindow - areawindow_high)):
    mx01, indx01 = max((waveArrSum[i,l], l) for l in
    range(indx00+areawindow_high, len(waveArrSum[i])))
    indx_Sb.extend([indx01]); amp_Sb.extend([mx01])
if(indx01 < (eventwindow - areawindow_high)):
    area_Sb.extend([sum(waveArrSum[i, indx01-areawindow_low:
    indx01+areawindow_high])*10])
else:
    area_Sb.extend([sum(waveArrSum[i, indx01-areawindow_low:
    indx01+areawindow_high])*10])
else:
    area_Sb.extend([0]); indx_Sb.extend([0]);
    amp_Sb.extend([0]);

if ((area_0a[i] > 0) & (area_1a[i] > 0)):
    tba.extend([(float((gain_correct*area_0a[i])-(area_1a[i]))
    / float((gain_correct*area_0a[i]+area_1a[i])))])
else:
    tba.extend([-2])

baseline_0 = np.array(baseline_0)
baseline_1 = np.array(baseline_1)
bl_stddev_0 = np.array(bl_stddev_0)
bl_stddev_1 = np.array(bl_stddev_1)
amp_0a = np.array(amp_0a)
amp_0b = np.array(amp_0b)
amp_1a = np.array(amp_1a)
amp_1b = np.array(amp_1b)
amp_Sa = np.array(amp_Sa)
amp_Sb = np.array(amp_Sb)
area_0a = np.array(area_0a)
area_0b = np.array(area_0b)
area_1a = np.array(area_1a)
gain_correct = gain_correct, \neventwindow = eventwindow, \neventnum = eventnum, \nlivetime = livetime, \ndeadtime = deadtime, \nruntime = runtime, \ntimestamp = timestamp, \nwaveArr = waveArr, \nwaveArrSum = waveArrSum)
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