

ABSTRACT

Title of dissertation: **MEASUREMENT OF DISSOLVED BETA
DECAY SOURCES IN THE LUX-ZEPLIN
EXPERIMENT**

John E. Armstrong, Doctor of Philosophy, 2025

Dissertation directed by: **Professor Carter Hall
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Weakly Interacting Massive Particles (WIMPs) are one of the most well-motivated dark matter candidates. Liquid Xe (LXe) time projection chambers (TPC) are the leading technology for probing the WIMP mass range. The LUX-ZEPLIN (LZ) experiment is a 10 tonne LXe TPC searching for the elusive WIMP dark matter. As detector masses increase to maximize sensitivity, background sources in the Xe, such as ^{85}Kr and ^{39}Ar , must be reduced to meet background requirements. These species are more difficult to quantify and require more stringent monitoring compared to previous generations of experiments. In this work, the techniques used to monitor ^{85}Kr and ^{39}Ar during commissioning and through LZ's WIMP Search 2024 science run (WS2024) are discussed. A mass spectrometry technique is used to measure 182 ± 26 ppq (g/g) ($^{nat}\text{Kr/Xe}$) during WS2024. A complementary measurement of an excited state decay of ^{85}Kr found a ^{nat}Kr equivalent concentration of 124^{+44}_{-37} ppq (g/g) ($^{nat}\text{Kr/Xe}$). The measured WS2024 Ar concentration is 1.10 ± 0.18 ppb (g/g) (Ar/Xe). LZ set a world leading limit on the interaction cross section across the expected WIMP mass range, with a minimum of $2.1 * 10^{-48} \text{ cm}^2$ at $36 \text{ GeV}/c^2$.

MEASUREMENT OF DISSOLVED BETA DECAY SOURCES IN THE
LUX-ZEPLIN EXPERIMENT

by

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Chapter 1: Introduction

Dark matter is a compelling but elusive topic in physics. It is generally agreed that some invisible form of matter not only exists but is more abundant than visible matter. Understanding the exact nature of dark matter would have tremendous implications for particle physics and cosmology. Many experiments have tried, and thus far, all have failed, to determine the exact nature of dark matter. If at first you do not succeed...

1.1 Dark Matter Evidence

1.1.1 Zwicky and the Coma Cluster

Fritz Zwicky is generally regarded as the first to coin the term dark matter ("dunkle materie"), though others (notably Kapteyn and Oort) used similar terms or described similar ideas before. In 1933, Zwicky sought to understand the redshift of galaxies in the Coma Cluster [1][2]. Zwicky proposed dark matter after noting the discrepancy between the expected and measured velocity dispersions of several galaxies in the cluster.

Zwicky's approach hinged on the virial theorem as a way to estimate the average kinetic energy of galaxies in the system. The virial theorem is valid for a system of particles bounded by a conservative force in a mechanically stationary state. The virial theorem is given by Eq. 1.1 where $\langle T \rangle$ and $\langle V \rangle$ are the average kinetic and potential energies of the system.

$$\langle T \rangle = -\frac{\langle V \rangle}{2} \quad (1.1)$$

Zwicky estimated the luminous mass of the cluster to be $M = 1.6 * 10^{45} \text{g}$, then calculated the expected average velocity of a galaxy in the cluster to be 80 km/s. This was in significant disagreement with measured dispersions of 1500 – 2000 km/s.

Zwicky proposed several explanations for the inconsistency. One was that the Coma Cluster would eventually disperse without a sufficient amount of matter binding it together. He noted that this was inconsistent with the velocity dispersion observed in isolated galaxies. All other explanations required some form of non-luminous matter.

1.1.2 Galactic Rotation Curves

Galactic rotation curves provide some of the most tangible evidence for dark matter. Based on the observed luminous mass distributions, the rotational velocity was expected to be relatively low near the smaller measurable radii, before increasing to peak at a given radius and falling at higher radii.

Galaxies can be imaged at different wavelengths. The first observations came primarily from the optical and radio wavelengths, as these are capable of penetrating the Earth's atmosphere. Optical measurements can indicate the location of the large bodies like stars. The radio measurements are primarily directed at observing the 21 cm wavelength. 21 cm photons are the product of the hyperfine transition and their presence is indicative of gaseous clouds of hydrogen.

Rubin studied the rotation curve of Andromeda in the optical range to over 100 arcminutes using a spectrometer developed by Ford in 1970 [3]. Roberts and Whitehurst (1972) did the same using radio observations [4]. Both measurements were consistent and indicated that the rotation curves did not fall at the highest observed radii, as would be expected

from their luminous mass distributions. Roberts compared these and other measurements of M81 and M101. He was one of the first to explicitly conclude that the mass to light ratio in galaxies is not constant as a function of radius but increases with increasing radii [5].

A considerable number of additional measurements in both the radio and optical wavelengths, and extending to higher radii have confirmed similar rotation curve structures. Radio measurements of the 21 cm line at radii that exceed the edge of the observable edge of galaxies (in the optical range) indicate that the mass excess extends to greater than the optical edge of galaxies. Fig. 1.1 is a compilation of 23 optical rotation curves measured by Rubin, all showing the rotation curves flatten at high radii.

The dark matter density profiles in galaxies are still estimated (in part) by rotation curve measurements. The most commonly used distribution for dark matter is given by the Navarro-Frenk-White (NFW) profile in Eq. 1.2 where ρ_s is the scale density and r_s is the scale radius [7].

$$\rho_{DM}(r) = \frac{\rho_s}{(r/r_s)(1 + r/r_s)^2} \quad (1.2)$$

1.1.3 Gravitational lensing and the Bullet Cluster

Light travels along geodesics in spacetime. Its travel will be influenced by large gravitational potentials like any other form of energy. Ignoring effects related to the expansion of the universe and assuming that the gravitational potential Φ is weak ($\Phi \ll c^2$), the metric for the potential can be approximated as a perturbation on the Minkowski metric. Gravitational potentials that meet this approximation cause *weak gravitational lensing* of the light. The metric is written in Eq. 1.3 [8].

$$ds^2 = -\left(1 + \frac{2\Phi}{c^2}\right)dt^2 + \left(1 + \frac{2\Phi}{c^2}\right)d\vec{x}^2 \quad (1.3)$$

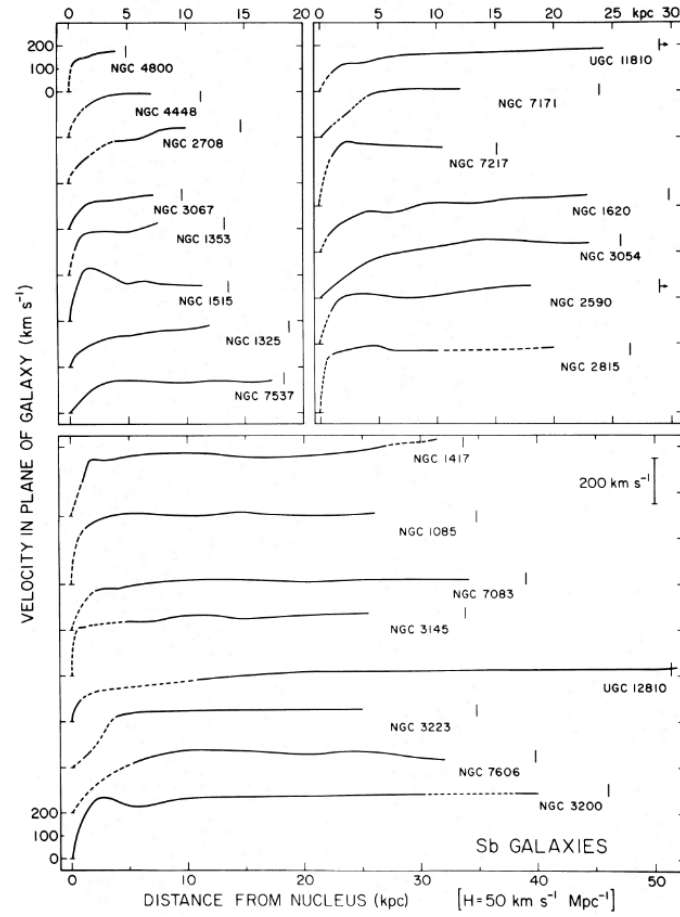


Figure 1.1: Measurements of 23 optical rotation curves are ordered from smallest galaxy size to largest. The curves generally flatten at high radii, indicating that excess non-visible mass must be present in the outer edges of the galaxy (image from [6]).

Setting the ds^2 term to zero indicates the light is traveling along a geodesic. The effective speed of light, c' , subject to the gravitational potential is given in Eq 1.4.

$$c' = \frac{d\vec{x}}{dt} = \sqrt{\frac{1 + 2\Phi/c^2}{1 - 2\Phi/c^2}} \approx c(1 + 2\Phi/c^2) \quad (1.4)$$

The effective index of refraction is $n = c'/c$. For a discrete prism with small deflection angles and an opening angle of ϕ , the deflection angle, α , can be approximated as $\alpha = \phi(n - 1)$. When applied to a continuous gravitational potential and applying several small angle approximations, the fundamental equation of lensing for light traveling with an impact parameter b is acquired: Eq. 1.5 [8].

$$\vec{\alpha}(b) = 2/c^2 \int_{-\infty}^{+\infty} \nabla_{\perp} \Phi dz \quad (1.5)$$

The spatial derivative, $\nabla_{\perp}$, is the potential gradient in the plane perpendicular to the direction the light is being viewed from, and $\hat{z}$ is the initial direction of travel of the light.

Gravitational shear is one manifestation of weak gravitational lensing that can be used to determine the mass distribution of the object causing the distortion. Gravitationally sheared objects are stretched tangential to the potential's center and (in the case of galaxies) their ellipticities deviate from isotropic distributions [9]. A procedure for inferring the mass distribution of objects causing the distortion is explained by Clowe (et al.) [10].

The Bullet Cluster is a particularly interesting galaxy cluster. It is one of the hottest known clusters. Optical and X-ray images of the cluster suggest that it was once two separate clusters that collided. Gravitational shearing around the cluster was used by Clowe (et al.) to infer the mass distribution [9]. The mass distribution contours are overlaid on the optical (left) and X-ray (right) images of the galaxy in Fig. 1.2.

Most luminous mass in the cluster is X-ray emitting, hot hydrogen gas. The X-ray data clearly indicates that the center of the luminous mass does not align with the center of the

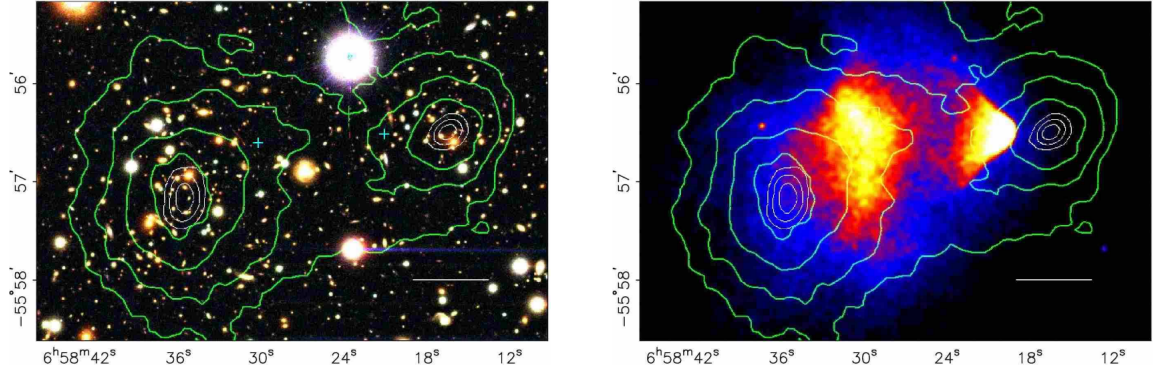


Figure 1.2: The left plot shows an optical image of the Bullet Cluster with the mass contours measured by weak lensing place on top. The right plot shows the same mass contours place on top of an X-ray image of the cluster. The three inner-most white rings in each mass distribution are the one, two, and three σ confidence intervals on the center of mass measurements from weak lensing. The white bar represents 200 kpc in the image. The mismatch between the X-ray image (highlighting most of the visible mass) and the mass contours is clear evidence of dark matter (image from [11]).

total mass. In the model of the two clusters colliding, the cluster that is currently displayed on the right approached from the left and vice versa. The majority of the luminous mass is found between the bulk of the two mass contours and suggests that when the collision occurred, most of the luminous matter self interacted (as expected) while any remaining mass passed relatively unimpeded.

Some theoretical alternatives to dark matter, such as modified gravitational theories, are able to explain galactic rotation curves. It is considerably more difficult for these theories to explain the Bullet Cluster. The most parsimonious explanation for the mass density profile is that a form of non-luminous matter, present in the original two clusters, passed by with little to no interaction, excepting gravity.

1.1.4 Cosmology and the Cosmic Microwave Background

The universe is observed to be expanding, homogeneous, and isotropic. The Friedmann-Robertson-Walker metric, given in Eq. 1.6, describes a universe that satisfies these three

conditions.

$$ds^2 = -dt^2 + a(t)^2 \left(\frac{dr^2}{1 - kr^2} + r^2(d\theta^2 + \sin^2\theta d\phi^2) \right) \quad (1.6)$$

The factor $a(t)$ describes the scale of the metric. The factor k is more interesting. It describes the curvature of the metric with $k > 0$ indicating a positively curved and *closed* universe, $k < 0$ indicating a negatively curved *open* universe, and $k = 0$ indicating a flat universe. If k is non-zero and normalized to 1, then a is roughly the curvature radius.

Einstein's equation for general relativity is given in Eq. 1.7, where $G_{\mu\nu}$, the Einstein tensor, is composed of the Ricci tensor, $R_{\mu\nu}$, and R is the Ricci scalar. G is given as Newton's gravitational constant.

$$G_{\mu\nu} = R_{\mu\nu} - g_{\mu\nu}R = 8\pi GT_{\mu\nu} \quad (1.7)$$

$T_{\mu\nu}$ is the stress energy tensor. It is diagonal and takes the form $T^0_0 = -\rho$ and $T^i_i = P$ for $i = 1, 2, 3$. Here ρ is the energy density and P is the pressure density.

Applying the Friedmann-Robertson-Walker metric to the Einstein equation will result in the Friedmann equations, Eq. 1.8 and Eq. 1.9.

$$H^2 = \left(\frac{\dot{a}}{a}\right)^2 = \frac{8\pi}{3}G\rho - \frac{k}{a^2} \quad (1.8)$$

$$\frac{\ddot{a}}{a} = \frac{4\pi}{3}G(\rho + 3P) \quad (1.9)$$

H in Eq. 1.8 is the (time varying) Hubble parameter. For a flat universe (thus far consistent with observations), $k = 0$ and the final term in Eq. 1.8 will vanish. The *critical energy density* can then be given by Eq. 1.10, where H_0 is the Hubble constant at present.

$$\rho_c = \frac{3H_0^2}{8\pi G} \quad (1.10)$$

Making use of the fact that $\nabla_\mu T^\mu{}_\nu = 0$, then generalizing $P = w\rho$ results in Eq. 1.11.

$$\dot{\rho} = -3H\rho(1+w) \quad (1.11)$$

There are three components to the energy density with three corresponding values of w : radiation (photons) with $w = 1/3$, matter with $w = 0$, and the cosmological constant (related to dark energy) with $w = -1$. Solving the differential equations, dividing each by the critical density, and substituting energy density components back into Eq. 1.8 gives the Hubble parameter in terms of the normalized components of the energy density today. This is shown by Eq. 1.12 where Ω_Λ is the fraction of the critical density of the cosmological constant Λ (expansion of the universe), Ω_m is the fraction of matter, and Ω_r is the fraction of radiation.

$$H^2 = H_0^2 \left(\Omega_\Lambda + \frac{\Omega_m}{a^3} + \frac{\Omega_r}{a^4} \right) \quad (1.12)$$

Understanding how measurements can be used to determine the fraction of each of these components requires a returning to the beginning of the universe. It is predicted that small quantum fluctuations developed before inflation, then expanded in size during inflation. The expanded fluctuations resulted in macroscopic spatial anisotropies. When energies were lower than required for photons to create electron positron pairs, but high enough to prevent electrons from binding with nuclei, the universe consisted of an opaque plasma of photons, baryons (nuclei), and electrons. The photons were coupled to the electrons through Thompson scattering and the electrons were coupled to the baryons through the Coulomb interaction.

The macroscopic anisotropies resulted in over-densities in the plasma. The attractive gravitational potential wells where the over-densities were located competed with the repulsive radiation pressure from the photon interactions. The two competing interactions caused oscillations in the plasma, known as *baryon acoustic oscillations*. When the temperature of the universe dropped enough, nuclei were able to combine with electrons, and the photons decoupled from the matter. This process is known as *recombination*. The process happened relatively quickly but not instantly. The mean free path of the photons rapidly increased before becoming effectively infinite at the *era of last scattering*. This occurred around 370000 years after the Big Bang [12].

A significant fraction of the released photons have been streaming in the same direction ever since. They are the single most valuable and one of the oldest sources of information used to assess the component energy density fractions. They now make up what is known as the *cosmic microwave background*. Integrating across the entire sky, the spectrum appears as a (now significantly redshifted) black body spectrum.

The cosmic microwave background is quite isotropic and corresponds to a temperature of 2.7255 K [12]. There are no significant temperature variations noted at the level of 0.01%¹. Improved precision and angular resolution reveal structure in the temperature fluctuations. The structure in the 2013 cosmic microwave background measured by the Planck Collaboration is shown in Fig. 1.3.

The image reveals fluctuations on the order of 10s of μK . It is necessary to return to the time before recombination to understand the source of these fluctuations.

The baryon acoustic oscillations created areas of compression or higher density, and areas of rarefaction or lower density. Areas with higher or lower densities at the time of recombination were at correspondingly higher or lower temperatures when their photons

¹This ignores the 3.36 mK dipole from Doppler boosting caused by the motion of the Solar System. The dipole contribution has been removed from Fig. 1.3.

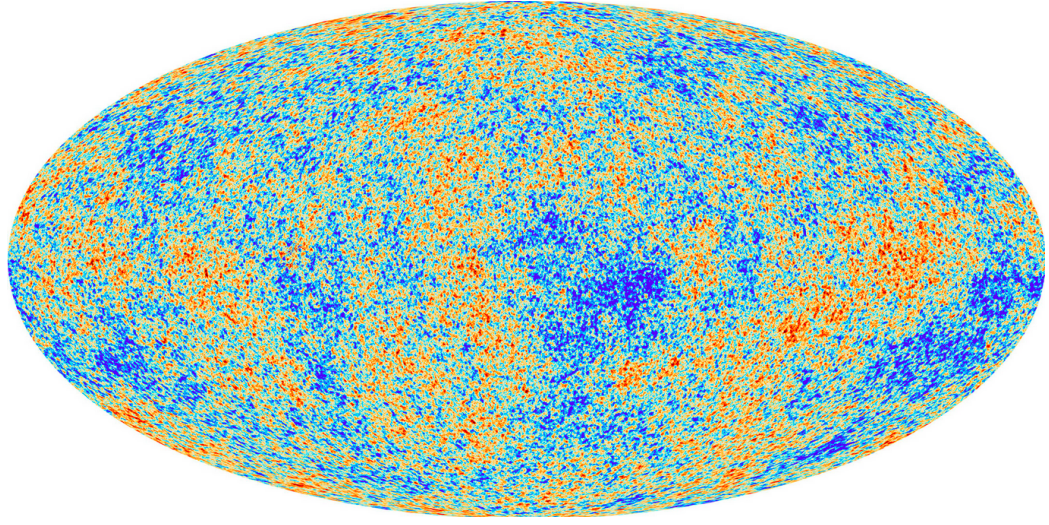


Figure 1.3: The cosmic microwave background measured by the Planck collaboration in 2013 is shown. Temperature changes in the spectrum vary from the measured average temperature 2.7255 K by 10s of μK (image from [13]).

were released.

Most modes of the acoustic oscillations will make no coherent contribution to the cosmic microwave background. However, oscillation modes that correspond to (nearly exact) low integer multiples of compression(s) plus rarefaction(s) over the time between the start of baryon acoustic oscillations and recombination are able to be detected. These are observed in the cosmic microwave background angular power spectrum. The cosmic microwave background angular power spectrum produced by the Planck collaboration in 2018 is shown in Fig. 1.4.

The baryon acoustic oscillations corresponding to integer extrema length scales naturally manifest themselves as spherical harmonics in the sky when viewed from Earth. The multi-pole moment of a spherical harmonic decomposition of the cosmic microwave background temperatures is indicated on the X-axis. The (absolute value of) temperature deviations are displayed on the Y-axis.

The first peak is associated with an oscillatory mode that compressed once, releasing

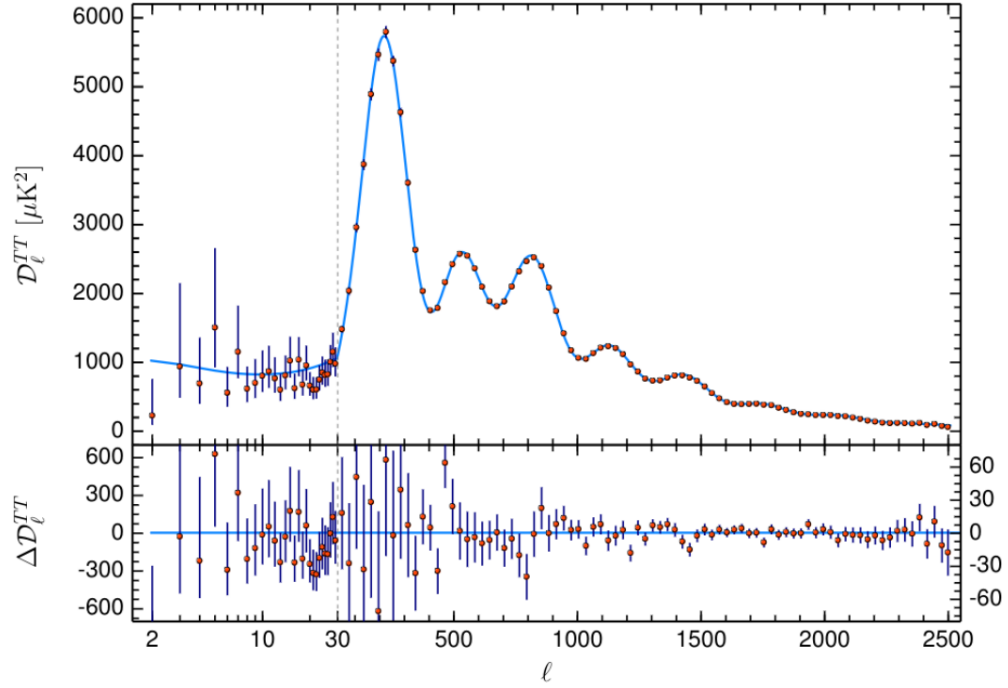


Figure 1.4: The angular power spectrum of the cosmic microwave background measured by the Planck collaboration in 2018 is shown. The height and position of the peaks are sensitive to changes in the dark energy, baryonic matter, and cold dark matter densities. The third peak exhibiting a height comparable to the second peak is a qualitative indicator of dark matter. This peak corresponds to a compression, rarefaction, and another compression of the baryon-photon plasma before recombination. The relative height of the second and third peaks indicates that some matter unaffected by radiation pressure continued to pool in the gravitational well while the baryonic matter rarefied (image from [14]).

its photons near peak compression (1/2 of a period). Thus, it has the longest wavelength and lowest multi-pole moment. The second peak corresponds to an oscillatory mode that compressed then released its photons near peak rarefaction. The third peak compressed, rarefied, compressed again, then released the photons.

Higher order peaks are generally expected to experience damping. One factor that contributes to this is the modest photon scattering that occurs during the recombination period. The scattering will add a degree of spatial smearing to the higher order peaks. As the size of spatial smearing approaches the wavelength of a given mode, the anisotropies of the mode will diminish.

The most qualitatively compelling argument for dark matter is the third peak. This corresponds to a second compression following a full oscillation (3/2 cycles). This peak is generally expected to be smaller than the second peak. However, if a source of mass that did not experience radiation pressure existed early in the universe, it could continue to gather in the gravitational well while the radiation and baryonic matter rarefied. The second compression's temperature deviation would be strengthened relative to the first rarefaction. The above argument generally holds for baryonic matter densities that are consistent with observations.

Many parameters affect the shape of the spectrum. Returning to Eq. 1.12, the radiation density, Ω_r , is currently negligible and the matter density, Ω_m , has been split into a baryonic matter component, Ω_b , and a cold dark matter component, Ω_c , that behaves in the way described above. The Planck 2018 data estimates the dark energy density to be $\Omega_\Lambda = 0.684 \pm 0.007$. The best estimate of the matter components from the 2018 Planck data are reported as a product of h^2 where $h = H_0/100$: $\Omega_b h^2 = 0.0223 \pm 0.0001$, and $\Omega_c h^2 = 0.120 \pm 0.001$ [14]. The baryonic matter density is $\Omega_b = 0.049$ and the cold dark matter density is $\Omega_c = 0.264$. This is very strong evidence for the existence of dark matter.

As a final note, dark matter consistent with the cosmic microwave background evi-

dence is expected to be *cold*. Cold is meant to indicate that the dark matter moves non-relativistically. Non-relativistic dark matter candidates are favored.

1.2 Dark Matter Candidates

While the existence of some form of dark matter is generally accepted, its exact nature is not well understood. A large number of theories have been proposed to explain the nature of dark matter. Currently, the two most well motivated, from the perspective of particle physics, are axions and weakly interacting massive particles.

Baryonic dark matter was one of the first proposed dark matter candidates. Most of these candidates fall into the class of massive compact halo objects (MACHOs). Baryonic MACHOs would include neutron stars, white dwarfs, brown dwarfs and objects similar. Microlensing measurements from the Magellanic Clouds by the MACHO (1997) and EROS (2007) collaborations indicate that objects with masses in the expected (MACHO) mass range cannot account for most of the dark matter in the Milky Way halo [15] [16]. Further, the cosmic microwave background angular power spectrum fit indicates that less than 5% of the energy density in the universe is baryonic and about 26% is non-baryonic cold dark matter. While baryonic dark matter may be a small fraction of the dark matter in galaxies, it cannot account for most of the dark matter in a given galaxy.

Most alternatives to dark matter involve modified Newtonian dynamics (MONDs). These theories stem from a proposal by Milgrom in 1983 [17]. The general idea involves a change to Newton's second law: $\vec{F} = m_g \vec{a}$ becomes $\vec{F} = m_g \mu(a/a_0) \vec{a}$ where $\mu(x \gg 1) \approx 1$ and $\mu(x \ll 1) \approx x$. These theories reproduce dynamics on the galactic level well but do not offer a compelling explanation for the behavior of the Bullet Cluster or the cosmic microwave background angular power spectrum.

1.2.1 Axions

Axions and axion-like particles are hypothetical light particles that could be dark matter. They are one of the two most well motivated dark matter candidates today. QCD Axions were initially realized as a solution to the strong CP problem. The strong interaction is not observed to violate charge-parity (CP) symmetry. However, the standard model Lagrangian includes an angle (usually denoted as θ) that should generally allow the strong force to violate CP. No CP violation is expected to occur if θ is exactly zero. Thus, the angle must be very small to be consistent with observations.

Peccei and Quinn proposed a solution to this problem. Their solution would add a new scalar field and chiral U(1) invariance [18]. The proposed symmetry would be broken below the electroweak energies. Both Wilczek and Weinberg noted that this symmetry breaking would result in a pseudo-Nambu-Goldstone boson, which Wilczek called the (QCD) axion [19] [20].

Axions and axion-like particles may have a wide range of masses. QCD axions with masses exceeding 1 eV have been ruled out. Two prominent models were developed to explain the cosmic origins of QCD axions: KSVZ and DFSZ [21] [22] [23]. The models also predict the axion-photon coupling, effectively setting a sensitivity benchmark for axion detection experiments. Some of the most favored remaining axion mass ranges have been ruled out at KSVZ and DFSZ sensitivities by haloscope experiments like the Axion Dark Matter eXperiment [24]. A large amount of parameter space has yet to be explored.

1.2.2 Weakly interacting massive particles

Weakly interacting massive particles (WIMPs) are the other compelling dark matter candidate. The term *weakly interacting massive particle* refers generally to a neutral, non-relativistic beyond standard model particle that interacts with standard model particles on

the weak scale (at most) [25]. The WIMP mass range is considered to extend from single GeV/c² to about 100s of TeV/c².

Most WIMP production theories suggest that WIMPs are relic dark matter, produced in the very early universe. When the temperature of the universe was greater than the WIMP mass, m_χ , WIMPs and standard model particles would have been in equilibrium. As the universe cooled, they would *freeze out* of equilibrium, fixing the WIMP abundance. This is required to happen before Big Bang nucleosynthesis to be consistent with the cosmic microwave background angular power spectrum measurements. Eq. 1.13 displays the Boltzmann equation describing the change in the WIMP number density n_χ , where H is the Hubble constant, σ_{ann} the WIMP annihilation cross-section, v is the WIMP velocity, and n_{eq} is the equilibrium density.

$$\frac{dn_\chi}{dt} = -3Hn_\chi - \langle \sigma_{ann} v_{rel} \rangle (n_\chi^2 - n_{eq}^2) \quad (1.13)$$

The dark matter relic abundance $\Omega_\chi h^2$ can then be written as Eq. 1.14 where T_0 is the present day temperature of the universe, h is the Hubble constant at present, ρ_c is the critical density from section 1.1.4, $x_f = m_\chi/T_f$ is the mass of the WIMP divided by the freeze out temperature T_f , $\bar{M}_P$ is the reduced Planck mass, and v_{rel} is the relative velocity of two dark matter particles in the center of mass frame [25]. The averaged product $\langle \sigma_{ann} v_{rel} \rangle_f$ is taken at the time of freeze out.

$$\Omega_\chi h^2 \approx \frac{m_\chi n_\chi T_0}{\rho_c} h^2 = \frac{T_0^3}{\rho_c} \frac{x_f}{\bar{M}_P} \frac{1}{\langle \sigma_{ann} v_{rel} \rangle_f} \quad (1.14)$$

Substituting in the best estimated values, including $\Omega_\chi h^2 = 0.12$ from Planck 2018 ($\Omega_\chi \equiv \Omega_c$) and a WIMP mass $M_\chi \approx 100 \text{ GeV}/c^2 - 10 \text{ TeV}/c^2$, gives Eq. 1.15 [14] [25].

$$\langle \sigma_{ann} v_{rel} \rangle_f \approx 3 * 10^{-26} \text{ cm}^3/\text{s} \quad (1.15)$$

This results in a weak strength cross-section ($\sim 10^{-36} \text{ cm}^2$) for a WIMP velocity of $v \approx 0.1c$. The realization that a weak scale annihilation cross-section and a velocity that is consistent with the expected WIMP velocity at freeze out results in the observed dark matter density is referred to as the *WIMP miracle*. The significance of the result has been debated [26].

One of the most noteworthy theories where WIMPs arise is supersymmetry. A few supersymmetric standard model partners are considered to be WIMP dark matter candidates. Though minimal supersymmetry has recently fallen out of favor due to the lack of supporting experimental findings, many other theories propose WIMPs or WIMP-like particles that could be dark matter candidates. These theories include universal extra dimensional theories, asymmetric dark matter theories, and Little Higgs models [27]. There are plenty of reasons to believe WIMPs may still be waiting to be discovered.

1.3 Thesis Outline

Dark matter is a significant outstanding problem in physics. There is overwhelming evidence for its existence but no direct understanding of its nature. WIMPs remain a leading particle candidate for dark matter. The remainder of this dissertation focuses on the WIMP detection experiment LUX-ZEPLIN.

Chapter 2 will introduce the LUX-ZEPLIN (LZ) experiment. The physics of particle interactions in liquid Xe will be explained. The dual phase liquid Xe time projection chamber detector technology is shown to be exemplary for WIMP detection. Other components of the LZ detector and their role in WIMP detection are also discussed.

Chapter 3 discusses the technique applied to monitor the purity of LZ Xe. Kr and Ar concentrations in LZ Xe are measured to within 10s of parts per quadrillion (g/g) using *cold trap mass spectrometry*. Xe purity is chronicled from the time before it entered LZ until

the end of LZ's WIMP Search 2024 science run. The Kr and Ar concentrations informing the LZ background priors for ^{85}Kr and ^{39}Ar in each science run are reported here.

Chapter 4 examines the methods used to measure the decay rate of an excited state of ^{85}Kr . This decay proceeds through ^{85m}Rb and provides a unique signature in the LZ detector. Simulations and data from the LZ detector are used to quantify the cut efficiency. The final results are shown and several sources of background are discussed to conclude the chapter.

Tritiated methane is injected into the Xe to calibrate the detector response to electrons. It must be effectively removed with the LZ noble gas purifier because it is a background for the WIMP search. Chapter 5 assesses methane removal in LZ. Measurements made using both the cold trap mass spectrometry technique from chapter 3 and data from the LZ detector are shown. The removal curve informing the number of expected tritium decays at the start of the WIMP Search 2024 science run is reported here.

Chapter 2: Dark Matter Detection and The LUX-ZEPLIN Experiment

Observation of dark matter could come in a variety of ways. They are summarized by the Feynman diagram in Fig. 2.1.

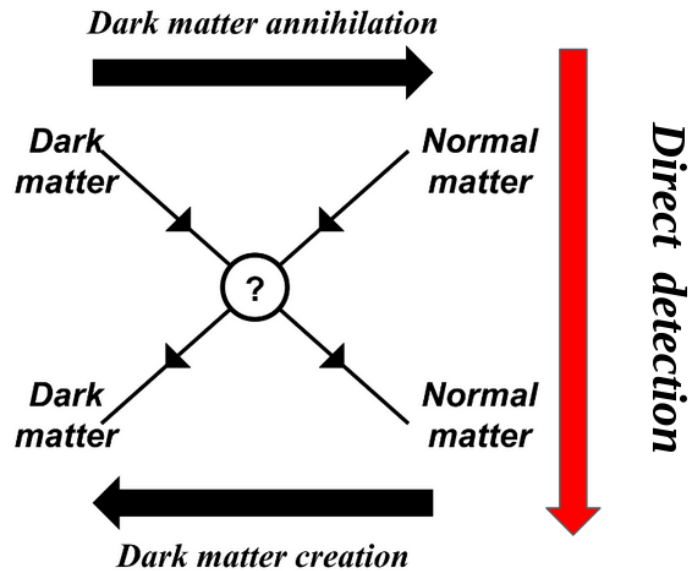


Figure 2.1: A hypothetical Feynman diagram for dark matter coupling to normal matter is shown. The diagram can be interpreted to suggest that dark matter annihilation and creation may be viable channels for finding evidence of dark matter. Direct detection experiments (like LUX-ZEPLIN) attempt to observe dark matter scattering off of normal matter.

Dark matter could self-interact and annihilate. An experiment may be able to observe the annihilation products to claim evidence of dark matter. It may be possible to smash normal matter together at high energies to create dark matter. A collider could create dark matter in this way and claim a missing mass signal as evidence of dark matter. The most straightforward way to detect (particle-like) dark matter would be to observe it scattering

off normal matter. This is referred to as direct detection.

The choice of target medium is the first design decision for a direct detection experiment. A WIMP interaction with an atom is expected to cause the target nucleus to recoil. A $30 \text{ GeV}/c^2$ mass WIMP scattering off of a Xe atom is expected to deposit up to 30 keV. Prior to the LUX-ZEPLIN experiment, the most promising and well motivated WIMP detection medium was liquid Xe (LXe). The 90% C.L. cross-section exclusion limits for a $50 \text{ GeV}/c^2$ WIMP by detection medium are shown as of 2017 in Fig. 2.2¹.

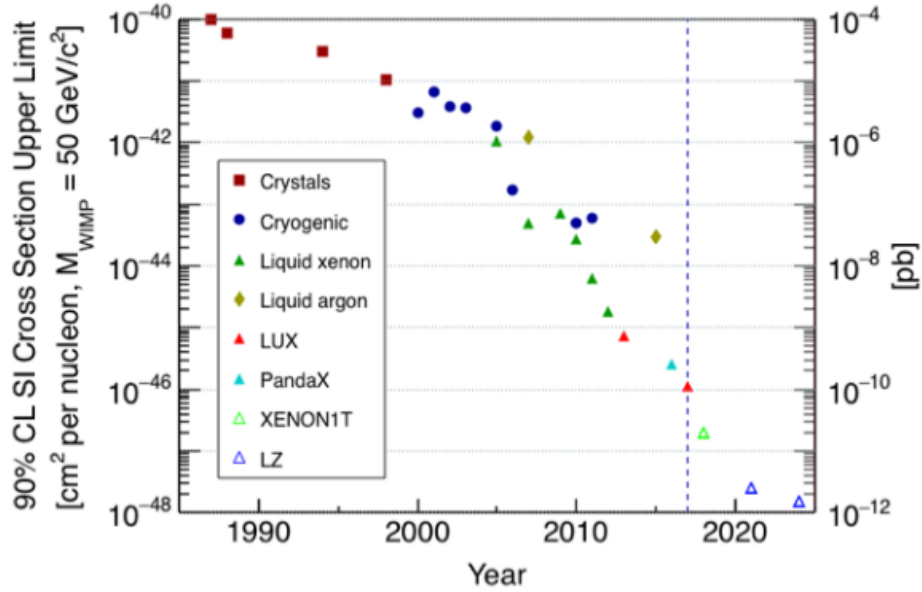


Figure 2.2: The 90% confidence (upper) limit on the scattering cross-section of a $50 \text{ GeV}/c^2$ WIMP measured by experiments using various detection media is shown. The square markers represent mostly NaI and Ge crystal experiments. The circular markers represent cryogenic Ge detectors. The triangle shaped markers (regardless of color) represent liquid Xe experiments and the diamond shaped markers represent liquid Ar experiments. Xe experiments have been dominant since 2010. The 2016 projected limits for XENON1T and LZ are also included in this plot (image from [28]).

LXe experiments outperformed others by over two orders of magnitude in 2017. The gap between Xe and other mediums has only widened since. Current limits show that

¹These cross-sections are determined using a standard set of assumptions regarding astrophysical parameters such as the local dark matter density and the WIMP particle velocity distribution. This will be true of all cross-section exclusion plots shown.

WIMP scatter interactions are limited to extremely low cross-sections; several experiments have ruled out (spin independent) cross-sections exceeding 10^{-46} cm^2 [29] [30] [31]. All are LXe time projection chamber dark matter experiments.

Xe is far better suited for detecting high mass WIMPs than any other medium because of high energy transfer efficiency. Liquefaction increases the Xe density to increase exposure. LXe is more dense than other liquid noble gases. These properties, along with others that will be discussed in the following sections, make LXe an obvious WIMP scattering target.

Section 2.1 gives an overview of the LZ detector and some of the main detector systems. Section 2.2 discusses time projection chamber design, interaction signals in LZ, Xe microphysics, and energy reconstruction. Various subsystems are described, including the Xe skin veto detector in section 2.3, the outer detector veto in section 2.4, and the Xe circulation system in section 2.5. Some basic background mitigation techniques will be explained in section 2.6. The chapter will conclude with a brief summary in section 2.7.

2.1 LZ Overview

LUX-ZEPLIN is an experiment designed to detect WIMP dark matter. It is housed on the 4850 ft level of the Sanford Underground Research Facility (SURF) in Lead, SD. It consists of a time projection chamber with a seven tonne active mass of LXe, an instrumented LXe skin detector, an instrumented outer detector, and an outer ultra-pure water shield. These pieces of the LZ experiment can be seen in Fig. 2.3.

Other pieces of the experiment (not seen in the figure) include the Xe circulation system, calibration source hardware, cryogenics systems, electronics readout and control, and vacuum systems.

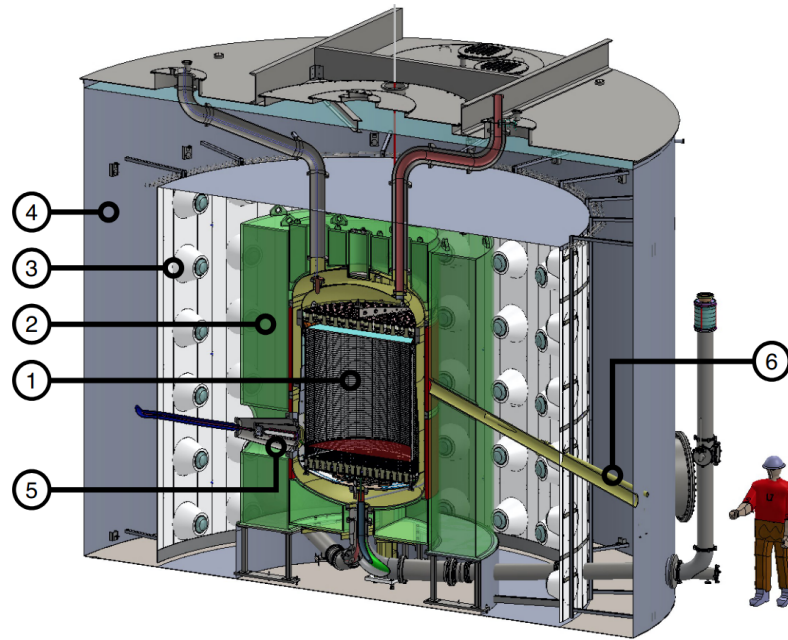


Figure 2.3: A diagram of the LZ detector is shown. At the center is the time projection chamber (1). The LZ Xe skin detector (not labeled) rests outside the gray time projection chamber walls but inside the yellow cryostat walls. The cryostat is surrounded by the green acrylic tanks (2), which hold gadolinium loaded liquid scintillator. Ultrapure water lies between the acrylic tanks and the Tyvek curtain and PMT array (3). The liquid scintillator tanks, water, PMTs and Tyvek all make up the LZ outer detector. More ultrapure water (primarily used for shielding) lies between the outside of the Tyvek curtain and the water tank wall (4). LZ's cathode high voltage connection (5) is shown attached to the bottom left side of the time projection chamber. A conduit pipe (6) for neutron calibration can be seen on the right side of the cryostat, extending to the water tank wall (image from [32]).

2.2 The LZ Time Projection Chamber

The heart of the LZ experiment is a ten tonne, dual phase, scintillation based liquid xenon (LXe) time projection chamber. A two phase liquid noble gas time projection chamber (TPC) is most commonly an upright cylinder. At the top and bottom of the cylinder are arrays of photo multiplier tubes (PMTs). Multiple sets of nearly transparent, thin wire grids are held at specific voltages to create vertical electric fields. In a dual phase (scintillation based) liquid noble TPC, there may be as many as five wire grids. From the bottom to the top, these are ordered: the bottom grid, the cathode grid, the gate grid, the anode grid, and the top grid. LZ only has four grids (no top grid). The liquid-gas boundary is designed to be between the tightly spaced anode and gate grids, near the top of the chamber. The space between the cathode and bottom grids is known as the *reverse field region* for obvious reasons. A diagram of a slice along the diameter of the LZ TPC can be seen in Fig. 2.4.

The LZ TPC has a height of 1.456 m (from cathode to gate) and an effective diameter of 1.456 m. The barrel of the cylinder is coated in polytetrafluoroethylene (Teflon or PTFE). Field shaping rings maintain electric field uniformity. The height of the liquid-gas boundary is set by three weir drain pipes. The inner cryovessel contains numerous temperature monitoring and control instruments, like resistive temperature devices, thermosiphons, and heaters. About seven tonnes of the ten tonne mass of LZ Xe is contained in the active portion of the TPC between the cathode and gate grids. The LZ TPC is described in extensive detail in [28].

A diagram of a particle interaction in the LZ TPC is shown in Fig. 2.5. A broad overview of the process is given here. A particle interaction with LXe can excite or ionize Xe atoms. *Prompt scintillation* light is released immediately at the location of the interaction. This light reflects around the TPC until it is either collected at a PMT or lost to absorption. Light collected from prompt scintillation is referred to as the *SI* signal. *Free*

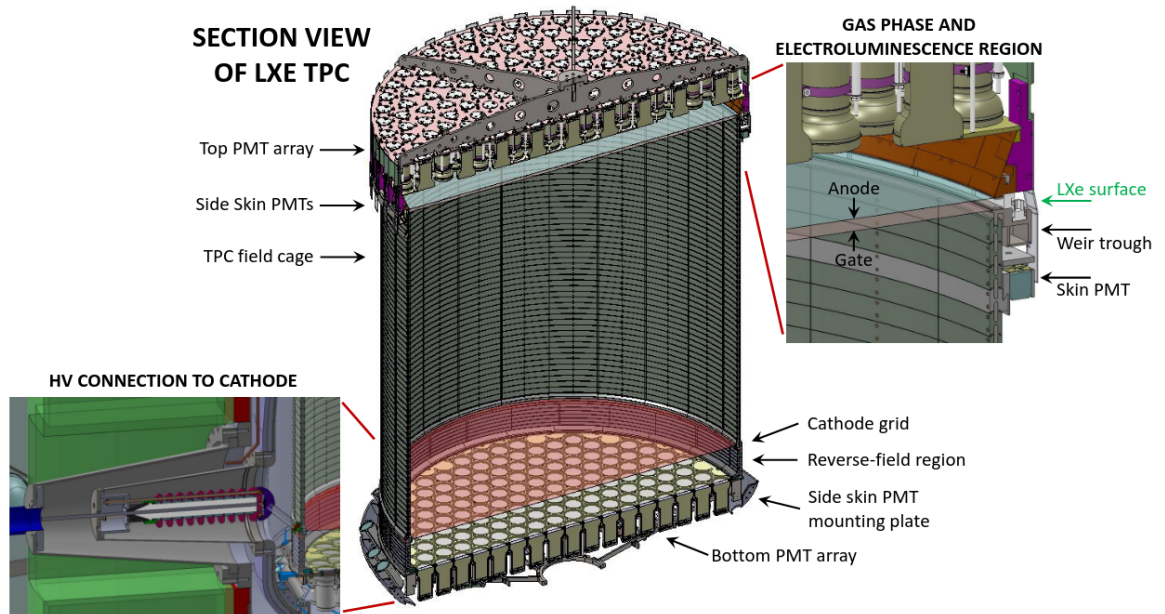


Figure 2.4: A cut away diagram of the LZ TPC is displayed. The PMT arrays are seen at the top and bottom of the cylinder. The cathode grid is shown near the bottom of the cylinder. The cathode's high voltage connection is shown in the inset on the left. The reverse field region between the cathode and bottom grids is indicated. The field cage creates the barrel of the TPC and spans most of the height of the TPC. The field cage is lined with Teflon. The top right inset indicates the position the tightly spaced gate grid, the LXe surface, and the anode grid. The weir fixes the liquid height between the two grids. Also visible are the skin PMTs, which are discussed in section 2.3 (image from [28])

electrons (or free charge) are also created at the interaction site. The electrons drift toward the top of the detector. Electrons that pass through the gate region and are extracted from the liquid electro-luminesce as they are accelerated through the gaseous region. This continues until they are collected on the anode. Light collected from electro-luminescence is referred to as the S2 signal.

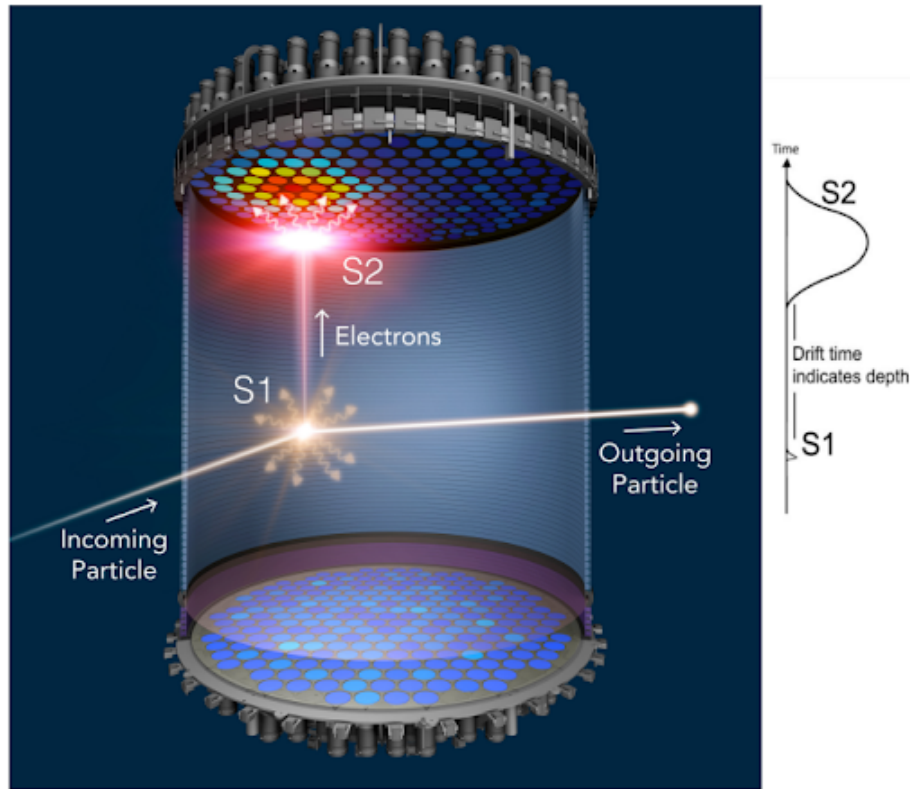


Figure 2.5: An illustration of a particle interaction in LZ is shown. A particle entering the detector and interacting with Xe atoms will produce prompt scintillation light at the site of the interaction. The collected prompt scintillation light is the S1 signal. The interaction will also produce free electrons, which drift to the top of the detector. Electrons that are extracted from the liquid will cause scintillation as they travel through the higher field gaseous region, before eventually being collected on the anode. The S2 signal from the gaseous scintillation is localized and used to determine the X-Y position of the event. The time between the S1 and S2 signals is used to determine the depth of the event (image from [28]).

The S1 and S2 signals are used to reconstruct the event position. The S2 signal's prox-

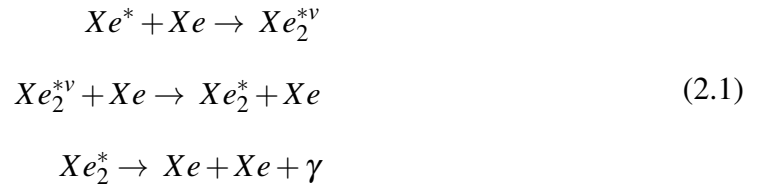
imity to the top PMT array allows the X-Y position of the event to be determined. The time between the S1 and S2 signals determines the depth of the event. Position reconstruction is important for the discrimination of backgrounds.

2.2.1 Xe interaction physics and its influence on the TPC design

The simplified overview above excludes several details regarding the physics of Xe interactions. Particles interacting with LXe will initially deposit energy in one of three ways: exciting the Xe, ionizing the Xe, or imparting the Xe with momentum (heat). LZ can measure the photons resulting from excitation and the charge freed by ionization but will not detect heat.

Scintillation light

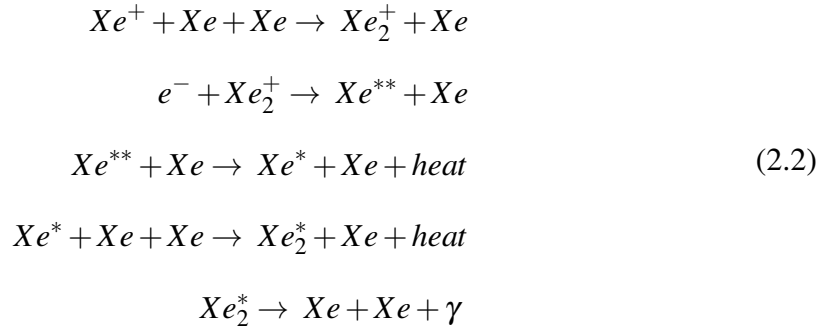
Ignoring what is lost to heat, energy from excitation and ionization remains. Excited Xe atoms, denoted as Xe^* , will nearly always form a diatomic bound excimer with a ground state Xe atom. The excimer is formed in an excited vibrational state and relaxes to an excited electronic state. This state decays by emitting a 178 nm photon,² on the timescale of tens of nanoseconds. This process is explained in [33]. Eq. 2.1 denotes the process.



Ionized atoms, Xe^+ , often immediately reform into molecular ions, Xe_2^+ . Electrons

²Note that this is the wavelength of the photon in vacuum, not in LXe. This will be referred to as 178 nm light throughout this chapter, but this is always in reference to its wavelength in vacuum.

freed by ionization can follow one of two paths: they can either recombine with Xe ions or remain free and drift to the top of the detector. The molecular formation and recombination process is outlined in Eq. 2.2.



Excited molecule recombination ends with the same process seen in the excited state formation and de-excitation. Both de-excitation and recombination occur within tens of nanoseconds [34]. The time difference between both sources of 178 nm light is imperceptible in LZ.

Several factors influence the recombination probability. The recombination rate depends on fluid density, electric field, particle energy, and track structure [35] [36] [37]. Roughly speaking, higher electric fields provide less time for electrons and holes to pair, reducing recombination. Recombination probability is generally higher when the linear energy transfer of the particle is higher because electrons and holes are more densely packed. However, areas of very high ionization density (greater than $10^3 \text{ MeV}/(\text{g}\cdot\text{cm}^2)$) show reduce light yield from excitation and recombination. The joining of two Xe^* resulting in a single Xe^+ through a process called *bi-excitonic quenching* may explain this observation [38].

The prompt scintillation photons travel through LXe relatively unimpeded. The two primary mechanisms that may affect photon propagation in the liquid are absorption and

Rayleigh scattering. The Rayleigh scattering length of a 178 nm photon in LXe is about 30 cm. Rayleigh scattering has no significant effect on the probability of any one photon being collected because it is an elastic process. Photon absorption in the bulk liquid is mostly due to impurities like H₂O and O₂. It is experimentally difficult to disentangle absorption and scattering lengths, but absorption lengths can exceed 100 cm [39]. LZ's purity should allow for absorption lengths that exceed 10 m [28].

Photons that reach the outer radius of the LZ TPC will encounter the PTFE lining the TPC barrel. 178 nm light propagating through LXe incident on a PTFE surface has been shown to have a reflectance that exceeds 95% when averaged across all angles [40] [41] [42]. Reflectance measurements of scintillation light in gaseous Xe incident on PTFE are slightly worse but are estimated to be between 75 and 85% [28]. PTFE is placed around the PMT bases on the top and bottom arrays.

Light can be absorbed by the four wire grids in the TPC. Each grid consists of a perpendicular set of woven wires. Each grid has a wire width of either 75 or 100 μm and a wire spacing of either 2.5 or 5.0 mm. The opacity of the bottom, cathode, and gate grids is between 3 and 4%, while the opacity of the anode grid is about 8% [28]. Their reflectance for 178 nm light is estimated to be poor (between 0 and 40%).

The liquid-gas boundary is relevant for light propagation. The critical angle for total internal reflection of 178 nm light at the Xe liquid-gas boundary is 36°. Prompt scintillation light is more frequently directed to the bottom PMT array.

The higher opacity of the anode grid, poorer light reflection at the gaseous Xe-PTFE, slightly lower coverage fraction of the top PMT array, and, most significantly, total internal reflection all contribute to a higher prompt scintillation light collection fraction at the bottom PMT array. The 241 3-inch bottom array PMTs are mounted in a hexagonal orientation. This is designed to maximize the photocathode coverage fraction, which reaches 54% in the bottom array [28]. The PMT arrangement is shown in Fig. 2.6.

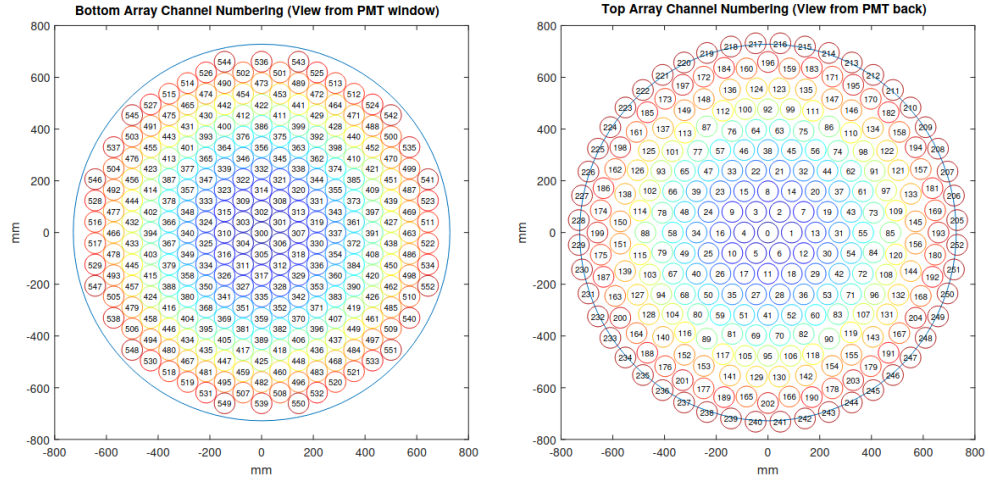


Figure 2.6: The arrangement of the bottom LZ PMT array is shown on the left. It is packed into a hexagonal structure to maximize PMT coverage at the bottom of the TPC where most of the S1 light is detected. The top LZ PMT array arrangement is shown on the right. The outermost PMTs are arranged in a circular manner and become more hexagonal toward the center. This improves position reconstruction near the walls, while maintaining a reasonable coverage fraction near the center of the detector. The top of the TPC is slightly wider than the bottom, so the top PMT array contains more PMTs despite being less densely packed. An outline of the shape of the bottom of the TPC is displayed as a cyan ring in both the left and right diagrams (image from [28]).

When a scintillation photon reaches the window of a PMT, it must still transmit through the window before it can be absorbed by the photocathode. LZ uses quartz windowed PMTs, which have an index of refraction of 1.57. Quartz is well matched to the 1.67 LXe index of refraction, allowing fairly good transmission through the bottom PMT windows [43]. Reflection within the window is possible.

Finally, the quantum efficiency of the PMTs must be taken into account. The quantum efficiency of a batch of the same model of PMTs used in LZ was measured to be $30.9 \pm 2.5\%$ when cooled to the LZ operating temperature [44]. Double photoelectron emission is possible at the Xe scintillation wavelength. This is estimated to occur for $22.6 \pm 2.0\%$ of PMT photoelectron emissions for the same PMTs under the same conditions [44]. The double photoelectron emission probability can be divided from the measured number of photoelectrons to acquire the measured scintillation signal in terms of photons detected (phd).

Losses from absorption in the LXe, on the grids, on the PTFE, and on inactive PMTs, as well as losses from the PMT quantum efficiency, limit the amount of collected scintillation light. The fraction of collected scintillation light, referred to as g_1 , was measured to be 0.114 ± 0.002 phd/photon in LZ's first science run [29]. The observed S1 signal (in phd) is related to the number of prompt scintillation quanta (resulting from both excitation and recombination) produced, N_{ph} , by this factor, as seen in Eq. 2.3.

$$N_{ph} = \frac{S1}{g_1} \quad (2.3)$$

An example of an S1 signal from LZ's event viewer is shown in Fig. 2.7.

The left plot shows the summed signal from all PMTs as a function of time. The S1 has a very sharp rise time and decays on the order of hundreds of nanoseconds. The amount of light collected by each PMT is shown on the right. Most light is collected by the bottom

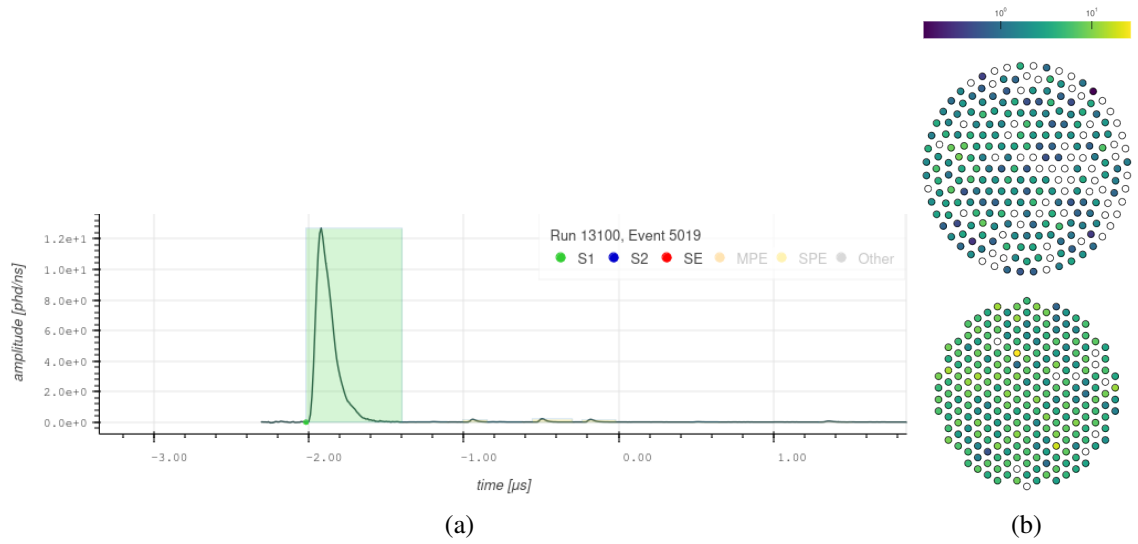


Figure 2.7: The left plot shows the sum of all PMT waveforms that contribute to the S1 pulse as a function of time. The width of the pulse is less than a μs . Its rise time is faster than its decay time, resulting in a non-symmetric shape. The pulse peak is about 12 phd/ns. The right diagram shows the PMT contributions to the summed pulse from the top array (at the top) and the bottom array (at the bottom). The intensities are higher at the bottom array, and there is no X-Y localization.

array and is not localized in X-Y space.

Free charge

Xe^+ ions and electrons that do not recombine drift toward the cathode or gate respectively. The majority of Xe^+ eventually neutralize by striking the cathode, acquiring an electron from its valence band. The free electrons will travel upward to the gate grid. The electrons may attach to electronegative impurities in the LXe, vastly lowering ion mobility. LZ measured the electron lifetime to be between five and eight ms for its first science run, which exceeded the total electron drift time (about $950 \mu\text{s}$) [29]. The fraction of electrons reaching the gate is dependent on depth and Xe purity.

Free electrons approach the gate in a cloud, with positions dispersed by the initial energy deposition and further spread by diffusion during drift. The electrons that reach and pass through the gate enter the 13 mm extraction and electro-luminescence region between the gate and the anode. The bottom 5 mm of the region is in the liquid, and the top 8 mm is in gas. The field in the extraction and electro-luminescence region is much higher than the field between the gate and the cathode. Further, the gaseous extraction region field is 1.96 times higher than the liquid extraction region field, due to the difference in the liquid and gas permittivity. For LZ's first science run, the extraction region (liquid) field was 3700 V/cm, compared to 193 V/cm between the cathode and the gate³ [29]. A photograph of the anode and gate grids prior to assembly in the TPC is shown in Fig. 2.8.

A reasonably high electric field is required for electrons to be efficiently extracted from the liquid into the gas. The potential difference between a free electron in vacuum and a free electron in LZ LXe is $0.67 \pm 0.05 \text{ eV}$ [45]. Additionally, the image charge at the liquid gas interface must be overcome to extract the electron. Only electrons with a mo-

³The LZ grid voltages changed several times after the first science run.

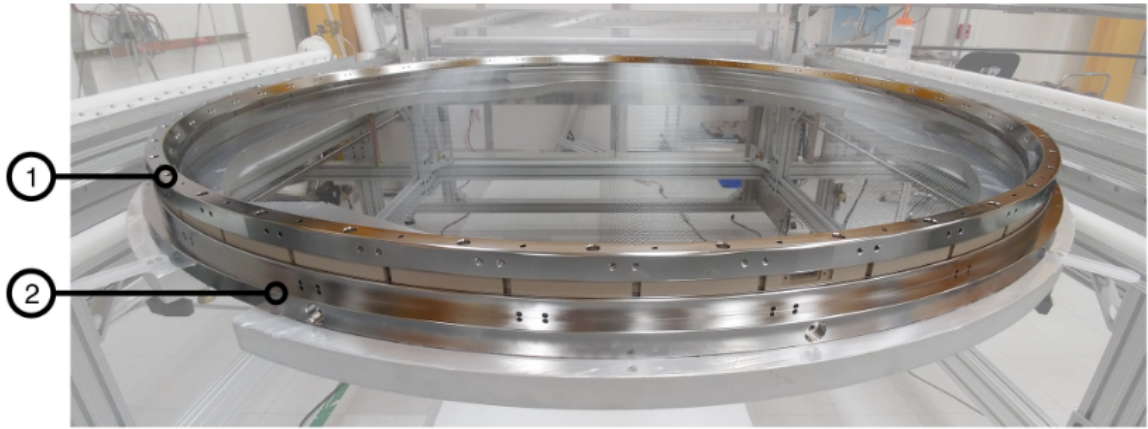


Figure 2.8: A picture of the assembled woven anode (1) and gate (2) grids that make up the extraction region is shown. Slight loss of transparency through the grids is seen from the photograph (image from [32]).

momentum projection perpendicular to the interface that exceeds the momentum necessary to overcome the barrier created by the potential difference and image charge will exit the liquid.

Electrons will change direction by scattering with Xe atoms. Though an electron may have sufficient energy to exceed the extraction threshold, its momentum perpendicular to the liquid surface may not be sufficient for the electron to be extracted the first time it approaches the liquid surface. Electrons that do not initially meet the momentum projection requirement are reflected back into the liquid phase, where they continue to (inelastically) scatter. The fraction of energy lost during each scatter is on the order of 0.1%, allowing the electrons to scatter many times and still be extracted. Tens of reflections occur on a ns timescale, and nearly all electrons with sufficient initial energy are eventually extracted [46].

Electrons subject to the 7300 V/cm field in the gaseous region will accelerate to speeds sufficient to excite the Xe atoms in their path and produce the secondary scintillation signal. The excitation signal is proportional to path length and produces scintillation light with a dominant wavelength of 171 nm (in Xe gas) when pressures exceed 1 bara [47]. The

electrons are eventually collected on the anode grid.

Most of the secondary scintillation signal is collected by the top array. The top array PMTs are arranged to maximize position reconstruction, particularly near the edge of the detector. PMTs at the outer radii are arranged in a circular manner, with the orientation progressing to hexagonal at the center. The TPC is slightly tapered, so the radius at the top is larger than the radius at the bottom. This accommodates 253 3-inch top array PMTs despite a less efficient packing orientation. The PMT orientations for both the bottom and top array are shown in Fig. 2.6.

The extraction efficiency of the free electrons, the gain resulting from the proportional scintillation, the collection efficiency of those scintillation photons, and the quantum efficiency of the PMTs are all quantified together as the factor g_2 . This relates an observed number of secondary scintillation photons, S_2 , to the quanta of free electrons produced (after recombination) N_{e^-} , via Eq. 2.4. For LZ's first science run, this was measured to be 47.1 ± 1.1 phd/electron [29].

$$N_{e^-} = \frac{S_2}{g_2} \quad (2.4)$$

A single electron extracted from the liquid will result in a roughly square pulse of $2 \mu\text{s}$ width. An S_2 signal is a sum of single electrons that have been smeared because of spread in the initial (spatial) charge distribution and diffusion. An example of an S_2 waveform from the LZ event viewer is seen in Fig. 2.9.

The left plot shows the summed PMT traces for the event as a function of time. S_2 widths depend on depth and are typically between 6 and $12 \mu\text{s}$. The S_2 shape is more symmetric than the S_1 . The majority of the light is detected by the top array. This event's S_2 signal is localized to the left side of the TPC. This S_2 is from the same event as the S_1 from Fig. 2.7. These S_1 and S_2 PMT waveforms are shown together in Fig. 2.10.

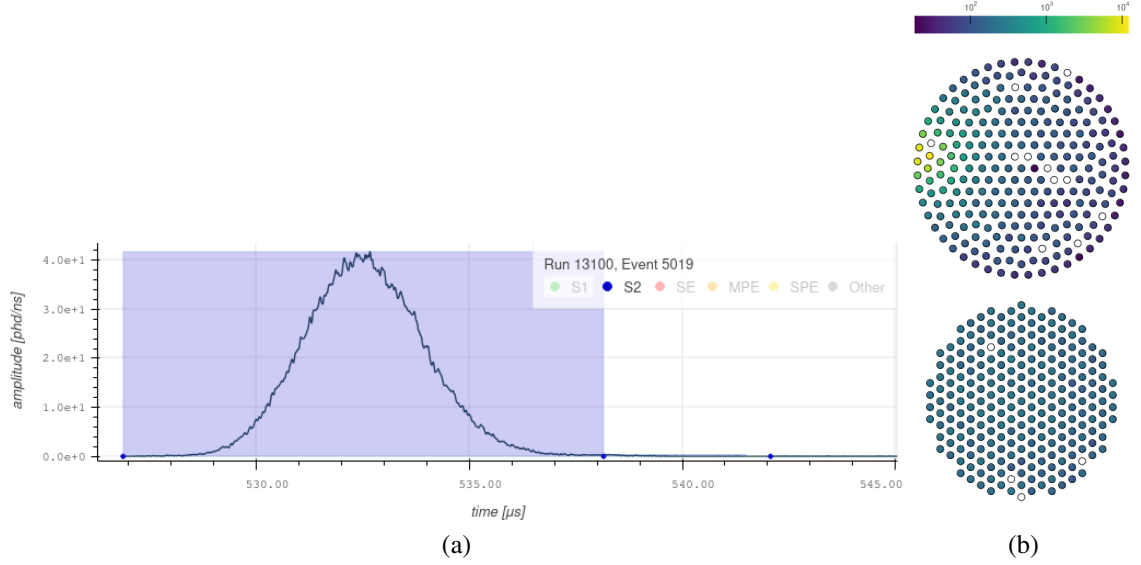


Figure 2.9: The left plot shows the sum of all PMT waveforms contributing to this S2 pulse as a function of time. The shape is far more symmetric than the S1 pulse. Both the width and the amplitude of this pulse exceed the width and amplitude of the corresponding S1 pulse shown in Fig 2.7. S2s are much larger than S1s because of the proportional gain from electro-luminescence. The PMT contributions to the summed pulse are shown on the right. The top array sees far more light, and the X-Y localization is clear.

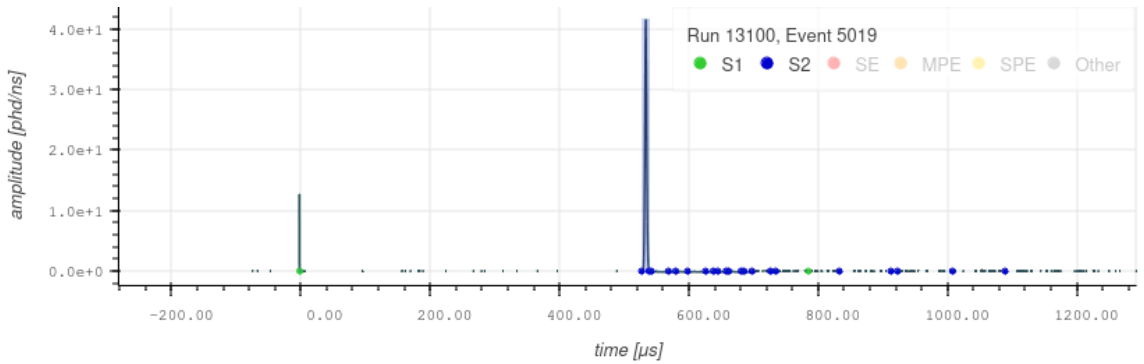


Figure 2.10: Shown are the summed S1 and S2 PMT waveforms as a function of time for the event discussed in Fig. 2.7 and Fig. 2.9. The time between the pulses ($\approx 500 \mu s$) indicates the depth of the event. The difference between the integrated pulse sizes is about two orders of magnitude.

The two pulses are separated by about $500 \mu\text{s}$. The maximum drift time in the TPC (from the cathode to the gate) was about $1050 \mu\text{s}$ when this event occurred, meaning the interaction that produced the event was about 0.75 m above the cathode. The S2 amplitude and width are much greater than the amplitude and width of the S1. The integrated S2 area is about $1.4 * 10^5$ phd, compared to $1.6 * 10^3$ phd for the S1. The large S2 area is the product of the gas scintillation gain and high efficiency for electron collection at the anode.

2.2.2 Energy reconstruction

The energy deposited (E_0) from an electron recoil interaction in LXe is given by Eq. 2.5, where E_i is the average energy to ionize for N_i ions, E_{ex} is the average energy to excite for N_{ex} excitons, and ϵ is the average energy lost to heat per electron. For LXe, ϵ is well known and relatively small.

$$E_0 = N_i E_i + N_{ex} E_{ex} + N_i \epsilon \quad (2.5)$$

The initial number of ionizations or excitations is not measured in a dual phase TPC. Instead, the quanta of prompt scintillation photons and free electrons are measured, subject to efficiencies and gain (from Eq. 2.3 and 2.4). These are related by the recombination fraction r using Eq. 2.6 and 2.7.

$$N_{ph} = N_{ex} + r N_i \quad (2.6)$$

$$N_{e^-} = (1 - r) N_i \quad (2.7)$$

Reconstructing energy is straightforward when the recombination fraction is known. Unfortunately, the mean recombination fraction depends on several parameters. Further,

repeated observations of mono-energetic events (with consistent detector conditions) produce S1 and S2 spectra with variances exceeding the variance expected for a Poisson process [48] [35].

The fluctuations in the light and charge signals from mono-energetic events are anti-correlated. This is unsurprising because recombination reduces the amount of free charge and equally increases the amount of prompt scintillation. When there is no quenching, the number of quanta before and after recombination is conserved, as noted by Eq. 2.8.

$$N_{ex} + N_i = N_{ph} + N_{e^-} \quad (2.8)$$

The W-value, $W = E_0/N_i$, is defined as the (total) energy deposited per ionization. Following [33], an analogous "scintillation W-value" can be defined, $W_s = E_0/N_{ph}$, for charge. W references the ionization produced before recombination. W_s is the post-recombination scintillation signal for zero field when all ions are assumed to recombine. In the zero field case, all excitons and ions are assumed to produce a single photon, $N_{ph} = N_{ex} + N_i$. Replacing N_{ph} in the definition for W_s gives Eq. 2.9, where W_s^{min} is the minimum energy required to produce a scintillation photon.

$$W_s^{min} = E_0/(N_i + N_{ex}) \quad (2.9)$$

Because quanta are conserved during recombination, Eq. 2.9 can be written in a more directly applicable form (with a slight change in notation) as Eq. 2.10. The total energy deposited is E , N_q is the number of quanta produced (as the sum of either N_{ex} and N_i or N_{ph} and N_{e^-}), W_q is the W-value for production of quanta, $S1_c$ and $S2_c$ are the (position corrected) S1 and S2 values, and $L(E)$ is the Lindhard factor. This generally holds for LXe TPCs [49].

$$E = N_q \frac{W_q}{L(E)} = (N_{ph} + N_{e^-}) \frac{W_q}{L(E)} = (S1_c/g_1 + S2_c/g_2) \frac{W_q}{L(E)} \quad (2.10)$$

$S1_c$ and $S2_c$ are modest corrections to the light and charge, determined by the positional dependence of light and charge collection. The corrected and uncorrected light and charge values varied by around 10% on average throughout the fiducial volume during LZ's first science run [29].

The Lindhard factor in this equation accounts for energy loss to heat. For electron recoils, this factor is constant in energy, and it has been shown that the number of quanta per unit energy is fixed [50]. Some conventions set the Lindhard factor to 1 for electron recoils, with heat losses built into W_q .

For nuclear recoils, the fraction of energy lost to heat is much higher and is not constant in energy [51] [52]. Analysis of many experiments across several decades indicate that the relationship between quanta and energy produced by nuclear recoils can be reasonably well described by a power law given by Eq. 2.11 [49]. Fitting to historical data, the exponent β is close to, but not consistent with, 1, implying $L(E)$ can be approximated by an equation that is linear in energy.

$$N_q = \alpha E^\beta \quad (2.11)$$

2.2.3 Electron and nuclear recoil discrimination

One attractive feature of LXe dual phase TPCs is their ability to discriminate between electron and nuclear recoils. WIMPs are expected to interact with Xe nuclei. The vast majority of radioactive backgrounds interact with electrons. Effectively discriminating between the two types of recoils is critical.

The ability to discriminate arises from the disparity in the exciton-ion ratio, N_{ex}/N_i , in

nuclear and electronic recoils and differences in recombination, which produce different N_{ph} and N_{e-} . The exciton-ion ratio is measured to be about one for nuclear recoils above 7 keV [52] [53]. For electron recoils, the observed ratio is 0.06 [54]. When events are plotted by $\log(S2_c)$ and $S1_c$ (the log is a common convention), the electron recoils and nuclear recoils separate into two distinct bands. This separation can be seen in Fig. 2.11.

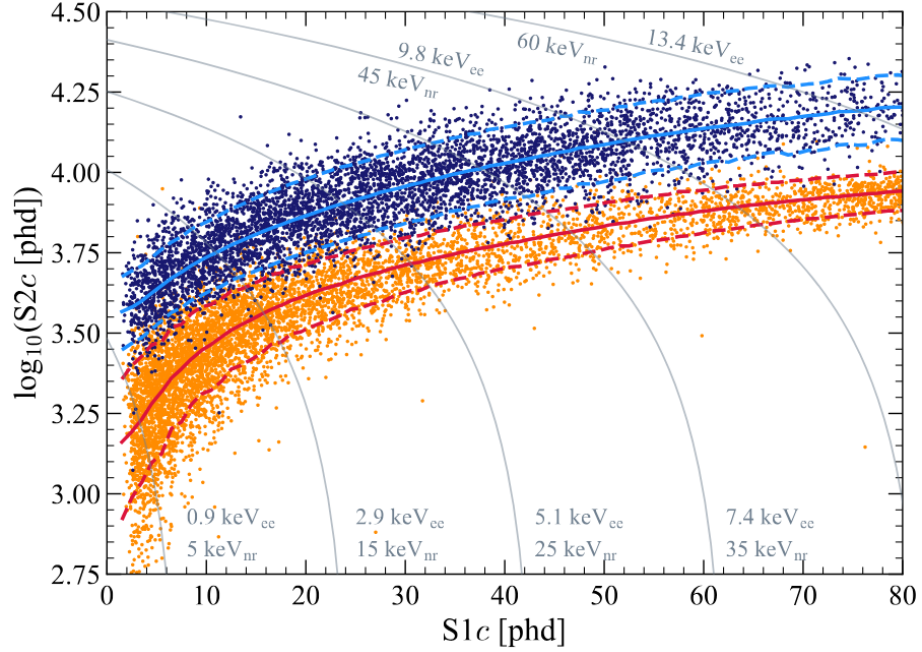


Figure 2.11: Calibration data from LZ's first science run is shown on a $\log(S2_c)$ vs $S1_c$ plot. The blue events were recorded during a tritium calibration and outline the (cyan) electron recoil band. Orange events are from the ^2H - ^2H neutron generator calibration and outline the (red) nuclear recoil band. Lines of equal energy for each respective recoil type are drawn on the plot (image from [29]).

The plotted events were recorded during calibrations following LZ's first science run. The electron recoil band is populated with (blue) tritium β -decay events. The nuclear recoil band is populated by (orange) neutron events produced by a ^2H - ^2H neutron generator. One of LZ's predecessors, the Large Underground Xenon experiment (LUX), observed 99.6% rejection of electron recoils, while maintaining 50% acceptance for nuclear recoils [55].

Lines of equivalent energy are also displayed on the plot. The true deposited energy

of a nuclear recoil is greater than the deposited energy of an electron recoil that produced an identical number of quanta because of the additional nuclear recoil energy lost to heat (captured by the Lindhard factor in Eq. 2.10). Deposited energy corresponding to a nuclear recoil is often denoted keV_{NR} , while deposited energy corresponding to an electron recoil is often denoted keV_{ER} .

2.3 The LZ Skin Veto

For LZ to be mechanically viable, there must be space between the TPC assembly and the titanium inner cryo-vessel (ICV) that houses the TPC. This *skin* region is also filled with LXe, providing both electrical insulation between the TPC and cryostat, and self shielding for the active volume. This region can also be instrumented. The skin consists of two sections: the *side skin* region that surrounds the barrel of the TPC and the *dome skin* below the TPC. The skin holds about two tonnes of Xe.

Many of LZ's backgrounds originate from sources that are external to or a part of the TPC. The skin Xe can help reject them. The skin volume is instrumented with 131 PMTs. 18 2-inch PMTs form a ring in the bottom dome, with 12 pointing away from the center and 6 pointing inward. 20 2-inch PMTs point up from the base of the side skin. 93 1-inch PMTs point down from the top of the side skin. The skin is a scintillation only detector since it has no gaseous Xe and no significant electric fields. All surfaces except the PMT windows and the cabling are covered in PTFE to maximize light collection. Fig. 2.12 shows the view from the top of the ICV, looking down into the skin prior to TPC installation. The bottom side skin PMTs are visible. Fig. 2.13 shows the outer portion of the assembled TPC. PTFE tiling used to enhance light collection in the skin is visible. The top side skin PMTs are also visible, recessed inside the ring above the TPC field cage.

The skin is optically isolated from the TPC. A simultaneous detection of scintillation

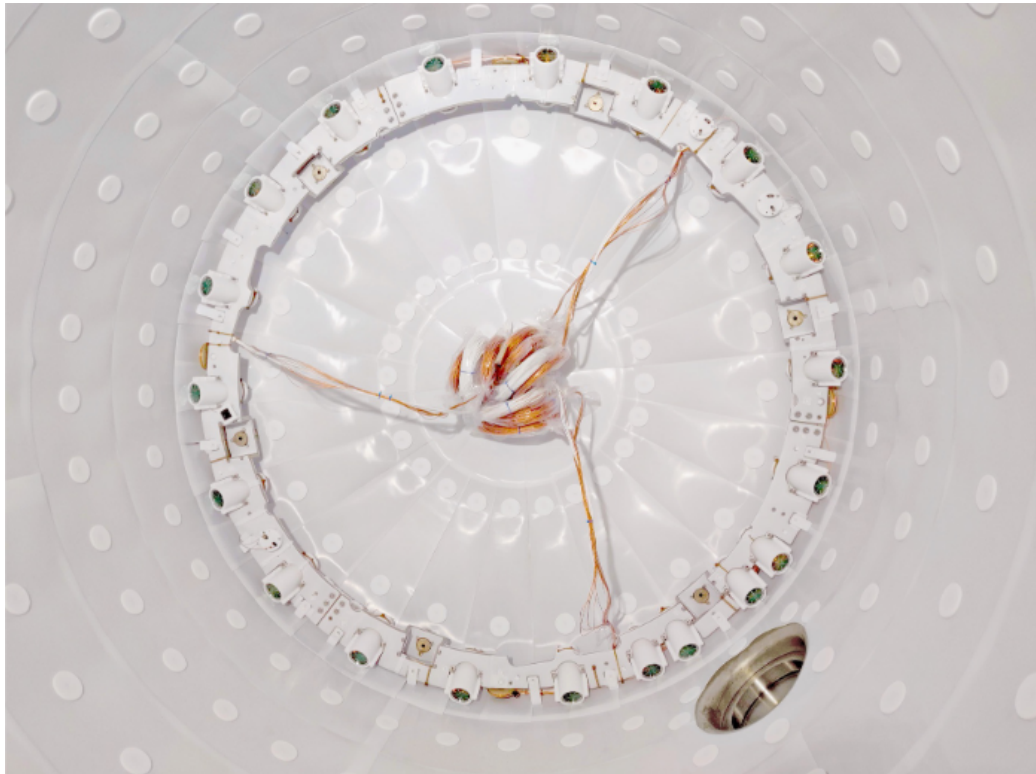


Figure 2.12: A photograph looking down at the 20 bottom side skin PMTs from the top of the inner cryovessel prior to the TPC's insertion is shown. These PMTs form a ring around the bottom of the cryostat. They are packed more densely near the cathode high voltage port (seen in the bottom right of this photo). The bottom dome PMTs are not installed (image from [32]).



Figure 2.13: An image of the LZ TPC before being inserted in the inner cryovessel is shown. Some of the 93 top side skin PMTs can be seen above the PTFE, pointing downward in the ring lining the top of the field cage. The bottom dome skin PMTs are not visible but are assembled under the bottom PMT array (image from [32]).

light from the TPC and the skin indicates a particle has scattered multiple times, which is inconsistent with a Xe-WIMP interaction. The skin has modest light collection efficiency and very poor energy and position resolution. Thus, the skin acts primarily as a coincidence veto to reject backgrounds that enter or exit the TPC.

The skin PMTs detected a signal during the event discussed in section 2.2.1, in Fig. 2.7, 2.9, and 2.10. The signal is seen in Fig. 2.14.

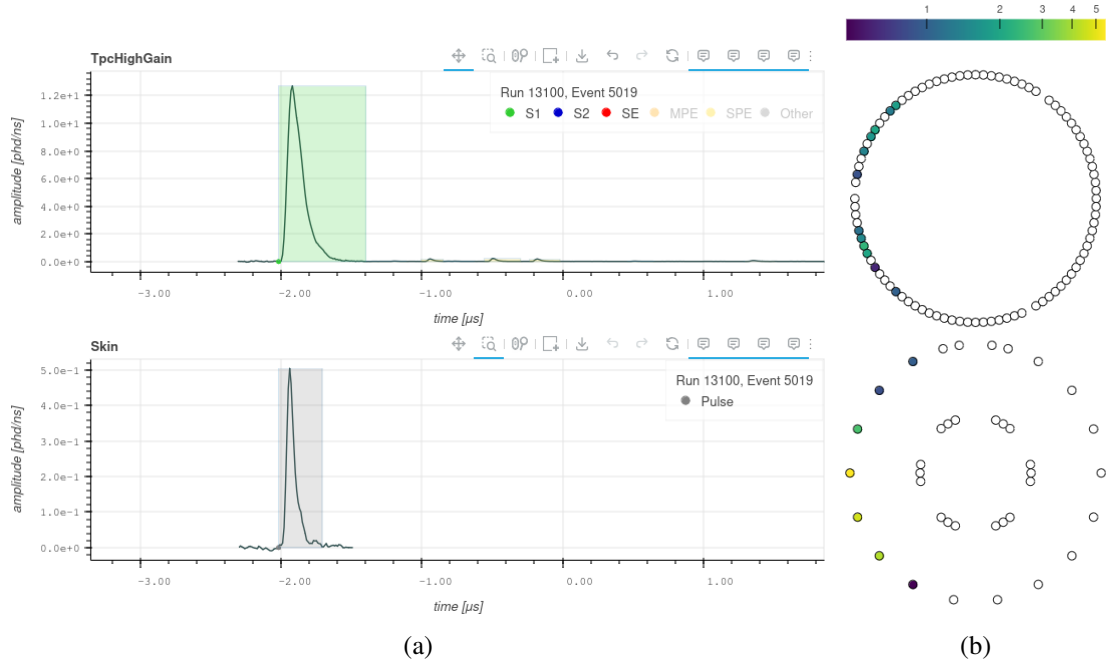


Figure 2.14: The summed PMT waveforms from the TPC and skin for the event discussed in Fig. 2.7, 2.9, and 2.10 are shown. The top plot on the left shows the S1 signal from the TPC (this was shown in Fig. 2.7). The bottom left plot shows the summed skin PMT waveforms for the same time interval. The coincidence implies at least two scatters occurred (at least one in both the skin and TPC). The PMT contributions from the top side skin (top right), bottom side skin (bottom right, outer), and dome skin (bottom right inner) are shown on the right diagram. The azimuthal position of each skin PMT ring corresponds to the azimuthal position of the TPC PMT arrays. The side skin PMTs suggest the interaction occurred near the $\theta \approx \pi$ region of the skin, close to the interaction location in the TPC. The bottom dome PMTs detected no signal.

The coincidence between the S1 and skin signals is very clear. The PMTs on the $\theta \approx \pi$

side of the skin detected the scintillation signal. Multiple scatters in roughly the same location indicate that this may have been a gamma that scattered in both the skin and TPC.

2.4 The LZ Outer Detector

Reviewing Fig. 2.3 is useful to visualize the components of the outer detector. A cluster of acrylic tanks, containing gadolinium loaded liquid scintillator (Gd-LS), immediately surround the cryostat. The scintillator tanks rest in a large water tank. The water tank contains about 228 tonnes of ultrapure water. The TPC and the cylindrical water tank have a common center axis.

A cylindrical cage-like support structure rests 282 cm from the center of the water tank and 115 cm from the outer edge of the acrylic tanks. The support structure is used to secure rows of 8-inch PMTs that detect light from the scintillator tanks. A total of 120 PMTs surround the acrylic tanks at six different heights and 20 different azimuthal positions. The PMTs protrude into the middle of the support cage such that the PMT window surfaces are about 84 cm from the acrylic tanks [28].

The support structure, the PMTs, and the floor are wrapped in Tyvek, and the ceiling is fashioned out of Tyvek to ensure maximum scintillation light collection. A low density foam is used to displace water near the geometrically complex portions of the cryostat and simplify the build geometry of the acrylic tanks. Fig. 2.15 shows a photograph taken inside the outer detector, before the water tank was filled.

Detector materials and the cavern walls may emit both gamma rays and neutrons. Neutrons in the TPC may cause a nuclear recoil and travel significant distances without scattering again. The primary purpose of the outer detector is to detect neutrons and veto neutron interactions. The outer detector is also used to study and estimate the neutron backgrounds it fails to reject. Gamma rays and, to a lesser extent, muons are also detected by the outer

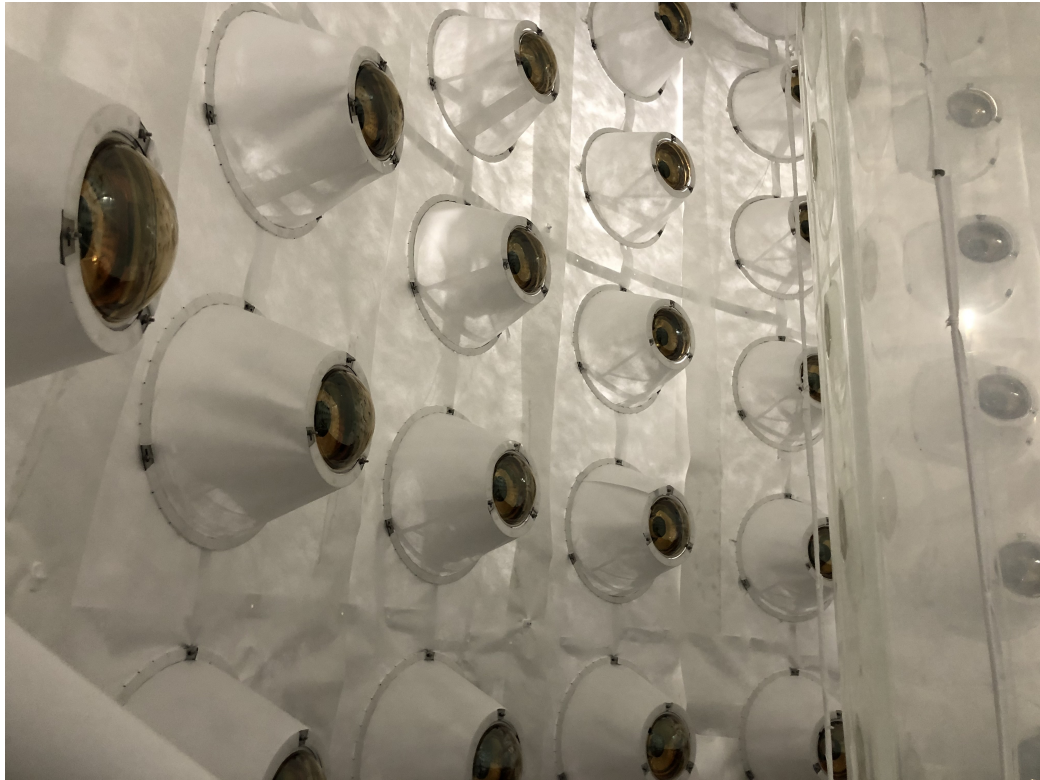


Figure 2.15: A photograph from inside the LZ outer detector is shown. The (empty) acrylic tanks are seen on the right side of the picture. The PMTs are seen protruding out of the Tyvek curtain. The PMT support structure lies behind the Tyvek curtain. The structure's shadow is visible on the Tyvek.

detector.

The liquid scintillator is a linear alkylbenzene solvent. Gammas in the liquid scintillator will induce scintillation, which can be picked up by the outer detector PMTs. The scintillator is doped with 0.1% Gd. Neutrons can be captured on H in the scintillator, but Gd has a much higher neutron capture cross-section: 49 kb compared to 0.33 b [28]. Gd releases three or four gammas with a total of about 8 MeV of energy, as opposed to a single 2.2 MeV gamma for H capture. The probability of all Gd capture gammas escaping the scintillator without causing scintillation is much lower than the probability of a single H capture gamma escaping. The scintillation response time to neutrons in the 0.1% Gd-LS is only 30 μ s, as opposed to 200 μ s for scintillator with no Gd [28]. Gd doping greatly reduces the fraction of neutrons that take an extended period of time to capture.

An important component of the outer detector veto system is its background. Any source of gamma rays in the cavern, including the cavern rocks, the PMTs, or the scintillator itself, could contribute to its trigger rate. High internal radioactivity will increase the fraction of time that outer detector veto is active, reducing live time. The measured outer detector rate above roughly 200 keV during LZ's first science run was 43 Hz, which is acceptable for the experiment [56].

2.5 The LZ Xe Circulation System

The Xe in the LZ experiment must be kept sufficiently pure. The Xe was cleaned before being introduced to the LZ detector, however there are mechanisms capable of increasing impurities, even during science operations. Xe must be actively cleaned during operation to ensure science goals are met.

Macroscopic amounts of impurities prevent Xe condensation. As mentioned in section 2.2, excess electronegative impurities can absorb prompt scintillation light, reducing

valve (not shown) is used to regulate flow. The compressor diaphragms and seals are all metal to minimize the often high Rn burden of rubbers. The compressors were intended to operate in parallel to deliver a Xe flow rate of 500 slpm. Maintenance schedules dictate that only one compressor is operated at a time, limiting flow to 370-400 slpm.

The LZ noble gas purifier (getter) immediately follows the compressors in the circulation flow path. The device uses zirconium material to capture and remove electronegative impurities in the Xe. Purification must occur in the gaseous phase because heating the zirconium is critical to ensure its effectiveness. The getter is discussed further in section 5.1.

The LXe tower is responsible for changing the phase of Xe as it enters and exits the TPC. Xe leaving the getter will enter the two phase heat exchanger, where it is cooled by Xe exiting the TPC. Xe that entered the heat exchanger from the gaseous portion of the circulation system is near or on the gas-liquid boundary as it exits the heat exchanger and enters the subcooler. The subcooler further cools the LXe to ensure it is sufficiently below the boiling point as it enters the transfer lines. The transfer lines direct the LXe to the ICV. LXe in the ICV spills over the weir drain pipes that maintain the liquid height. The spill-over LXe travels back to the Xe tower, where it rests in the reservoir. This Xe flows back into the two phase heat exchanger, where it is warmed by Xe entering from the gaseous portion of the circulation system. The LXe tower and TPC are outfitted with numerous temperature monitoring and control devices, like resistive temperature detectors (RTDs), thermosiphons, and heaters. All circulation components involving LXe are placed in an insulating vacuum.

Several breakouts are necessary to extract cables from the TPC. These breakouts contain pockets of gas that would be isolated if not for the flow paths leading to the Rn removal system. The system consists of a column filled with 10 kg of nitric acid etched, synthetic charcoal. The system uses chromatography to sequester Rn. The column is cooled to 190 K to increase sequestration time. Flowing at 0.5 slpm, the system holds Rn for 12.7 days

[32]. The Rn removal system location is chosen to mitigate Rn emanating from the cable breakouts, despite the modest flow rate.

2.6 Background Discrimination Techniques

Any successful rare event search must effectively reject backgrounds. Several general sets of event selection cuts are applied in the LZ experiment. These have been referenced throughout this chapter but are explicitly stated here.

The probability of a WIMP scattering off of a Xe atom in LZ is incredibly low. The probability of a WIMP scattering twice in the same time window is nonexistent. Any event that scatters multiple times in the detector is likely a gamma ray or neutron and is rejected.

A 30 GeV WIMP is expected to deposit between 5-30 keV_{NR}. This deposition is mass dependent, with higher mass WIMPs capable of depositing greater energies. Though the tails of high mass WIMP recoil energy spectra may stretch beyond 60 keV_{NR}, the majority of WIMP interactions are expected to deposit less energy. An energy cut is not explicitly used to reject backgrounds, but cuts on $S1_c$ and $S2_c$ are used to reject events that exceed an energy roughly corresponding to 55 keV_{NR}. The combination of the $S1_c$ and $S2_c$ cuts is used to define the WIMP search region of interest (ROI).

Discrimination between electron and nuclear recoils is discussed in section 2.2.3. Electron recoil band events are not explicitly cut from the analysis but are used to quantify electron recoil backgrounds. Electron recoils can leak into the nuclear recoil band. Each event is assigned a probability of being a nuclear or electron recoil based on its observed $S1_c$ and $S2_c$. The low probability of events in the electron recoil band being WIMP events is reflected in the profile likelihood fit, rather than via outright rejection.

Many of the detector materials contain radioactive isotopes. Every candidate detector material was screened to verify its radioactivity is relatively low, but screening cannot re-

move all radioactivity. Gammas and neutrons may also enter from outside the detector. Xe is self shielding, and sources of radioactivity are more abundant near the detector walls, so backgrounds are lower near the center of the detector. A WIMP's interaction probability is spatially uniform in the TPC. A positional (fiducial) cut, removing the outer edges of the detector, rejects a high fraction of external and wall related backgrounds.

Veto cuts from the skin and outer detector are applied. Any event with coincidence in the TPC and either the skin or the outer detector is rejected. Neutrons represent a potentially dangerous background because they recoil off of the nucleus and have a nontrivial probability of scattering only once in the TPC. The high neutron capture cross-section of Gd in the outer detector liquid scintillator tanks is important for rejecting neutrons. Gammas are less likely to travel large distances in LXe, so the skin provides slightly more Xe for rejecting or absorbing gammas. The effect of the fiducial cut, skin veto, and outer detector veto on events in the ROI in LZ's first science run are shown in Fig. 2.17.

Events passing all cuts are shown as solid black dots. Events that fail only the fiducial volume cut are shown in gray. Events in blue fail the outer detector cut, while events in red fail the skin cut. The excess of events near the walls is evident from this plot. The higher event density near the high radius edge of the fiducial volume is heavily mitigated by the vetoes (particularly the skin veto).

Events that pass all the cuts during LZ's first science run are displayed in $\log(S2_c)$ vs $S1_c$ space in Fig. 2.18. The electron recoil band is shaded in gray, the nuclear recoil band sketched in red, and the expected location of a $30 \text{ GeV}/c^2$ WIMP event is shown in purple. The fitted number of $30 \text{ GeV}/c^2$ WIMP signal events during LZ's first science run is $0^{+0.6}$.

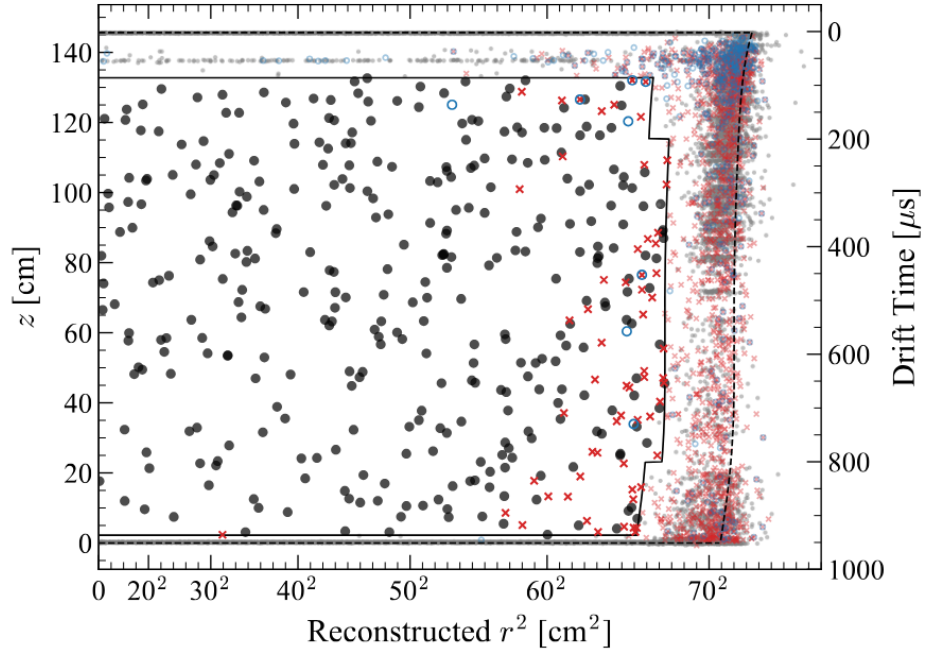


Figure 2.17: A plot of the positions of LZ science run 1 events passing all cuts except the fiducial, skin veto, and outer detector veto cuts is shown. The corresponding drift time is also indicated on the right axis. The fiducial volume is outlined in solid black, and the estimated wall position is outlined in dashed black. Events may be reconstructed outside the estimated wall position. Events that pass all cuts are marked in black. Events failing the skin cut are shown as red "x"s, events failing the outer detector cut are shown as blue "o"s, and events which pass both but are outside the fiducial volume are shown in gray. Radioactivity from detector construction materials results in a large number of events near the walls (image from [29]).

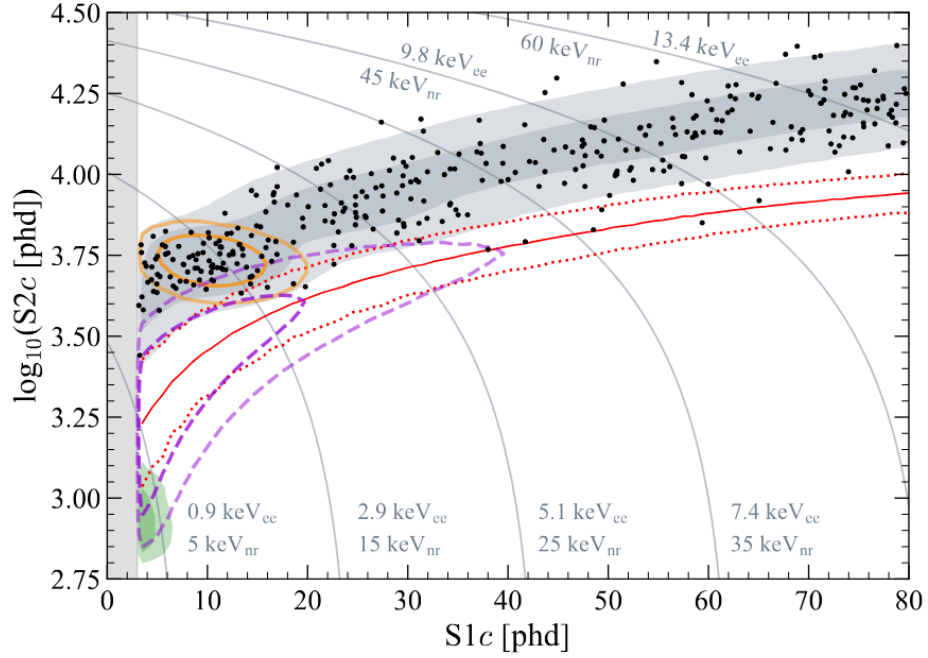


Figure 2.18: A plot of events passing all cuts in $\log(S2_c)$ vs $S1_c$ space for LZ's first science run is shown. The one and two sigma expected distributions are shown for the electron recoil band (gray), a $30 \text{ GeV}/c^2$ WIMP (purple), ^{39}Ar (orange), and ^8B solar neutrinos (green). The red bands indicate the median, 10th, and 90th percentiles of the nuclear recoil band. Bands of equal energy are plotted for each recoil type. As expected, the vast majority of events are in the electron recoil band. A handful of events at higher energies appear in the nuclear recoil band. Increasing the WIMP mass would expand the WIMP probability contour to higher energies along the nuclear recoil band, but a significant fraction of the WIMP interaction probability density would remain at low energies (image from [29]).

2.7 Summary

Liquid Xe time projection chambers are the leading technology in the field of direct detection of dark matter for the WIMP mass range. LXe TPC experiments continue to probe lower WIMP scattering cross-sections that remain inaccessible to other detector types. LZ is a LXe TPC experiment designed to set world leading cross-section limits across the WIMP mass range.

The LZ TPC exhibits good light and charge collection. The systems surrounding the LZ TPC, including the skin and outer detector vetoes, help reject backgrounds. LZ's Xe circulation system reduces Rn rates and maintains high Xe purity. All parts of the experiment made necessary contributions to the world leading limit set after LZ's first science run,⁴ as shown in Fig. 2.19. LZ is well suited to continue setting world leading limits on the scattering cross-section in the WIMP mass range.

⁴This limit has since been surpassed. This will be discussed in the conclusion.

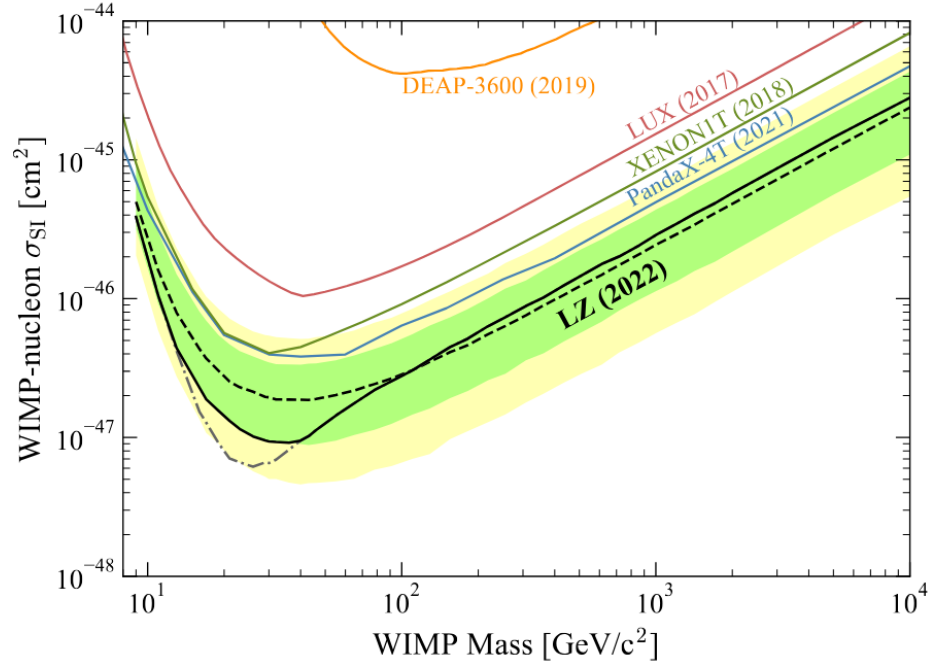


Figure 2.19: The (spin independent) WIMP cross section exclusion curves as a function of WIMP mass for different experiments when LZ’s first WIMP search publication was submitted are shown. The solid black line indicates the 90% confidence limit. The dashed black line indicates LZ’s median sensitivity with the green and yellow, indicating the ± 1 and 2σ contours. Inconsistency in the shape between this and previous limit curves (particularly the heavier exclusion of WIMPs between 15 and 50 GeV/c^2) is due to an absence of events in the $< 25 \text{ keV}_{NR}$ portion of the nuclear recoil band, seen in Fig. 2.18. The measured result in this mass range (noted by the dot-dashed gray line) is power constrained to the experiment’s -1σ projected sensitivity. The result was world leading in the WIMP mass range (image from [29]).

Chapter 3: Cold Trap Mass Spectrometry

LZ maintains high cleanliness standards for its ten tonnes of Xe. A noble gas purifier (getter) actively removes non-noble impurities during normal operation. Noble impurities are more difficult to address. The two noble impurities of greatest interest to LZ (excluding Rn) are Kr and Ar. While the common isotopes of each of these gases are not particularly problematic, atmospheric Kr and Ar both contain radioactive isotopes that may contribute to LZ's background.

^{85}Kr has an isotopic abundance of $2 * 10^{-11}$ ($^{85}\text{Kr}^{nat}\text{Kr}$) [57] [58]. The isotope decays with a 10.78 year half-life to ^{85}Rb . The decay has a Q-value of 687 keV, and the most common decay path is via β - decay directly to the ^{85}Rb ground state. ^{39}Ar has an isotopic abundance of $8 * 10^{-16}$ ($^{39}\text{Ar}^{nat}\text{Ar}$). This isotope decays via β - decay to ^{39}K , with a Q-value of 565 keV. Both of these decays contribute to LZ's electron recoil backgrounds. An excess of electron recoil events will spill over into the nuclear recoil band and limit LZ's potential for discovery. Better measurements of ^{85}Kr and ^{39}Ar improve the constraint of the dominant and degenerate ^{214}Pb β background. Despite their low abundance, ^{85}Kr and ^{39}Ar dictate the ^{nat}Kr and ^{nat}Ar requirements in LZ.

LZ's initial Kr requirement was 15 parts per quadrillion (ppq, measured in $\text{g}_{\text{Kr}}/\text{g}_{\text{Xe}}$) at the start of operation, with ingress limited to 5 ppq (g/g) per year [28]. The initial Ar requirement at the start of science runs was 450 parts per trillion (ppt, $\text{g}_{\text{Ar}}/\text{g}_{\text{Xe}}$), with no expressed limit for yearly Ar increase [28]. The estimated ^{214}Pb background allowed the starting Kr requirement to be relaxed to 300 ppq (g/g). There was no expressed revised

limit for Kr ingress, but ingress during the experiment's lifetime is ideally smaller than the relaxed starting requirement. The starting Ar concentration was also relaxed but not stated. ^{39}Ar backgrounds are generally subdominant. Relaxing the requirements had little impact on the WIMP search sensitivity.

Removing noble impurities from (bulk) noble gases is non-trivial. There is no mechanism to significantly reduce noble impurities from Xe in the LZ detector. All LZ Xe was purified off site prior to being delivered to SURF. Purification occurred at SLAC using a charcoal chromatography system, designed to clean large amounts of Xe [59]. This Xe was then shipped to SURF to be delivered into the LZ detector.

Monitoring the Kr and Ar concentrations of the delivered Xe and Xe within the LZ detector during commissioning and operation was critical to meeting experimental goals. Though less critical, it was also useful to measure other species, like N_2 , CH_4 , and He. Detecting Kr concentrations with accuracy on the order of tens of ppq is not trivial. The cold trap mass spectrometry technique described in [60] was used to do this. The technique, its application, and its contribution to the LZ experiment through May of 2024 are described in this chapter.

Section 3.1 gives a brief explanation of sources of Kr ingress. Section 3.2 gives a general overview of the cold trap mass spectrometry technique. Sections 3.3 and 3.4 explain the hardware and procedures used to measure impurities in Xe. Measurement signals and analysis techniques are described in section 3.5. The methods for calibrating the systems are given in section 3.6. Section 3.7 describes sources of uncertainty, describes how measurement uncertainties are evaluated, and lists the evaluated uncertainties for each system in each measurement mode. The system automation and integration in the LZ slow controls framework is explained in section 3.8. Section 3.9 describes relevant results and includes a discussion on the implications of each. The chapter concludes with a brief summary in section 3.10.

3.1 Ingress Mechanisms

Kr and Ar concentrations do not remain constant after Xe is loaded into the LZ detector. While concentrations cannot be reduced, they can certainly increase. Sources of Kr and Ar ingress must be properly understood prior to filling the detector to ensure the Xe remains sufficiently pure throughout the experiment's lifetime.

The sources of Kr or Ar ingress can be characterized as internal or external. External sources of Kr and Ar are often leaks into the Xe plumbing from outside air. Dry air is about one percent Ar (by mass) and about three parts per million (ppm) Kr (by mass). The characteristic air ratios are observed when a leak is present, though electronegative air components are greatly diminished if Xe is circulated through the getter. The ingress from a leak appears linear on time scales that are short relative to the time scale it takes concentrations to equilibrate with air.

Internal sources are defined as sources that exist within the Xe volume. Plastics in the TPC are exposed to air during construction. They absorb the air gases then release them after the detector is sealed. Most welds in the circulation system plumbing outgas Ar because they were made with an Ar purged welder. Other possible sources of internal impurity ingress are virtual leaks and trapped volumes. The ingress from an outgassing plumbing component appears as exponential ingrowth and diminishes as the impurities in the solid plumbing component approach equilibrium with Xe volume. Outgassing still appears linear over timescales that are short relative to the ingrowth time constant. The entire LZ circulation system was evacuated from March 2020 to June 2020, following assembly of the ICV. This pumping time allowed impurities to diffuse out of plastics and be removed from the circulation system, effectively reducing internal sources of ingress.

The presence of impurity ingress heightens the importance of monitoring Kr and Ar concentrations. A quick response to a sudden leak could prevent irreversible Xe contamina-

tion that may be fatal to the dark matter sensitivity. Understanding outgassing is necessary to estimate the Kr and Ar backgrounds.

3.2 General Technique

The primary measurement device of the cold trap mass spectrometry systems is a Residual Gas Analyzer (RGA). LZ uses a Stanford Research Systems RGA200. This vacuum device can only operate at or below pressures on the order of 10^{-5} mbar. The RGA ionizes and detects residual impurities of a given mass-to-charge ratio (AMU/q). Mass-to-charge ratio is often simply referred to as "mass" in this chapter.

A simple setup could measure the concentration of an impurity in a bulk gas using a leak valve. Leaking gas into the RGA volume at a rate that yields an RGA pressure just below the device's maximum operational pressure would maximize sensitivity to impurities. The sensitivity of this hypothetical setup would be governed by the RGA's dynamic range of about five to six orders of magnitude. The implied sensitivity is about one to ten parts per million (ppm). This is eight to nine orders of magnitude from the desired sensitivity of 10s of ppq.

The relatively high freezing point of Xe can be used to vastly increase the sensitivity to impurities. Bulk Xe flowing into a liquid nitrogen cooled cold trap freezes on the cold trap walls. The Xe partial pressure at the trap outlet is reduced to the vapor pressure of ice Xe at LN temperatures: 2.5×10^{-3} mbar. While this pressure is still too high for the RGA, additional plumbing impedance can be added to reduce the pressure to levels acceptable for RGA operation. Kr will pass through the trap relatively unimpeded. An illustration of this is shown in Fig 3.1.

A mass flow controller (MFC) is used to regulate the Xe flow rate into the cold trap. A cold trap will enhance sensitivity by six to seven orders of magnitude, to the single ppt

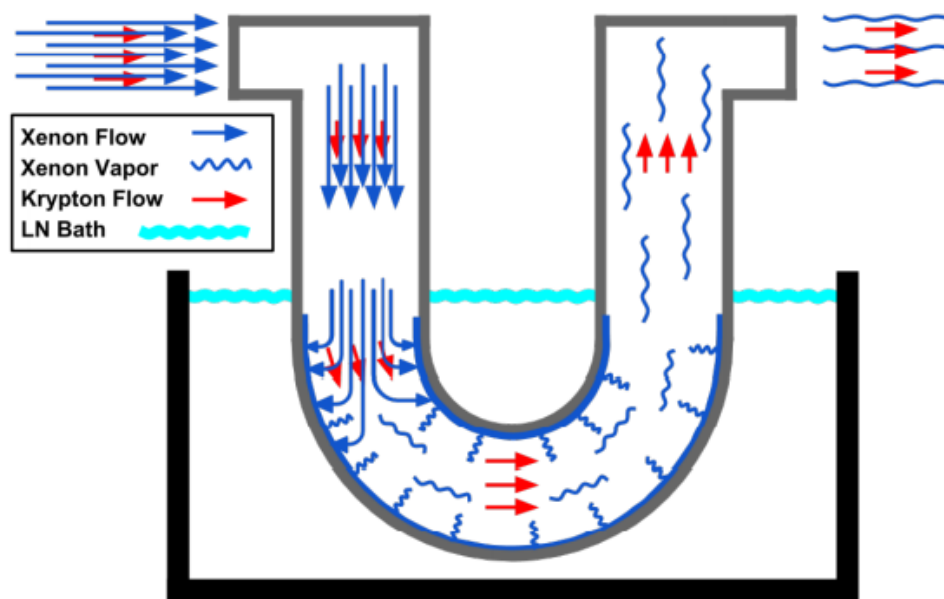


Figure 3.1: A diagram depicting the process of bulk Xe gas and trace Kr passing through a liquid nitrogen cooled cold trap is shown. Bulk Xe (darker blue arrows) and trace Kr (red arrows) enter the cold trap from the left side. When reaching the level of the liquid nitrogen bath (denoted by the light blue line), the bulk Xe begins to freeze to the walls of the trap. Kr will pass through the trap nearly unaffected, while the Xe ice acts as a source of constant vapor pressure. Only the Kr (or other impurities) and the Xe vapor will reach the cold trap exit (image from [61]).

scale. The Kr sensitivity can be pushed to 100s of ppq by flowing for longer periods of time and integrating the Kr signal. The limiting factor on the Xe flow rate is the trap's ability to quickly freeze the bulk Xe. In practice, it is possible to reach flow rates of several standard liters per minute (SLPM) before bulk Xe sneaks through the cold trap.

The sensitivity can be further improved by placing impedance valves before and after the RGA. This can be illustrated by a simplified argument, using the electrical circuit analogy. Xe behaves like a voltage source, with its *potential* regulated by the Xe vapor pressure from the cold trap. Kr acts like a current source, with its flow regulated by the MFC. The impedance of a valve between the cold trap and the RGA is Z_1 , and the impedance of a valve between the RGA and the pump is Z_2 . These valves are labeled IV1 and IV2 in Fig. 3.2. The impedance of both valves must be adjusted such that the Xe pressure at the RGA does not increase. If the impedance of both valves increases $Z_i \rightarrow C * Z_i$, the pressure at the RGA, P_{RGA} , for the *voltage source* (the pressure source, in this case Xe) will not change. However, P_{RGA} for the *current source* (the flow source, in this case Kr) will increase by a factor of C . The argument breaks down at higher impedances. Not much is gained beyond factors of C that exceed 20 [61]. This is because of a decrease in Kr throughput through the cold trap.

A representative plumbing and instrumentation diagram (P&ID) for a cold trap mass spectrometry system can be seen in Fig. 3.2. This diagram includes some additional plumbing bypasses and an additional pumping location.

3.3 Hardware

LZ employs two cold trap mass spectrometry *sampling systems* to measure the purity of LZ Xe. Both systems operate in similar ways but are differentiated by their hardware. The first system is referred to as the Mobile Sampling System (MSS). The second is the

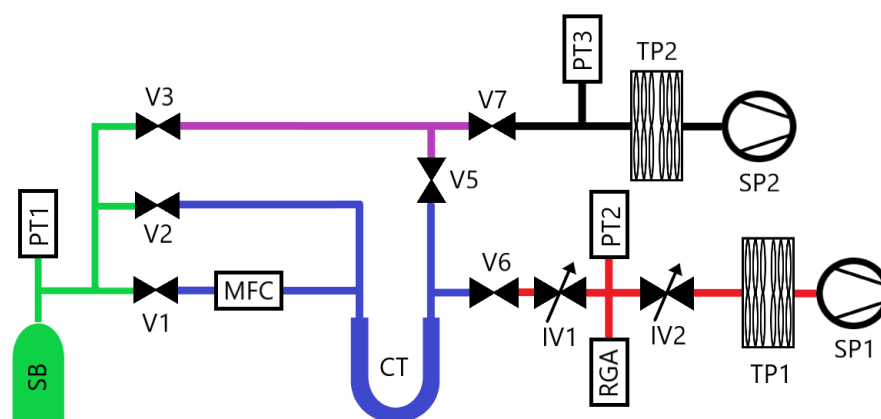


Figure 3.2: A schematic diagram of the plumbing and instrumentation for a generic cold trap mass spectrometry system is shown. This excludes all input and return plumbing. Xe is put into sample bottle "SB". The mass flow controller is denoted "MFC". The blue "U" labeled "CT" represents the cold trap. The red plumbing represents the RGA vacuum plumbing, where the RGA and a pressure transducer are denoted "RGA" and "PT2" respectively. "IV1" and "IV2" are impedance valves which increase sensitivity when properly tuned. The turbomolecular pump "TP1" and the scroll pump "SP1" are also shown. A utility pumping setup using pressure transducer "PT3", turbo pump "TP2", and scroll pump "SP2" is available for other pumping purposes when a higher impedance pumping path is not desirable. Other bypass plumbing is shown as well.

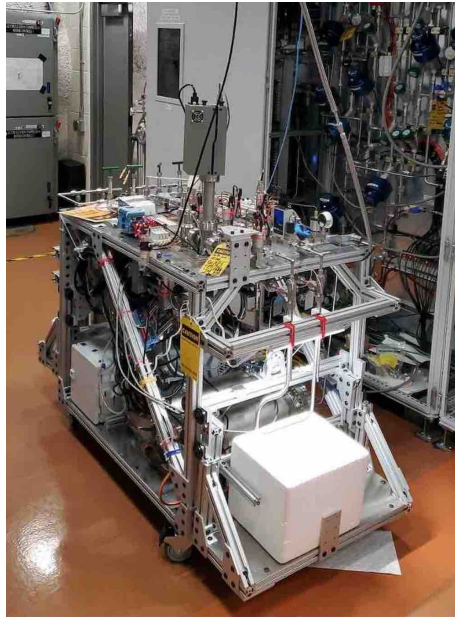
Stationary Sampling System (SSS). A residual gas analyzer is the core measurement device in both systems.

The MSS is designed to be a flexible mass spectrometry system, capable of being moved from one location to another. Consequently, the MSS is mounted on casters. It is depicted in Fig. 3.3 (a). Its cold trap is a 3/8" outer diameter, stainless steel stocking-shaped trap, which is seen in Fig. 3.4 (a). The trap is cooled by a liquid nitrogen bath. The bath rests on a shelf that can be raised or lowered with a hand crank. The MSS uses a 0.5 L or 7.6 L sample bottle to accommodate a wide range of Xe sample sizes. The system also allows for a wide range of sampling pressures via a high pressure inlet port. Xe is recovered either internally to a local 7.5 L cryopumping bottle or externally to the LZ Storage and Recovery Vessel. The MSS was the primary mass spectrometry system during LZ commissioning.

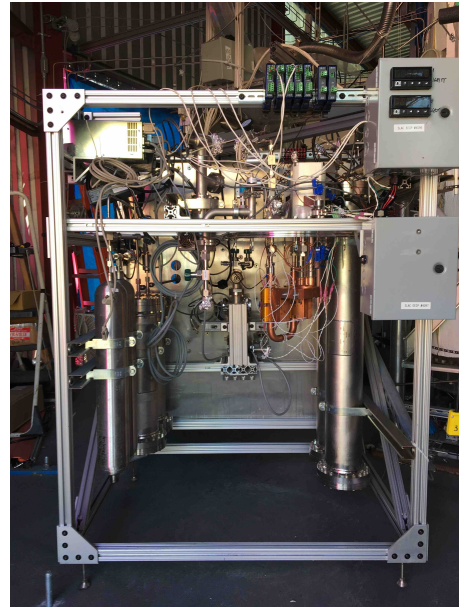
While less flexible than the MSS, the SSS is designed for frequent and periodic operation. It can be seen in Fig. 3.3 (b). Unlike the MSS (which requires an on-site operator to pour liquid nitrogen and adjust pressure regulators), making measurements with the SSS is intended to be fully automated. The SSS uses a 3/4" inner diameter copper cold trap, seen in Fig. 3.4 (b). This is cooled by a Cryomech PT60 Pulse Tube Refrigerator. The cold trap has heaters and RTDs (resistance temperature detectors) in thermal contact with the trap input and output. The heaters are regulated by PID loops controlled by RTDs to adjust the trap temperature. The cold trap and its adjacent components reside in a cryostat. A vacuum insulation blanket fashioned around the cold trap reduces radiative heating from the cryostat walls. The cryostat is evacuated by a turbo pump during operation.

The SSS is permanently plumbed into a port that allows for easy access to gaseous Xe from several locations in the Xe circulation system. The SSS is designed to return Xe to the circulation system via two 7.5 L return bottles. The SSS is the primary mass spectrometry system during LZ science operations because of its automation capability.

Both systems use a Teledyne Hastings HFC 300 series mass flow controller (MFC) to



(a)

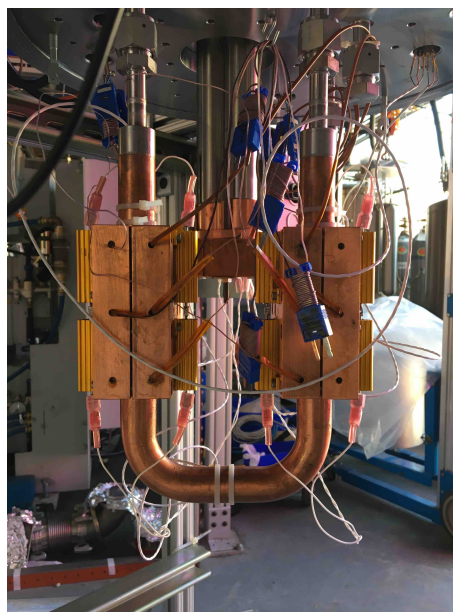


(b)

Figure 3.3: A photograph of the Mobile Sampling System at SURF is shown on the left. The cold trap and the styrofoam dewar which submerges the cold trap in LN can be seen in the lower right corner. The dewar rests on a shelf that can be raised and lowered via a winch. The RGA is oriented vertically on the system's top platform. A photograph of the back side of the stationary sampling system is shown on the right. The copper cold trap, turbo pumps, and several large sampling volumes are visible. The main plumbing control panel is on the front of the system and is not seen in this photograph. The insulating cryostat has been removed for this picture.



(a)



(b)

Figure 3.4: A picture of the MSS "stocking" shaped stainless steel cold trap is shown on the right. It is cooled by raising a styrofoam dewar filled with liquid nitrogen around the trap. Also shown are RTDs used to monitor liquid level height. A picture of the SSS "U" shaped copper cold trap is shown on the left. This trap sits in a cryostat, suspended from the vessel's top flange. The cold head used to cool the trap is seen behind the trap. Scalloped copper blocks transfer heat from the trap inlet and outlet to the cold head. Heaters and RTDs are attached to the scalloped block.

meter Xe from the sample bottles into the cold trap, and both systems use an RGA200 from Stanford Research Systems. Each system has two pumping chains. On the MSS, these consist of an Agilent Technologies TwisTorr 84 FS turbo pump, with high vacuum pressure monitored by an Agilent Technologies IMG100 inverted magnetron gauge and rough vacuum monitored by Agilent Technologies 531/536 thermocouple vacuum sensors. The SSS pumping chains use Edwards nEXT85D turbo pumps. The turbo pumps have been backed by a variety of roughing pumps, including Edwards nXDS10i/nXDS6i scroll pumps and Varian SH-110 scroll pumps. Vacuum pressures are monitored with a combination of pressure transducers, including IMG100s and Edwards WRG-Ss for higher vacuum, and Edwards APG100s for lower vacuum. Macroscopic sample bottle pressures (ranging from 0.5 to 3 bara) are monitored by an MKS Baratron 722B capacitance manometer in both systems. The majority of the valves on both systems are pneumatically actuated and remotely operable. Each system contains a bottle to hold calibration Xe.

The MSS arrived underground in 2019 and was the only available system before the fall of 2021. The SSS was initially installed at SLAC for use in LZ Kr removal operations. The Kr removal operations concluded in September of 2021, and the SSS arrived at SURF shortly after. It was operational in November of 2021.

3.3.1 RGA

A brief discussion of the RGA is informative to help explain Xe gas purity measurements. RGAs are composed of an ionizer, a quadrupole mass (ion) filter, and an ion detector. The ionizer produces a stream of relatively columnated positive ions of all gas species present in the vacuum space. These enter the quadrupole mass filter. Ions which successfully pass through the quadrupole mass filter reach the ion collector. A diagram of this setup can be seen in Fig. 3.5.

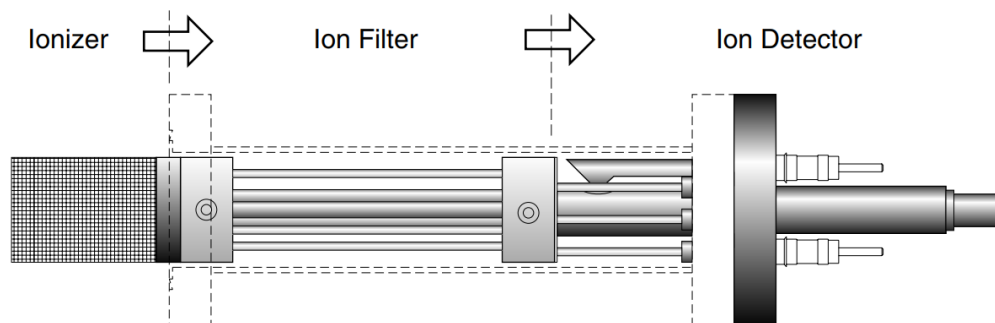


Figure 3.5: A diagram of major components of the RGA is shown. The ionizer end of the probe protrudes into the gas volume of interest. Ionized molecules enter the ion filter, where they are selected by their mass-to-charge ratio and are collected by one of two channels in the ion detector (image from [62]).

The RGA's ionizer consists of a ring-shaped filament, coaxially encircling a cylindrical wire mesh grid anode. Both are enclosed in a cylindrical wire mesh repeller cage. A schematic of this is seen in Fig. 3.6. The ionizer is separated from the rest of the RGA body by the focus plate, positioned on one circular face. The negatively charged filament is resistively heated to emit electrons, which ionize molecules. These electrons are accelerated away from the negatively charged filament and outer repeller cage and toward the inner anode grid. Most electrons pass through the anode grid without striking a wire. They are, again, accelerated back into the anode by the potential between repeller cage and anode grid. The electrons oscillate until they strike a wire, ionize an atom, or are recaptured on the filament. This process creates an over-density of electrons at the ionizer's center axis. Molecules moving through the anode grid can be struck by these electrons and positively ionized. The ions are drawn to the electron over-density at the center axis and are driven to the negatively charged focus plate. Appropriately aligned ions successfully pass through the small hole at the center of the focus plate and move into the quadrupole mass filter.

The quadrupole mass filter is composed of four hyperbolically shaped electrodes. A cross-section of the electrode orientation is shown below in Fig. 3.7. Rods on opposing

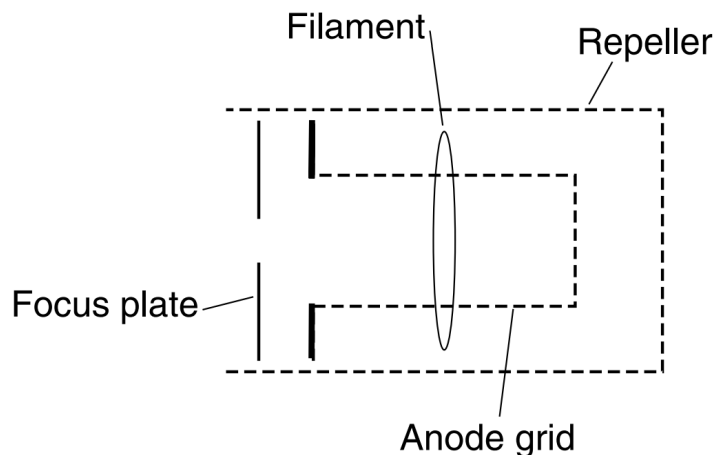


Figure 3.6: A side view of the RGA's ionizer is displayed. The filament ring emits electrons, which are accelerated toward the anode grid. Electrons are most abundant at the axial center of the anode grid. Molecules are ionized in the anode grid and are driven toward the negatively charged focus plate. If ionizer components were displayed in Fig. 3.5, the focus plate would sit to the right side of the ionizer section, dividing the ionizer from the quadrupole mass ion filter (image from [62]).

sides have the same potential applied to them, while adjacent rods have potentials of the opposite sign. The total applied potential is a superposition of both a DC and an RF component (U and V respectively), of the form $\phi = \begin{bmatrix} + \\ - \end{bmatrix} (U + V \cos(\omega t))$.

The transverse motion of the ions with respect to DC and RF voltages can be described by the Mathieu Equation:

$$\frac{d^2 u}{d\xi^2} + (a_u - 2b_u \cos(2\xi))u = 0 \quad (3.1)$$

Roughly speaking, u is a cartesian coordinate, ξ is related to a scaled time component, and a_u and b_u are related to the DC and RF components of the field. There are factors of $1/m$, $1/\omega^2$, and q inside of a and b . This equation can be solved numerically. The RGA200 has a fixed operating frequency, ω , of 2.7648 MHz.

Light ions tend to stay in phase with the RF component of the field better than heavier ions and oscillate with increasing amplitudes. Raising the RF amplitude causes these

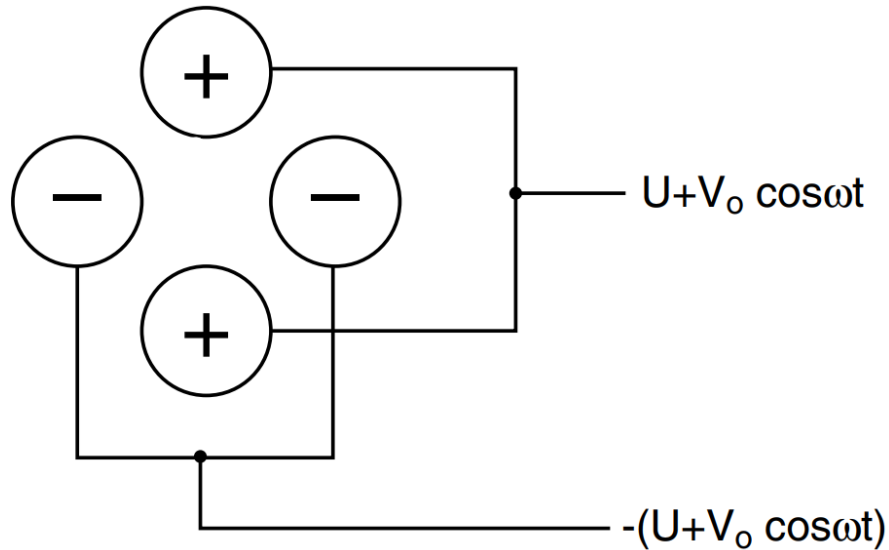


Figure 3.7: A cross-sectional view looking down the center axis of the RGA's quadrupole mass filter is shown. Electrode voltage orientations are given. The electrodes in the RGA quadrupole mass filter are actually hyperbolically shaped wedges, not cylindrically shaped rods as shown here (image from [62]).

lighter ions to collide with the positive electrodes. Heavier ions are less affected by the RF component and less likely to be driven into the positive electrodes. Instead, they are more likely to be destabilized by the DC component of the negative electrodes. The light ions are susceptible to the DC component of the negative electrodes as well, but under the appropriate initial conditions, they can be stabilized by the RF component of the negative electrodes. Therefore, increasing the DC component drives heavy ions into the negative electrodes, and increasing the RF component drives light ions into the positive electrodes. The delicate tuning of these two components allows for only a chosen mass-to-charge ratio to pass through the mass filter.

Ions permitted by the quadrupole mass filter pass through the RGA's grounded exit plate and reach the ion collector. The collector has two channels: a Faraday cup and a continuous dynode electron multiplier (also referred to as the CDEM or CEM). The Faraday cup rests on-axis and has a maximum operating pressure of 10^{-4} mbar. The CEM sits slightly off

axis and is capable of amplifying the incoming ion signal by several orders of magnitude more than the faraday cup. The CEM has an adjustable high voltage setting and can only be used when the pressure at the RGA is less than 5×10^{-6} mbar. An example signal output generated from the CEM while setting the the quadrupole mass filter to scan through individual mass-to-charge ratios can be seen in Fig. 3.8. This type of scan is referred to as an *analog scan*.

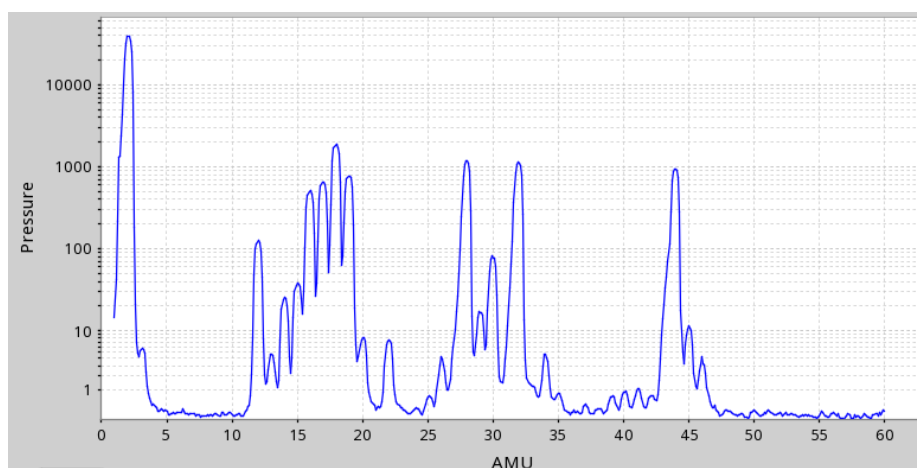


Figure 3.8: An example of an RGA analog scan with partial pressure (roughly given in picotorr on the y-axis) plotted for each atomic mass (mass-to-charge) is shown. The scan ranges from 1 to 60 AMU/q. The three prominent water peaks can be seen at 16, 17, and 18 AMU/q. N₂ (28 AMU/q), O₂ (32 AMU/q), and CO₂ (44 AMU/q) are also noted in this scan. The large peak at H₂ is seen in all vacuum systems.

A few effects related to the RGA are relevant for interpreting its data. The ionizer is capable of doubly ionizing a given atom or molecule. This is particularly relevant for easily ionized atoms like Xe. "AMU/q 62" and "AMU/q 68" are often used as tracers for ¹²⁴Xe and ¹³⁶Xe respectively, and are referred to as ⁶²Xe and ⁶⁸Xe in this chapter. These species are relevant for Xe purity measurements.

It is also possible for the ionizer to fragment molecules into component atoms or molecules. Each molecular species will exhibit a characteristic fragmentation pattern. An example of the water fragmentation pattern is seen in Fig. 3.8. Peaks are present at every

atomic mass between 16 and 20 AMU/q, with 18 AMU/q being 74% of the total contribution to the spectrum. HO (17 AMU/q) and O (16 AMU/q) fragments account for about 17% and 8% of the total spectrum. This fragmentation effect is particularly relevant for measuring CH₄, which has a nominal mass of 16 AMU/q (the atomic mass of oxygen). AMU/q 16 is a fragmentation product of many common species, including O₂ and water. AMU/q 15 is a much cleaner tracer of CH₄ and accounts for 39.5% of the total methane signal. Cold trap mass spectrometry measurements in chapter 5 use AMU/q 15 to measure the removal time of natural CH₄.

RGAs are susceptible to a variety of systematic effects, including gain degradation, noise, saturation, and baseline shift. The RGA CEM gain degrades over time. The vapor pressure of Xe ice at 77 K should remain constant, so the Xe vapor pressure is used to monitor the CEM gain. Based on the observed Xe ice signal, the CEM voltage is adjusted to set the observed signal to a chosen value. Generally, the voltage adjustments are needed only once every few weeks. This is discussed further in sections 3.5 and 3.6.

The RGA200 has a parameter known as the *noise floor*, which determines the signal integration time for a given mass measurement. Increasing this integration time allows the RGA to better average out noise, improving accuracy. This is discussed further in section 3.4.

Baseline shifts are systematic shifts in RGA behavior and response to all masses. Gases contributing to RGA signals at or near saturation will affect measurement of less abundant or absent gas species. Both saturation effects and baseline shifts are monitored by observing an atomic mass where no species are expected to be present. For this work, AMU/q 87 is frequently used. Baseline shifts and examples of how they affect measurements are discussed in sections 3.5 and 3.9.7.

3.4 Procedure

The method for making a measurement with the sampling systems begins by drawing a batch of Xe (a sample) into the sample bottle and the cold trap, as seen in Fig. 3.2. Samples range in size from 5 to 100 g. The cold trap is isolated from the sample bottle and cooled to 77 K. Once sufficiently cooled, the cold trap is pumped on to remove impurities from the frozen Xe. The cold trap is opened to the RGA. The partial pressures immediately rise, then fall and stabilize over several minutes, indicating that the majority of the impurities in the cold trap have been pumped out. *Background* data is taken after the pressure traces have stabilized. The background data is reflective of the measured signal from clean Xe ice and the local plumbing. Xe is then introduced into the cold trap from the sample bottle at a constant flow rate for a set time period (typically five minutes), while RGA measurements continue. A few more minutes of data are taken after flow ends. The RGA is then valved off and Xe is safely warmed back to the sample bottle to conclude the measurement.

Three major modes of measurement and RGA operation are used. *Low sensitivity analog scanning* is one measurement technique. This less sensitive technique was used exclusively during the early phases of LZ commissioning with the MSS. An analog scan is used to measure the partial pressures across a wide range of masses (technically AMU/q, see Fig. 3.8). The RGA noise floor parameter must be relatively high (allowing for faster scanning but less accuracy) to ensure Xe is not exhausted before all partial pressures are measured. This technique is sparingly used in this thesis and will not be discussed further.

Pressure vs time (PVT) scanning gives a time history of a small number of species. PVT scanning is used for all LZ Xe that has been processed for Kr removal. Scanning fewer masses allows for a lower RGA noise floor, increasing sensitivity. When only certain impurities are of interest, PVT scanning is more sensitive than analog scanning. An example of a PVT scan is seen in Fig. 3.9.

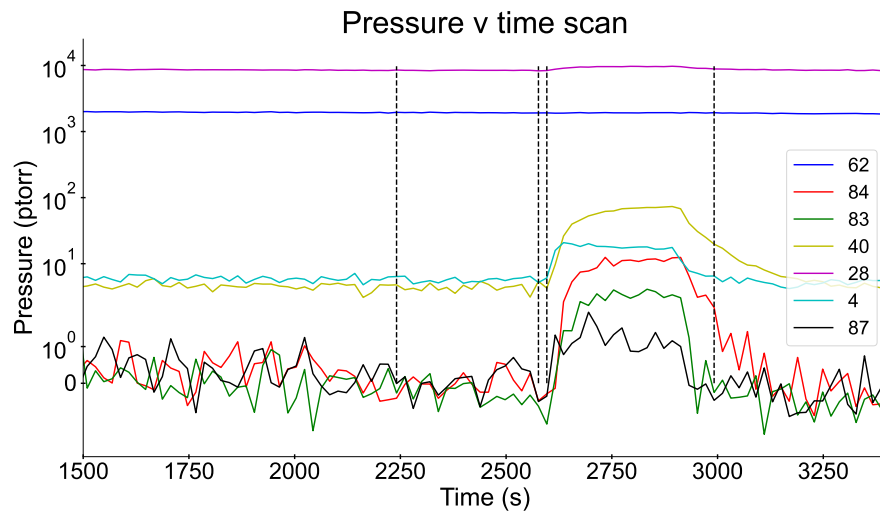


Figure 3.9: An example PVT scan for seven different masses is shown. Important masses include AMU/q 62 (doubly ionized ^{124}Xe), ^{84}Kr , and the baseline at AMU/q 87. Two analysis windows are shown by the dashed black lines. The window encapsulated by the first two dashed lines beginning around 2250 s is the background window. Here, the RGA is observing clean Xe ice in the cold trap. The window between the third and fourth dashed black lines ending around 3000 s is the flow window. As Xe flows into the cold trap at the start of the flow window, partial pressures of most gas species rise. This includes the baseline at 87 AMU/q, indicating a slight systematic shift in RGA response. ^{62}Xe remains flat throughout the flow period, as expected. Most partial pressures drop toward the end of the flow period after flow is stopped. The flow window extends just a bit beyond the end of flow. The background and flow windows are integrated and compared to a calibration reference measurement to determine the concentration of a given impurity within a particular run.

When impurities are in the range of 10s of ppt or greater, the Faraday cup is sufficient to detect them, even at low flow rates. The flow rate is set to 0.1 SLPM for Faraday cup measurements. PVT measurements using the Faraday cup at *low* flow rates are referred to as *high sensitivity PVT scanning* measurements. Using the Faraday cup avoids complications with CEM gain degradation. Gases in LZ measured with high sensitivity PVT scans include Ar, He, N₂, and CH₄.

Achieving the highest sensitivity to Kr requires the RGA's electron multiplier and flow rates between 1.5 to 2 SLPM. Because the partial pressure of Xe ice should remain constant, the RGA's electron multiplier is tuned to give a ⁶²Xe pressure of a chosen value. This mode of operation is called *ultra-high sensitivity PVT scanning*.

Both PVT measurement techniques are necessary to detect all species of interest for LZ. Taking an ultra-high sensitivity measurement of Xe with impurity concentrations that can be easily viewed with high sensitivity sampling will cause RGA saturation. Saturation often leads to baseline shifts (mentioned in section 3.3) or other poor systematic RGA behavior that can be severe enough to invalidate the Kr measurement. LZ Xe must be treated in a way that preserves the Kr while removing other impurities before any Kr measurement.

The most efficient method for measuring all species of interest is as follows. First, an approximately 100 g batch of Xe is pulled into the sampling system. A high sensitivity measurement is made to assess the concentrations of N₂, Ar, CH₄ and He. The Xe ice formed from this measurement is warmed and recovered to the sample bottle. Next, a procedure referred to as a *static pump* is performed. The static pump procedure reduces impurities like N₂, He, and Ar, with little effect on Kr. This will be discussed further in section 3.4.1. Next, an ultra-high sensitivity measurement is performed and Xe is rewarmed. Finally, the Xe is recovered from the sample bottle.

The impurity concentrations of a batch of Xe are necessarily reduced during a measurement because the gas pumped away (ultimately the gas detected by the RGA) is enriched

in impurities. The concentration cannot be reduced by more than the sample fraction that is flowed into the cold trap. For this reason, the flow rate for high sensitivity measurements is chosen to minimize the quantity of Xe that enters the cold trap. 100 g of Xe corresponds to about 17 standard liters of Xe gas. The lowest flow rate the MFC can properly regulate is 0.1 SLPM. Flowing at 0.1 SLPM for a five minutes implies that the total Kr loss from a low sensitivity measurement is less than 3%. An ultra-high sensitivity *calibration* measurement is also preceded by a high sensitivity measurement and a static pumpout, so small corrections from both of these procedures are built into the calibration.

3.4.1 Xe cleaning methods

The sampling systems slightly clean Xe during a measurement, but cleaning methods like *static pumpouts* and *clean runs* more efficiently clean Xe. Removing all traces of detectable impurities from Xe is useful when calibrating the sampling systems. As discussed above, it is also desirable to remove certain impurities while preserving Kr.

Freezing Xe will trap impurities in the Xe ice. The gaseous phase will always be out of static equilibrium with the solid phase when pumped; the solid phase constantly sources molecules. Xe's freezing point is primarily governed by Van der Waals interactions. The strength of Van der Waals interactions between Xe and other noble gases increases as the mass of the interacting atom increases [63]. Thus, more massive noble gases, like Kr, are more tightly bound to the frozen Xe and have a lower probability of escaping the solid phase Xe than He. In this way, Xe ice behaves like a chromatographic stationary phase medium. The smaller species, like He, escape the Xe ice faster, while larger atoms, like Kr, diffuse out more slowly.

The process of freezing all the Xe in a given batch, then pumping on the volume (after sufficiently cooled), is referred to as a static pumpout. Static pumpouts lasting half an hour

do not appreciably affect the Kr concentration but reduce the He concentration by orders of magnitude. An example of a PVT scan for a static pumpout is shown in Fig. 3.10.

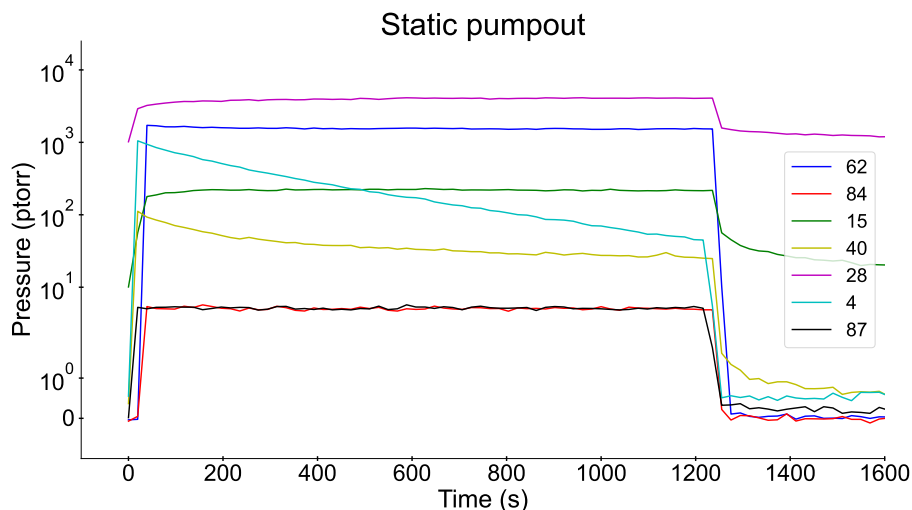


Figure 3.10: An example of an RGA PVT scan during a static pumpout is shown. The Xe ice vapor pressure (62) is constant. Kr (84) and the baseline (87) read the same value throughout the scan, indicating that Kr is not detected by the RGA or being pumped away. He (4) and Ar (40) reduce as the gases are removed. All concentrations abruptly drop when the RGA is valved off from the Xe ice, after 1200 seconds

The most effective way to reduce *all* impurities is to flow into the cold trap at three to four SLPM, while pumping. This operation is referred to as a clean run. Higher flow rates reduce entrainment of impurities. The flow rate is limited by the cold trap's ability to continue freezing the incoming Xe and maintain the outlet Xe vapor pressure. Clean runs can be used to clean Xe to concentrations below the limit of detection of each sampling system. This is useful when calibrating.

3.5 Signals and Analysis

The RGA pressure vs time data is analyzed in the following way. Two time windows are established based on the start time of Xe flow into the cold trap: the *background window*

preceding the flow and the *flow window* during Xe flow. These windows are pictured as dashed black lines in the pressure vs time scan in Fig. 3.9. The start of flow can be identified by the sudden rise of most gas species in the plot between 2500 s and 2750 s. Flow lasts exactly five minutes.

For high sensitivity and ultra-high sensitivity measurements, the *raw pressure* for a species of atomic mass (per charge) A is determined by taking its instantaneous partial pressure ($p_i(A)$) and subtracting the instantaneous baseline pressure ($p_i(87)$) at each point in the background window (from t_1 to t_2) and flow window (from t_3 to t_4). AMU/q 87 is used to track changes in the behavior of the RGA's systematics and is subtracted from the species of interest. Each quantity is multiplied by the time interval between data points (dt , this is nearly constant for all bins), then summed across the full flow or background window. These summed pressures are divided by the respective total integration times to determine an average pressure for a given mass in either the flow or background window, $P_{flw}(A)$ or $P_{bkg}(A)$. This is written in Eq. 3.2 and Eq. 3.3.

$$P_{flw}(A) = \frac{1}{t_4 - t_3} \sum_{i=1}^{N-1} 1/2 * [p_i(A) - p_i(87) + p_{i+1}(A) - p_{i+1}(87)] * dt \quad (3.2)$$

$$P_{bkg}(A) = \frac{1}{t_2 - t_1} \sum_{i=1}^{N-1} 1/2 * [p_i(A) - p_i(87) + p_{i+1}(A) - p_{i+1}(87)] * dt \quad (3.3)$$

The average background pressure ($P_{bkg}(A)$) is subtracted from the average flow pressure ($P_{flw}(A)$) to find the raw signal pressure $P_{sample}(A)$ for a given species.

$$P_{sample}(A) = P_{flw}(A) - P_{bkg}(A) \quad (3.4)$$

The concentration is determined using Eq. 3.5, where $C(A)$ is concentration of species A , F_{cal} is the calibration factor from the appropriate reference calibration measurement,

$m(A)$ is the (atomic) mass of the species A , and $P_{cal,bkg}(Xe)$ and $P_{bkg}(Xe)$ are the average background Xe pressures of the calibration and current measurement respectively. Again, ^{68}Xe (doubly ionized ^{136}Xe) is used to track the Xe pressure for high sensitivity measurements, and ^{62}Xe (doubly ionized ^{124}Xe) is used for ultra-high sensitivity measurements.

$$C(A) = P_{sample}(A) m(A) F_{cal} \frac{P_{cal,bkg}(Xe)}{P_{bkg}(Xe)} \quad (3.5)$$

F_{cal} and $P_{cal, bkg}(Xe)$ are determined by a single calibration reference measurement. F_{cal} has dimensions of $[1/(mass * Pressure)]$ to give $C(A)$ in $[mass/mass]$. Section 3.6 will discuss how F_{cal} is calculated. The final fraction involving $P_{cal, bkg}(Xe)$ and $P_{bkg}(Xe)$ is used to make small gain corrections between the calibration and current measurements because the Xe pressure of Xe partial pressure of all measurements should be constant.

These corrections are generally small. In the case of the ultra-high sensitivity measurements, the CEM voltage is adjusted prior to the measurement to set the Xe pressure to the desired value. The voltage adjustments are somewhat coarse, so the factor compensates. In the case of high sensitivity measurements, the CEM is not used and the factor is intended to account for other changes to the Xe pressure signal.

3.6 Calibration

The primary goal of the calibration is to obtain the factors F_{cal} and $P_{cal}(Xe)$ in Eq. 3.5. A single calibration measurement is used as a reference for subsequent measurements. Each non-calibration measurement uses the calibration factor and background Xe pressure from that reference to convert an observed signal to a concentration. A calibration is referenced until a new calibration is performed or any major system changes occur. Statistical error on the calibration measurement propagates (as a systematic) to all measurements using that calibration as a reference.

Sampling system calibration gases are prepared by mixing a known amount of a given impurity with a known amount of clean Xe to give a precise concentration for the mixture. All gas volumes on the system are measured prior to mixing. A macroscopic quantity of Xe is cleaned to an immeasurable impurity concentration and stored in the *sample bottle volume*. The impurity gas source is introduced into another known *impurity volume* (previously at vacuum). A reference diagram is included in Fig. 3.11.

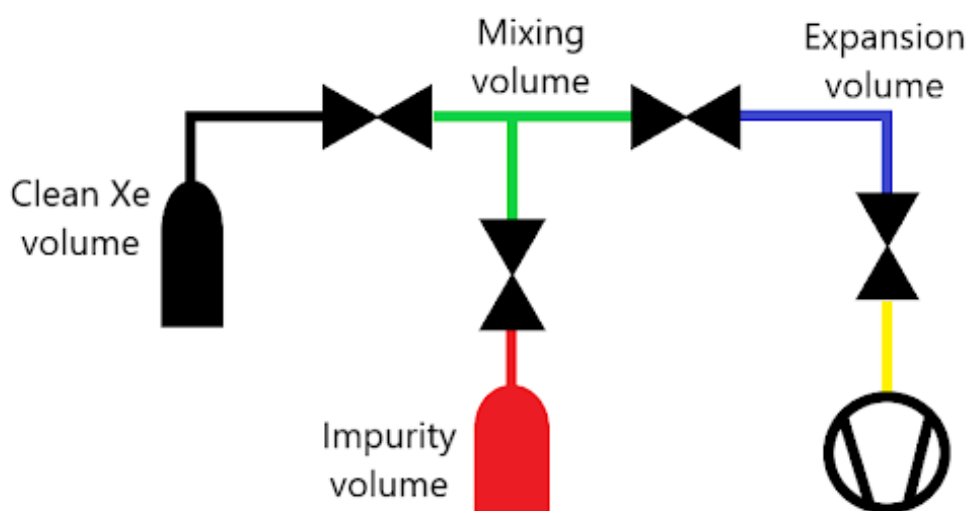


Figure 3.11: A schematic diagram of the calibration mixing setup is shown. Initially the clean Xe volume is filled with clean Xe, and the impurity volume is filled with the impurity mixture. The mixing volume and expansion volumes are initially evacuated. All valves begin closed. The impurity volume is opened to allow a chosen amount of pressure into the mixing volume. The valve separating the impurity volume from the mixing volume is then closed. If dilution expansions are required to reduce the mixing volume pressure, the mixing volume is opened to the expansion volume, then closed off again to cut the pressure in the mixing volume. The expansion volume is then pumped out. The dilution expansion process can be repeated until the mixing volume has reached the desired pressure.

The pressure of the impurity gas and clean Xe is recorded. In some cases, the impurity is diluted to reach the desired concentration. This is done by opening the impurity volume to an *expansion volume* (previously at vacuum), then reisolating the impurity volume and evacuating the expansion volume. This process is referred to as a *dilution expansion*. After

the desired impurity quantity is reached, the gas is mixed by freezing the bulk Xe and the impurities in a cooled cold trap and warming to expand back into the sample bottle volume. The known quantity of the impurity and the clean Xe are used to calculate the concentration of the calibration. After mixing, the calibration mixture is measured like any other measurement.

The F_{cal} is calculated by setting C to the mixed concentration (determined by the pressures and volumes), calculating the raw pressure P_{sample} , and setting the Xe line correction factor (the final fractional term) equal to 1 in Eq. 3.5. Assuming the instrumentation and plumbing configuration for a sampling system does not change, F_{cal} should not change significantly on a month-long timescale. Monthly calibrations are sufficient to account for changes when the CEM is required to make the measurement. The RGA exhibits more stability over long periods of time when the CEM is not used. Calibrations for measurements that do not use the CEM are less frequent, but should happen once every three months.

An ideal calibration concentration is about a factor of five to ten greater than the measurement range. For LZ Kr, typical measurement concentrations are on the order of 100s of ppq, and calibration concentrations are on the order of single ppt. This calibration range has several benefits. First, it minimizes the influence of irreducible statistical error that would increase the fractional uncertainty on smaller measurements. Repeated measurements of Xe with imperceptible amounts of Kr show variation of about 20-30 ppq for the SSS. This error is fractionally smaller for larger concentrations and, therefore, slightly higher concentrations reduce systematic uncertainty from the calibration factor. Second, this calibration concentration range avoids potential systematic scaling nonlinearities. The measured RGA signal size is not linear with concentration across three or more orders of magnitude. The calibration concentrations should be relatively close (within one to two orders of magnitude) to the intended measurement concentrations.

For Kr calibrations with the SSS, the impurity gas is Xe with about 200 ppt (g/g) of Kr.

Making a 1 ppt Kr calibration with the SSS requires mixing quantities of about 200:1 of clean Xe to impurity gas. The procedure for mixing to this ratio is relatively simple given the mixing volume to clean Xe volume ratio. Kr calibrations generally require no dilution expansions to reach the desired calibration concentration.

Many dilution expansions are required if the impurity gas is a (nearly) pure species. Pressures cannot be accurately measured by the mixing volume pressure transducers after just a few dilution expansions. Each dilution expansion reduces the quantity of impurity by the fraction $V_{mixing}/(V_{mixing} + V_{expansion})$. This fraction must be relied on to calculate the impurity quantity. Any uncertainty in this fraction goes like the power of the number of volume expansions in the calculation of the final concentration. Error from the volume expansions in the final concentration calculation results in error on F_{cal} and is adopted as a systematic by all measurements that use the impurity mixture as a calibration source.

3.7 Uncertainties

The uncertainty on the measured concentration depends upon the sampling system and measurement mode. Possible sources of statistical error include RGA noise, statistical error in MFC regulation, and anything that could be affected by mechanical noise (from pumps resting on the lower deck of the MSS). The statistical uncertainty is determined empirically. The error bars shown on all plots within this chapter are strictly statistical unless specified otherwise.

The uncertainty due to calibration (from F_{cal}) is the dominant systematic uncertainty. Other possible sources of systematic error include, but are not limited to, incomplete pumpouts during calibrations, variation in ice formation, recent history of the RGA filament and plumbing, MFC offsets and nonlinearities, procedural errors, and other RGA systematics. These can be studied by cross calibrating with other sampling systems.

Dedicated studies characterize the system uncertainties. When there is insufficient data in the measurement regime being studied, approximations or interpolations are relied on to estimate uncertainties. The statistical uncertainty on an individual measurement is modeled as having a fractional uncertainty σ_{stat}^{frac} proportional to the measured concentration C and a constant (absolute) uncertainty σ_{stat}^{abs} . The quoted statistical error on a measurement, σ_{stat} , is given by Eq. 3.6.

$$\sigma_{stat} = \sqrt{(\sigma_{stat}^{abs})^2 + (\sigma_{stat}^{frac} * C)^2} \quad (3.6)$$

For concentrations much greater than the sampling system limit of detection but well below the point of RGA saturation, the fractional term, $\sigma_{stat}^{frac} * C$, will dominate the right hand side of Eq. 3.6. The total statistical uncertainty approximately equals the fractional component in this case. At concentrations nearing the level of RGA saturation, uncertainties are not well behaved, and Eq. 3.6 cannot be applied.

Cold gas circulation Kr measurements are used to inform the estimation of σ_{stat}^{frac} for ultra-high sensitivity MSS measurements. These measurements are comfortably above the MSS limit of detection. The details of this sampling campaign are discussed in section 3.9.2. To summarize, the Kr concentration was expected to rise linearly in time. This assumption is confirmed by Kr measurements taken across the five month cold Xe gas circulation period. The data can be seen in Fig. 3.16.

A 3% error on the measured Kr concentration gives a p-value of 0.51. Thus, 3% is chosen to be the ultra-high sensitivity measurement fractional statistical error for the MSS. A similar method was used with Ar to determine the high sensitivity PVT scanning statistical uncertainty with the MSS of 10%. The results are shown in Fig. 3.18.

The SSS ultra-high sensitivity fractional uncertainty was determined by mixing a large batch of calibration Xe and repeatedly measuring the batch. These measurements yield

a standard deviation of about 5% of the mean value for SSS ultra-high sensitivity sampling. This is not unexpected, as the SSS flows at a slightly lower flow rate for ultra-high sensitivity measurements and is slightly less sensitive than the MSS.

$\sigma_{stat}^{frac} = 0.1$ is used for SSS high sensitivity measurements. This estimate is consistent with SSS He measurements taken during the most stable period of LZ's first science run liquid Xe (LXe) circulation: late January of 2022 to late April 2022. The results are shown in Fig. 3.20. He measurements in this period averaged 95.7 ppt with a standard deviation of 9.5 ppt. Observations of He throughout the LXe circulation period reveal that He measurements are easily influenced by the circulation system conditions. This implies 0.1 is an upper limit on the fractional statistical uncertainty of SSS high sensitivity measurements. However, circulation system configuration changes in this period were minute and the chosen value is sufficient. These measurements are discussed in more depth in section 3.9.5.

Sampling systems can be used to clean Xe to undetectable impurity concentrations. In the limit of concentrations that are small relative to the sampling system's limit of detection ($C \approx 0$), σ_{stat}^{abs} will dominate the uncertainty ($\sigma_{stat}^{abs} \approx \sigma_{stat}$). Repeated measurements of Xe with undetectable levels of Kr were performed with the MSS to estimate σ_{stat}^{abs} . The mean measured concentration is found to be less than 1 ppq with a standard deviation of about 6 ppq. This indicates 6 ppq is a reasonable estimate of the MSS ultra-high sensitivity σ_{stat}^{abs} . A histogram of these measurements is shown in Fig. 3.12.

The SSS has undergone many configurations changes and part replacements since it was first operational in November of 2021. These configurations do not necessarily result in the same statistical uncertainty. The RGA used to make all science run 1 measurements was rendered inoperable in May of 2022. This occurred before a dedicated study to determine the configuration's ultra-high sensitivity σ_{stat}^{abs} could be conducted. A later SSS study revealed $\sigma_{stat}^{abs} = 30$ ppq using a different RGA and pumping configuration. Assuming SSS LXe circulation Kr measurements made with this RGA are linear with respect to time,

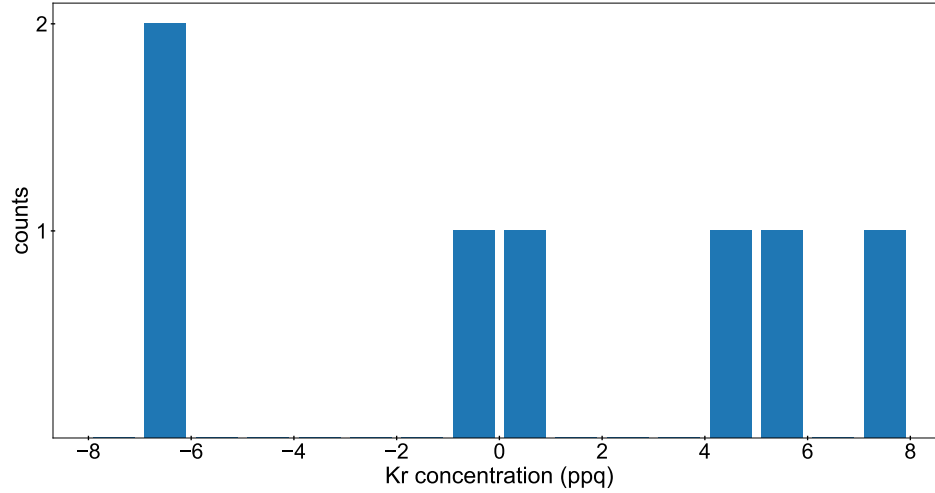


Figure 3.12: A histogram of repeated MSS measurements of Kr-free Xe is shown. This test took place over several days in June of 2021. The average of all measurements is less than 1 ppq, indicating no detectable systematic offset. The standard deviation is about 6 ppq. This is used to estimate σ_{stat}^{abs} .

the p-value of a linear fit will give information about σ_{stat}^{abs} for ultra-high sensitivity SSS measurements.

A linear fit to all SSS LXe circulation Kr measurements from November 2021 to May 2022 using $\sigma_{stat}^{abs} = 30$ ppq and $\sigma_{stat}^{frac} = 0.05$ gives a p-value of 0.99, indicating 30 ppq is an overestimate for this configuration. Using the MSS estimate, $\sigma_{stat}^{abs} = 6$ ppq and $\sigma_{stat}^{frac} = 0.05$, the p-value of 0.0001 implies 6 ppq is an obvious underestimate. $\sigma_{stat}^{abs} = 20$ ppq and $\sigma_{stat}^{frac} = 0.05$ yields a reasonable p-value: 0.43.

The same caveats mentioned regarding He measurements still apply here. The measured impurity concentrations may still be sensitive to thermodynamic changes. This period is relatively stable, and Kr measurements appear more stable during thermodynamic changes, indicating that 20 ppq is likely an appropriate estimate of σ_{stat}^{abs} .

All SSS ultra-high sensitivity measurements following the configuration change and RGA replacement in May of 2022 use $\sigma_{stat}^{abs} = 30$ ppq. Many configurations changes have

occurred since. A study of the uncertainties for each configuration change was not possible. The 30 ppq estimate is periodically crosschecked with incoming measurements. The most recent crosscheck occurred during WIMP Search 2024 (WS2024). This is detailed in section 3.9.7. Context is needed to properly explain the measurements, but a brief summary will be given here. A linear fit was made to several different subsets of WS2024 Kr measurements. These measurements are shown in Fig. 3.21. The p-values of fits to these different subsets are given in Table 3.6. A few of these subsets include quantitatively unreliable measurements because of high baseline drift. Other subsets include measurements in time periods when RGA behavior was known to be erratic. The bottom row in the table is the most reliable subset of measurements and yields a p-value of 0.46.

For high sensitivity measurements, the second term in Eq. 3.7 is generally much greater than the first. The fractional statistical error is approximated to be the total statistical error in this case.

Systematic error is modeled as a fractional term, which is shown in Eq. 3.7.

$$\sigma_{sys} = \sigma_{sys}^{frac} * C \quad (3.7)$$

The systematic error on any measurement is primarily due to the calibration. Any calibration will require either an impurity mixture to calibrate with or a series of dilution expansions. Both are potential sources of error. Further, all calibrations on the cold trap mass spectrometry systems are fundamentally measurements with statistical error. This error will propagate to every subsequent measurement that uses a given calibration as a reference.

The systematic error for ultra-high sensitivity measurements is conservatively estimated at 15% of the measured value. Due to additional difficulties with calibrating high sensitivity measurements, the systematic uncertainty is conservatively estimated at 20%. These

difficulties are discussed at length in section 3.9.8. Statistical and systematic errors are added in quadrature to obtain the total error on a measurement.

The error estimates are summarized in Table 3.1.

	MSS			SSS		
	High	Ultra-High		High	Ultra-High	
	Fractional	Absolute	Fractional	Fractional	Absolute	Fractional
Statistical	10%	6 ppq	3%	10%	30 ppq*	5%
Systematic	20%	0	15%	20%	0	15%

Table 3.1: Error estimates for the two sampling systems are summarized here. The estimates are divided by system (in the top row), sensitivity (in the second row). The fractional and absolute components of both the statistical and systematic uncertainties are indicated. No absolute uncertainty is applied to the high sensitivity measurements. The quoted value on the absolute component of the SSS ultra-high sensitivity statistical uncertainty is the uncertainty after May 2022. Prior, the absolute component of the statistical on SSS ultra-high sensitivity measurements was estimated to be 20 ppq.

3.8 Sampling System Control

This section provides a general, simplified overview of the sampling system control interfaces, particularly the automation code and interlocks. Most LZ device inputs and outputs are interpreted by a Siemens Programmable Logic Controller. The experiment uses the Inductive Automation program, *Ignition*, as a visual control interface for users to read and control different devices. A device can be controlled directly through Ignition or through the PLC. These two programs act together to allow users to effectively manage operations in LZ.

The PLC receives a signal from a device output, writes the value to a *symbol*, processes the symbol (this may involve smoothing or scaling to convert a voltage reading to a output pressure value, for example), then writes the processed output to a variable *database*. Ignition reads from the PLC’s variable database(s) and outputs the values in a way that

is easily digestible to the user. A user can also tell Ignition to write to the PLC variable database. The PLC sends signal commands to devices based on the writable variables contained within the PLC database. Both the PLC and Ignition hold variables that are not associated with a device, and both support some degree of scripting code. The PLC is generally unaware of Ignition, except in the instant that Ignition is writing to the PLC.

The PLC process cycle time is ten milliseconds, compared to Ignition's refresh and execution rate of once every one to ten seconds (depending on the device). The PLC will continue to function properly in the event of communication failure between the underground and the surface, or between Ignition and the PLC. The PLC is far more robust against crashing than Ignition. The PLC's communication methods with system devices are inherently more reliable than Ignition's. For all these reasons, devices, interlocks, and scripting are all preferentially run through the PLC.

It is possible and sometimes necessary to control devices directly through Ignition, without the PLC. RGAs can be operated in a few ways, but the most common is via serial communication. LZ is not capable of running serial devices through the PLC. A VLink serial-to-ethernet converter is used to convert RGA communications to ethernet, which can be interpreted by Ignition. Nearly all SSS devices are connected directly to the PLC. The inability to connect the most important part of this system (the RGA) directly to the PLC creates challenges for protecting the device and automating the SSS.

The MSS is managed entirely through ignition. In this case, most device inputs and outputs are interpreted through ADAM modules, attached to the MSS itself. The ADAM modules are connected to a switch on the system. The MSS RGA is connected into the same switch through a serial-to-ethernet converter. All MSS communication with slow controls are routed from the switch, through a single ethernet cable, to the data acquisition hardware. This allows the MSS to be swiftly moved around the Davis Cavern, with only one communication cable requiring relocation.

3.8.1 System Automation

The MSS and the SSS were first used with minimal automation. Automation mechanisms were built up over time to better protect system hardware, better control procedural timing, and reduce the time burden on the operator. The (lighter) MSS automation was completed in Summer of 2021. The SSS automation was implemented and quality assurance checked over the course of many months. The SSS automation was completed in early 2024.

Protecting the system from any unexpected failure is the most critical purpose of the automation framework. *Interlocks* monitor sensors and quickly respond to protect devices, if necessary. The PLC provides the fastest and most reliable interlocking capability, but the MSS interlocks are necessarily written into the Ignition framework. Most MSS interlocks monitor the condition of the system pumps. If a pump is showing signs of degraded performance or outright failure, the interlocks turn off the RGA filament and CEM, then turn off the system turbo pumps to prevent damage. Failure of a pump during a time of communication failure could render the RGA inoperable, but periods of communication failure are rare. The MSS also has a *tell-tale* system to alert users of a blown rupture disc. An activated tell-tale will trigger a system lockdown to avoid contaminating LZ Xe.

The SSS interlocks are written into the PLC. The SSS has interlocks similar to those on the MSS to protect pumps and the RGA, but several interlocks ensure Xe is not warming at inappropriate times. Both the MSS and the SSS present obvious potential to create high internal pressures that may blow rupture discs. Unexpected warming of the cold trap while open to the RGA will over-pressure both the RGA and the turbo pump. The MSS avoids these situations by relying on procedures and an attentive operator to monitor liquid nitrogen levels. The PLC is left responsible for avoiding over-pressure in the SSS. The pulse tube refrigerator has no mechanism to indicate whether it is actively cooling. Thus,

the PLC monitors the cold trap temperature while the trap is open to the RGA to prevent damage to the RGA. Both 15 L sample bottles and 7.5 L return bottles are opened to the cold trap if the pressure in the cold trap nears rupture disc pressures at any time. One additional element of protection is gained by placing the RGA power on a relay controlled by the PLC. The relay activates to immediately remove power from the RGA if there is any danger to the device.

The MSS is limited in its procedural automation potential. An operator must be physically present to adjust regulators, pour liquid nitrogen, and turn a small number of manual valves. Filling, returning, and performing a static pumpout with the MSS is not automated. Automation is only used for high sensitivity and ultra-high sensitivity PVT scans. All automation code is written using a jython script, capable of interfacing with and activating from Ignition. Prompts tell the user when to raise and lower the cold trap or pour LN. The procedure will timeout and abort if the user does not quickly respond to a prompt, keeping the RGA and system components safe.

3.8.2 SSS Procedural Automation

All LZ (sub)systems use a *Process Control Narrative* (PCN) to document their PLC inputs, outputs, interlocks, and automation scripts. The SSS has two PCNs: one for the PLC and one for Ignition. The automation code was written to ensure as many steps as possible are performed by the PLC, however, changes to RGA settings must be made in Ignition.

The level of controls for the SSS automation are sorted into a hierarchy. *Steps* are at the bottom of the hierarchy. PLC steps strung together make PLC *procedures*. PLC procedures and Ignition steps are pieced together to make *functions*. These functions come together to make *operations*, and a series of operations will make a *run*. The diagram in Fig. 3.13

visually indicates the levels and where the code for each level is written.

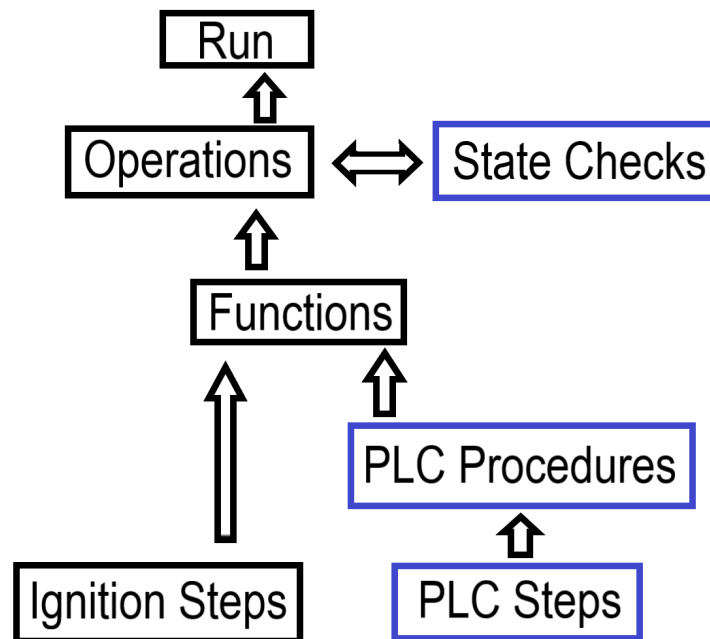


Figure 3.13: A diagram indicating the sampling hierarchy of controls is shown. The most fundamental units of automation are near the bottom of the diagram. Each successive level is comprised of the units below, indicated by the arrow(s) directed at that level. The items outlined in black are written in Ignition, while the items outlined in blue are written into the PLC. State checks written into the PLC are called by Ignition at the beginning and end of an operation.

Steps are the most fundamental actions performed by the automation. These include opening valves, waiting for a condition to be satisfied, turning off devices, or changing RGA settings. They can be either Ignition steps or PLC steps depending on whether the RGA is involved. Each step that involves waiting for a condition to occur has a timeout. Timeouts are meant to protect the SSS if something unexpected occurs and to prevent Ignition or the PLC from hanging indefinitely if the condition cannot be met.

A string of PLC steps that are always intended to occur sequentially, without interruption, are combined into PLC *procedures*. A PLC procedure is activated when its corresponding *initialize* (PLC) variable is set to true. The initialize variable is set to false when the procedure terminates. These procedures have minor checks to ensure the proper condi-

tions before initialization and after completion. Procedures may terminate in a variety of ways: a failed initial check or final check, a timeout during a given step, or successful completion of a given run. A first fault variable is set when a procedure terminates to indicate the step in which it terminated.

Because of the incompatibility of RGA control and the PLC, Ignition steps (usually these are RGA feedback or control) must be combined with PLC procedures to make functions. The primary purpose of this level of control is to construct useful system actions from smaller units of code lower in the hierarchy. Functions are written in and called by Ignition. Functions receive parameters from the user. The parameters map to variables that are defined in both Ignition or the PLC (for example fill pressure, RGA CEM high voltage, flow rate). There is only one type of check on the function level that will be discussed later in this section. If the RGA is not involved in a particular function, then the function only exists to access PLC procedure initialize variables. No PLC procedures can run while an interlock is active.

While functions are useful actions with variable inputs, operations weave functions together into larger, more useful, modular blocks of automation. Operations are also defined strictly in Ignition. An operation will perform a very detailed state check at its start and end. The state checks exist as a single boolean variable defined within the PLC. There are three PLC defined state checks: the pre-fill state, the pre-sample state, and the post-sample state. Operations are grouped into types defined by their starting and ending state checks. These are denoted in Table 3.2.

A single operation may consist of one to five functions. A single function may consist of one to five procedures. There are operations made of only a single function that is composed of one PLC procedure. This is done to maintain consistency of the automation framework and to utilize features of each level of control in a self consistent way.

A few examples can illustrate the benefits of this framework. Only two operations allow

Operation Type	Starting state check	Ending state check
I	Pre-fill	Pre-sample
II	Pre-sample	Pre-sample
III	Pre-sample	Post-sample
IV	Post-sample	Pre-fill

Table 3.2: State checks that define the operation type are shown in the table above. The three states are pre-fill, pre-sample, and post-sample.

the sampling system access to the LZ circulation system. Both of these operations consist of a single function, which calls a single PLC procedure. While these two operations must be called from Ignition, the state check (governed by the PLC) allows the PLC to act as the gatekeeper that authorizes execution. The PLC also maintains control of all valve actuation, as this is performed on the level of the PLC procedure. Thus, the PLC exerts maximal control over any automation accessing the circulation system. When an operation's first action is an Ignition step, the PLC must still authorize the action (on the level of the operation, by a state check) before Ignition proceeds.

A run is a series of operations. The operations comprising a run are queued by the user prior to executing the run. The operation ordering is valid if the system's current state matches the first operation's starting state and any operation's ending state matches the following operation's starting state. A run may end after any operation, but a run must end if an operation's ending state is the pre-fill state. This requirement forces the user to be attentive to the system before drawing more Xe.

An *abort* may be required at any point in the control sequence. Two types of aborts can occur: a *hard abort*, or a *soft abort*. Both aborts terminate the current procedure, but only hard aborts force the system into its *safe state*. Soft aborts simply leave the system in the state it is in. Aborts occur when a state check fails, a condition check exceeds an elapsed amount of time, a system interlock fires, or the user initiates an immediate abort.

Soft aborting is often more convenient and preferred if the system is in a reasonably safe state when the abort triggers. Both types of aborts can be initiated manually. In the case of a failed check or a timeout, the abort type is predetermined. All aborts are written in the PLC.

Ignition has no intrinsic mechanism for learning that a PLC procedure has aborted; Ignition only knows if a PLC procedure is active. If a function dictates that another procedure should run after the aborted procedure ends, Ignition may attempt to initiate the next procedure. The *run queue kill flag* is used to inform Ignition of an abort. The PLC sets the flag as a part of the abort sequence. Ignition checks this flag before every function level action.

One final noteworthy feature is the *sss ana* variable. This variable cycles through a set of values as a measurement is made. Each value corresponds to the timestamp of an action that is relevant to analyzing the measurement. Prior to automation, analysis was done by manually exporting the RGA data and defining time windows by hand. This analysis variable is used to indicate timestamps when RGA data should be exported, analysis windows should be defined, and relevant device outputs should be recorded. This variable allows all SSS analysis code to execute by simply defining a query time range and confirming a few assumptions about each measurement. The automation framework successfully protects the system, improves procedural consistency, maximizes system efficiency, and reduces the burden on the system operator.

3.9 Results and chronology

All LZ Xe was first *dekryptonated* via chromatography at SLAC. Dekryptonation reduces Kr concentrations to 100s of ppq, which is necessary to meet LZ's rigorous purity requirements. The dekryptonated Xe was transported to SURF in *storage packs*. Each of the twelve storage packs are measured prior to being introduced into the circulation system.

The SSS remained at SLAC to aid with dekryptonation operations until all Xe was cleaned. The MSS was the primary tool for analyzing the cleanliness of the circulation system until the SSS was moved to SURF in the fall of 2021.

While Xe was dekryptonated at SLAC, the circulation system was commissioned at SURF. A number of critical detector commissioning time periods occurred prior to the Xe arriving on site. The first major operational period was a circulation system test. The circulation test used several components of the LZ circulation system and a *test cryostat*, with about one percent capacity of the full LZ cryostat to circulate and liquefy Xe.

Circulation test Xe was not dekryptonated but was still required to pass modest purity standards. The MSS measured the purity of candidate Xe and searched for circulation system leaks. The system was used in low sensitivity analog scanning mode to track many gaseous species at once. The getter was not used during the circulation test, allowing the MSS to reliably use N₂ to detect leaks. The fraction of Ar ingress to N₂ ingress matching the Ar to N₂ fraction in air of 0.012 (by mass) was a clear signature of an air leak.

The MSS observed that N₂ concentrations exhibited a strong dependence on the pressure in the test cryostat when liquid was present. No correlation between the N₂ concentrations and date of the measurement was seen. The observation was not related to a leak or ingress but was likely due to a pressure dependence on the N₂ distribution between two phases of Xe. These measurements are seen in Fig. 3.14. Operational periods prior to the arrival of dekryptonated Xe are not discussed further in this chapter.

3.9.1 Commissioning campaigns

Following the circulation test, the next stage of circulation system commissioning was gas circulation through the LZ ICV. Dekryptonated Xe was exclusively used from this point onward to minimize absorption of excess Kr into ICV plastics. Undesirable electronega-

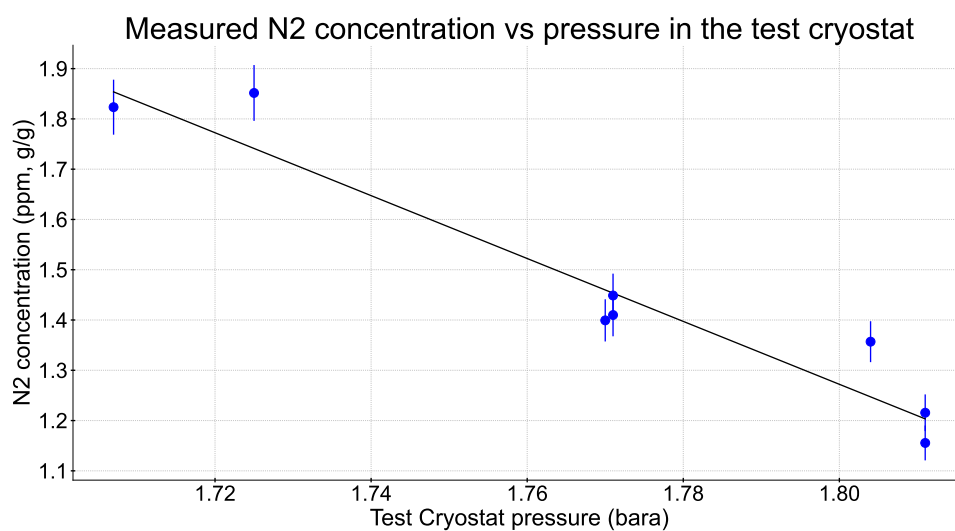


Figure 3.14: Measured concentrations of N_2 are plotted against the test cryostat pressure here. There is no significant correlation between measurement date and pressure. The measured N_2 concentrations are approximately linear with respect to the test cryostat pressure for the pressure range observed. These measurements were made with the MSS in the summer of 2020. These are the only measurements in this thesis that use the low sensitivity analog scanning technique.

tives are removed by flowing through the LZ getter. Thus, N_2 cannot be used as a tracer for air leaks.

Storage packs were delivered to SURF from fall 2020 to July 2021. The dekryptonated Xe was first introduced to the ICV and circulated at room temperature (around 293 K) in December of 2020. Cooling of the ICV and Xe tower started in early February of 2021. Steady temperatures, ranging from 185 to 191 K, were reached later in the month. Cold gas was circulated until nearly all Xe was delivered to site. The ten tonne Xe fill began in July of 2021, and the detector was fully filled by mid September of 2021.

3.9.2 Kr measurements before the science runs

The first major sampling task was to measure the incoming dekryptonated Xe. Initially, all individual cylinders in every storage pack were intended to be measured. These plans were later scaled back after seeing results from a few cylinders. The goal of these measurements was to verify that the Xe was not contaminated when transported from SLAC to SURF.

Only storage pack 8 Xe was used for the room temperature and cold gas circulation periods. Three cylinders of storage pack 8 were directly measured, with two measured in combination. MSS measurements made at SURF are compared with measurements made at SLAC in Table 3.3. The remaining storage pack 8 cylinders were measured indirectly, as part of other measurements. The results are in agreement and, more importantly, indicate no Kr ingress occurred in transit.

Room temperature gas circulation commenced after the candidate Xe was verified to be sufficiently clean. This circulation period allowed for testing of circulation system components. The primary goal of the cold trap mass spectrometry systems at this time was to quantify impurity ingress.

Cylinder	SURF (MSS) measure (ppq (g/g) Kr)	SLAC measure (ppq (g/g) Kr)
1	682 ± 104	520 ± 54
2 and 3	39 ± 9	24 ± 15

Table 3.3: A comparison of measurements taken at SLAC and at SURF for cylinder 1 and a combination of cylinders 2 and 3 from storage pack 8 is shown. Both statistical and systematic uncertainties are included in the reported uncertainty. Cylinder 1 was confirmed to be less pure than cylinders 2 and 3. The SURF and SLAC measurements are consistent, indicating the Xe was not contaminated during transport.

One noteworthy difference between ingress from an air leak and ingress from outgassing of detector plastics is that the latter is temperature dependent. Outgassing is roughly expected to follow the Arrhenius equation, implying an ingress rate decrease of a factor of 2 for every 10 K drop in detector temperature. Comparisons of the room temperature and cold gas circulation measurements offer further insight into the sources of ingress.

Kr measurements from a 40 day period are used to calculate the room temperature gas ingress rate. Temperatures in the ICV fluctuated from 292-294 K at this time. Room temperature gas circulation Kr mass ingress measurements are shown in Fig. 3.15.

The expected linear trend is confirmed by these measurements. The fitted mass ingress rate for Kr can be normalized to an ingress rate in 10 T of Xe to compare with the goal. The room temperature Kr ingress rate is $450 \pm 10_{(stat)} \pm 70_{(sys)}$ ppq/y (g/g) in 10 T of Xe. This is nearly two orders of magnitude higher than the original experimental design goal of 5 ppq/y (g/g).

Cold gas circulation began in February of 2021 and lasted until July of 2021. The purpose was to exercise and characterize the circulation system cryogenics before liquefying Xe. Many measurements were made in similar thermodynamic configurations to understand the circulation system Kr ingress rate.

The MSS measured Kr across the five month period. ICV temperatures varied from

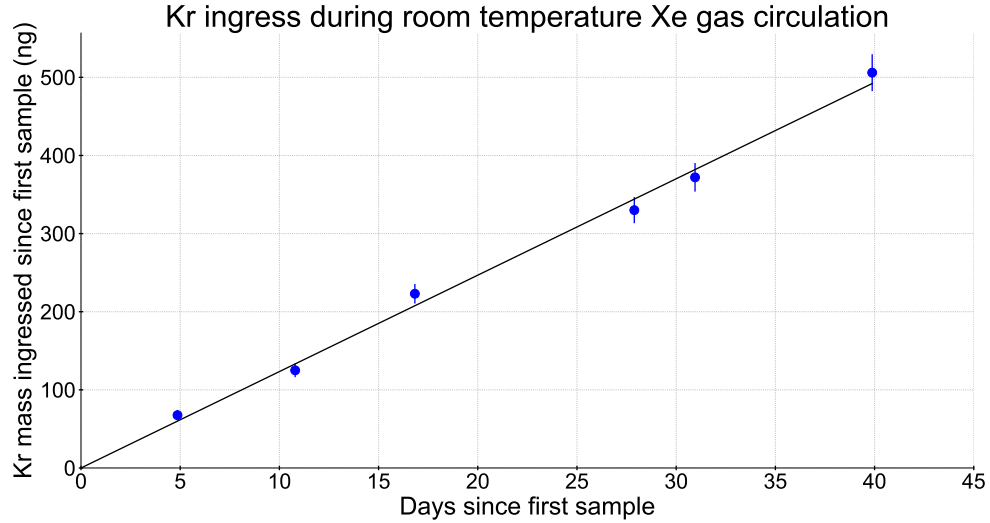


Figure 3.15: The Kr mass ingressed in the circulation system during the room temperature (293 K) gas circulation period is shown. The fitted mass ingress rate is $450 \pm 10_{(stat)} \pm 70_{(sys)}$ ppq/y of Kr (g/g) in 10 T of Xe. The measurements were made with the MSS between December 2020 and February 2021.

185-191 K in that time. Kr measurements are shown in Fig. 3.16. As described in section 3.7, this well-behaved data set was also used to estimate the statistical error on ultra-high sensitivity MSS measurements.

The fitted slope is about of 5 ppt/y (g/g). When accounting for the mass difference between a detector filled with gas (around 93 kg) and the total mass of LZ, the ingress rate is 49 ± 7 ppq/y in 10 T of Xe (g/g). This is an order of magnitude less than the 450 ± 70 ppq/y (g/g) observed during room temperature circulation. While this is not as low as the original experimental design (5 ppq/y), this ingress rate is sufficient for further operations.

The Arrhenius equation predicts greater than four orders of magnitude in outgassing ingress reduction for a temperature drop of 105 K. This was not observed. First, only the cooled portions of the circulation system should exhibit an ingress reduction. Only the ICV and portions of the Xe tower are cooled (see section 2.5 for further details). The dominant source of outgassing in LZ is the TPC, specifically the TPC plastics. However, other

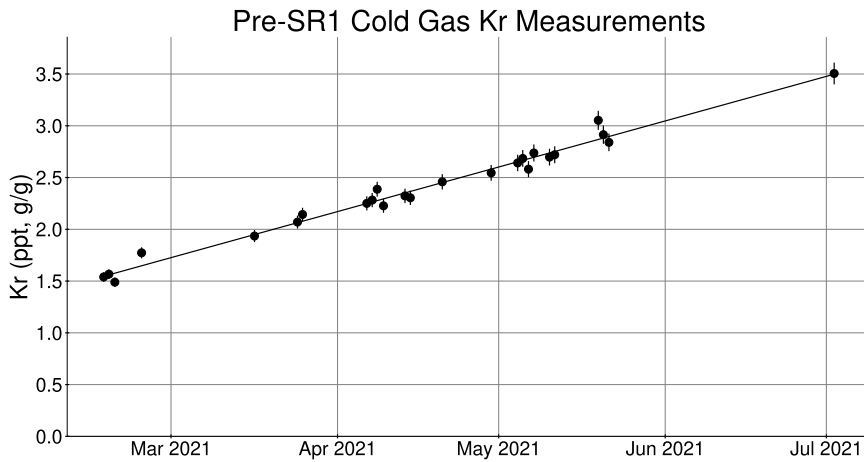


Figure 3.16: Kr measurements from LZ during the "cold gas" circulation period are shown. The circulation system was filled with about 93 kg of Xe, and the ICV was cooled between 185 and 191 K. Adjusting to an ingress rate in 10 tons of Xe, the Kr ingress rate is 49 ± 7 ppq/y (g/g). This sets an expectation for Kr ingress throughout the lifetime of the experiment.

outgassing sources like the compressors experience no reduction. Second, there are (very small) known leaks, and their ingress is not diminished by reducing the temperature. These two measurements prove that the majority of the ingress observed during room temperature gas circulation was the result of outgassing from the TPC.

The cold gas ingress rate is expected to be quite close to the liquid circulation ingress rate. The cold gas circulation temperatures (about 185-191 K) are only slightly higher than the liquid circulation detector temperature (172-177 K). For the same mass of Kr ingressed, a much larger increase in Kr concentration will be observed in 93 kg of Xe than in 10 T. This yields a much smaller uncertainty on the fitted ingress rate in 93 kg than would be observed in 10 T over the same time period. For cold gas circulation, there are no additional complexities from having two phases of Xe in the circulation system. This result sets a rough expectation for Kr ingress during LZ's lifetime.

With the exception of storage pack 8, each storage pack sample was drawn simultane-

ously from all twelve gas cylinders in the pack. Drawing a thoroughly mixed 100 g gas sample from twelve gas cylinders, each with a different pressure and concentration, is non-trivial. The procedure for drawing Xe from the storage packs was altered several times during the measurement campaign. The slight procedural variations may produce minor systematic fluctuations in the measurements. These fluctuations are not expected to have a significant impact on the final mass-averaged storage pack concentrations.

The individual storage pack measurements made at SLAC and SURF (with the MSS) are seen in Fig. 3.17 and are tabulated in Table 3.4. The total Xe mass of each storage pack and the pack mass in LZ are also included in the table.

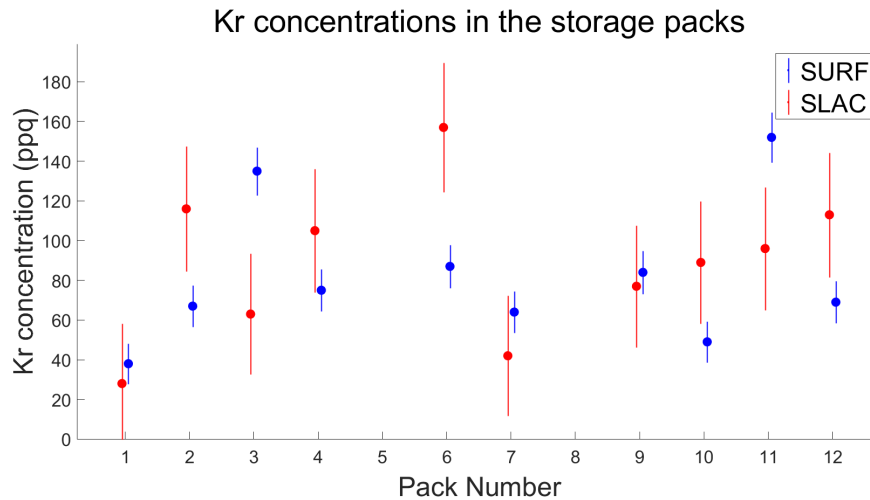


Figure 3.17: Individual storage pack measurements before and after transport from SLAC to SURF are compared. The measurements are mostly consistent. The error bars shown are strictly statistical. The SURF MSS measurements have a larger systematic uncertainty but a smaller statistical uncertainty than the SLAC measurements. The mass averaged Kr concentration for all storage packs measured at SURF is 117 ± 18 ppq. The total mass averaged Kr concentration for the SLAC measurements is 123 ± 10 ppq. The two results are in agreement. The SLAC average is calculated using the SURF measurement of storage pack 5, and the SURF average is calculated using the SLAC measurement of storage pack 8. See also Table 3.4.

As was the case with the SURF measurements, the methods for drawing a well mixed batch of Xe from the storage packs at SLAC changed over time. This may contribute some

Storage Pack	Mass (kg)	Mass Used (kg)	MSS Kr (ppq)	SLAC Kr (ppq)
1	558	550.2	38	28
2	941	933.2	67	116
3	972	964.2	135	63
4	982	940.7	75	105
5	808	766.7	482	N/A
6	983	941.7	87	157
7	989	981.2	64	42
8	289	193.2	N/A	176
9	969	961.2	84	77
10	971	963.2	50	89
11	952	944.2	152	96
12	972	964.2	69	113
Avg (storage packs)	10474	N/A	117	123
Residual	88	88	3380	N/A
Avg in LZ (w/ resid)	N/A	10191	144	151

Table 3.4: Storage pack Kr measurements made with the MSS at SURF and the SLAC sampling system are compared. The "Mass" is the mass of Xe in each storage pack. The "Mass Used" is the mass from each storage pack that was sent into LZ. "Residual" refers to the Xe leftover in the detector after the circulation test. The average of the storage pack measurements is the concentration weighted by the "Mass" column. The average in LZ is the average concentration, weighted by the "Mass Used". This is the expected starting science run 1 Kr concentration. In cases when no measurement was available from one of the locations, the other location's measurement was used to calculate the average. The reported science run 1 Kr concentration from the storage pack measurements is 144 ppq (g/g) with an error of ± 22 ppq (g/g).

small error in both data sets. Using measurements taken at SURF (along with the SLAC measurement for storage pack 8), the mass average purified concentration of all packs as they arrived at SURF is 117 ± 18 ppq (g/g). The dominant uncertainty is the 15% systematic error associated with the MSS calibration. The SLAC measurements (using the SURF measurement of storage pack 5) averaged 123 ± 10 ppq (g/g). The SLAC measurements have less systematic error. The individual pack measurements are in agreement.

The individual measurements and the mass-weighted average from the two different cold trap mass spectrometry systems are consistent. Adding in the Xe that remained after the cold gas measurements and weighting for the amount of Xe used from each storage pack, the expected starting science run 1 Kr concentration is 144 ± 22 ppq (g/g). The storage pack measurements combined with the cold gas measurements establish an expected Kr concentration over the experiment's life of $144[ppq] + (49[ppq/y] * t[y])$, where t is the time since the start of science run 1 (December 23, 2021).

Xe is drawn from specific locations in the gaseous portion of the circulation system during regular LZ operations. The circulation system is dynamic, large, and complex, and multiple phases of Xe are present. Impurities may partition such that the Xe drawn during regular operations is not indicative of the true average impurity concentration. For example, the impurities may preferentially dissolve in the LXe. In the LUX experiment, measured Kr concentrations remained stable throughout the life of the experiment, but were a factor of four greater than the average Kr concentrations measured prior to filling [64]. This is an indication that Kr preferentially remained in the gas phase in LUX. The storage pack mass average and the initial liquid circulation measurements can be compared to understand how impurities partition.

3.9.3 Ar measurements before the science runs

Ar concentrations may exceed Kr concentrations by several orders of magnitude and still be a negligible component of LZ's background budget. Regardless, it is important to quantify and monitor the Ar concentrations. The Ar measurements may offer insight into the behavior of non-Kr impurity species in the circulation system.

The first useful Ar measurement campaign is the cold gas circulation period. Measurements from this period are shown in Fig. 3.18.

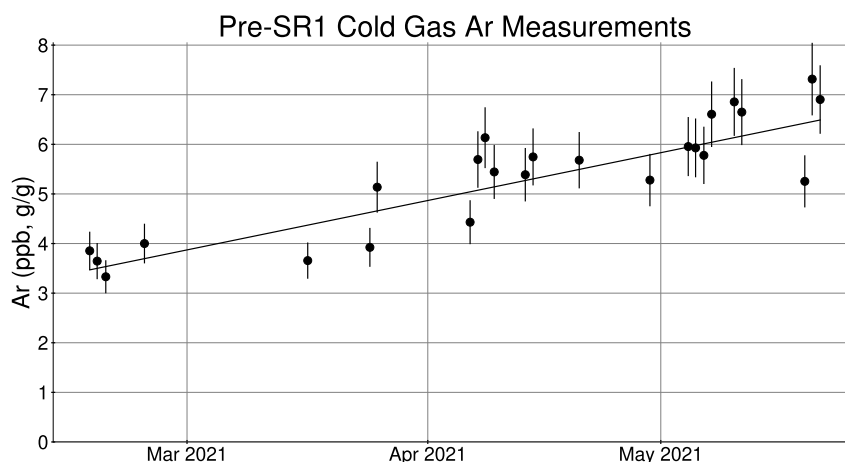


Figure 3.18: Ar measurements from LZ during the cold gas circulation period are shown. The circulation system was filled with about 93 kg of Xe and the ICV was cooled between 185 and 191 K. The Ar mass ingress in this period should be very similar to the Ar mass ingress after LZ is fully filled. Correcting to an ingress rate in 10 tonnes of Xe, the Ar ingress rate is 110 ± 20 ppt (g/g). This sets an expectation for Ar ingress throughout the lifetime of LZ.

The measured Ar ingress rate normalized to 10 tonnes of Xe is 110 ± 20 ppt/y (g/g). There is no reliable room temperature Ar ingress rate to make a comparison. This measurement sets a much more precise expectation for LZ's Ar ingress rate than would be garnered from early measurements during full 10 tonne liquid circulation.

Ar was measured in the storage packs when they arrived at SURF. The storage packs,

their total masses, and the mass that entered the circulation system from each storage pack are included in Table 3.5.

Storage Pack	Total Mass (kg)	Mass Used (kg)	MSS Ar (ppt)
1	558	550.2	38
2	941	933.2	228
3	972	964.2	1850
4	982	940.7	206
5	808	766.7	359
6	983	941.7	1190
7	989	981.2	1990
8	289	193.2	500
9	969	961.2	681
10	971	963.2	208
11	952	944.2	944
12	972	964.2	747
Residual	88	88	11000
Avg in LZ (w/ residual)	N/A	10191	890

Table 3.5: Storage pack Ar measurements made with the MSS at SURF are shown. The "Mass" is the mass of Xe within each storage pack. The "Mass Used" is the mass from each storage pack that was sent into the circulation system. "Residual" refers to the Xe leftover in the detector after the circulation test. The average in LZ is the average concentration, weighted by the "Mass Used". This is intended to reflect the starting expected science run 1 Ar concentration. The reported science run 1 Ar concentration measured from the storage packs is 890 ppt (g/g) with an error of ± 180 ppt (g/g).

The mass-weighted Ar concentration including residual Xe from the cold gas circulation is 890 ± 180 ppt (g/g) at the start of science run 1. As with Kr, the storage pack and cold gas circulation measurements combine to set a slope and intercept for the expected Ar concentration in LZ of $890[ppt] + (110[ppt/y] * dt[y])$.

3.9.4 Kr measurements from LZ's first science run

Xe liquefaction and the full ten tonne Xe fill of LZ began in July 2021 and ended in September 2021. Cold trap mass spectrometry sampling capabilities were limited during

this time period. Despite this, Kr concentrations were clearly observed to drop, as storage pack Xe diluted the more Kr rich residual Xe remaining from cold gas circulation. The first purity measurements while circulating LXe were made on September 15, 2021. LZ Science Run 1 (SR1) officially began on December 23, 2021.

The MSS made initial measurements in this time period. The SSS was transported from SLAC to SURF in September of 2021 and was operational by November of 2021. Kr measurements with both systems from the start of LXe circulation through the end of SR1 are shown in Fig 3.19. The expected initial Kr concentration and the time window defining SR1 are indicated.

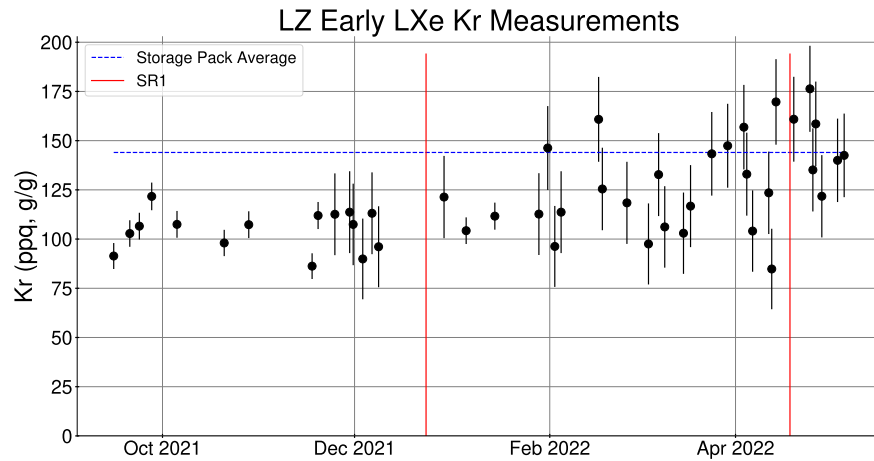


Figure 3.19: Kr measurements from immediately after the full 10 ton fill of LZ until May 6, 2022 are shown. The dashed blue line indicates the 144 ppq expectation from the storage pack measurements. The area between the vertical red lines indicates when SR1 occurred. The measurements with smaller error bars are made with the MSS, while the measurements with larger error bars are made with the SSS (see section 3.7 for more on this). The displayed error bars on all measurements are strictly statistical. The storage pack measurements initially fall slightly below the 144 ppq expectation before rising at the end of SR1.

The measured Kr concentrations are not far from the expected Kr concentrations. This implies that, unlike in LUX, the measured Kr concentrations can be considered indicative of the true average concentration in the detector. While Kr measurements are initially lower

than the storage pack expectation, they rise slightly near the end of SR1.

The reported natural Kr concentration in LZ during SR1 is 144 ± 22 ppq (g/g). This is measured directly from the storage packs. Kr ingress during SR1 is negligible.

3.9.5 Ar and He measurements from LZ's first science run

Ar and He measurements from the start of LXe circulation through the end of SR1 are shown in Fig. 3.20.

Early Ar measurements during liquid circulation are considerably lower than the expectation set by the storage pack measurements. The average Ar concentration during SR1 is 60.8 ± 12.2 ppt (g/g). The fraction $f = C_{Ar}^{SP}/C_{Ar}^{SR1}$, where C_{Ar}^{SP} is the concentration in the storage packs and C_{Ar}^{SR1} is the concentration in SR1, is about $14.6 \pm 0.8_{stat}$. The order of magnitude disparity between expected and measured Ar concentrations is not fully understood. Like with the Kr observation in LUX, the leading hypothesis is that the Ar preferentially dissolves in the liquid phase of the Xe. This implies Ar in the gaseous phase of Xe (where all measurements are drawn) will be depleted.

This effect is plausibly quite sensitive to changes in circulation system thermodynamics. Large variations in N_2 concentrations are correlated with the test cryostat pressure when LXe was in the test cryostat, seen in Fig. 3.14. SR1 thermodynamic changes can also be noted by observing the TPC pressure. Measured Ar concentrations show large variation before December 2021 when detector thermodynamics were regularly adjusted. The variation slowed in mid-December as changes were halted and vanished as the detector stabilized. Ar measurements remain nearly constant throughout SR1.

He measurements also display this behavior. The sharp rise in measured He concentrations after SR1 directly corresponds to an intentional change in circulation system thermodynamics to increase convection in the TPC. Evidence of a similar effect in Ar measure-

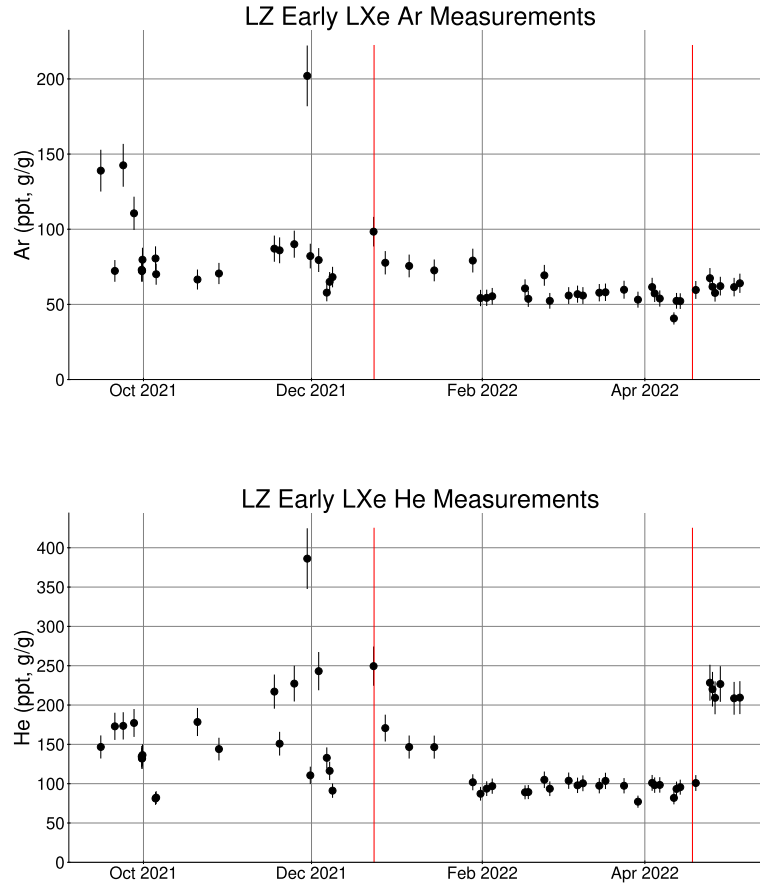


Figure 3.20: Ar (top) and He (bottom) measurements following the full 10 ton fill of LZ until May 6, 2022 are shown. SR1 is the period between the vertical red lines. Ar measurements prior to the start of SR1 display excessive variation. The variance decreases when SR1 begins as detector thermodynamics settle. The sudden drop in concentrations of both species at the end of January 2022 is indicative of a change in systematics associated with calibrations (see section 3.9.8 for more on this). All measurements from approximately February onward have identical calibration related systematics. These measurements indicate that the observed Ar concentrations in the gaseous phase Xe are affected by circulation system thermodynamics. Like Ar, the measured He concentration falls well below the expectation from the storage pack measurements. Also like Ar, the He measurements show large variation before settling after the start of SR1. The sharp jump after the end of SR1 directly corresponds to a significant and intentional change to detector thermodynamics to promote convection within the TPC. This plot is strong evidence that changes to detector thermodynamics influence the measured concentration of He in the gaseous phase of LZ.

ments following SR1 is not as obvious. Still, the clear effect in He, the pressure dependence in the N₂ concentrations, and the variation in the pre-SR1 Ar measurements all support the idea that the fraction of Ar dissolved in the liquid is affected by circulation system thermodynamics.

One alternate explanation for the order of magnitude discrepancy is related to the storage pack measurement procedure. Cylinders in the storage packs are connected by a manifold. Xe moves from the manifold to the Xe storage panel, then through the very long (220 ft) storage room transfer line to the Xe delivery and recovery panel, where it is pulled into the MSS.

Individual cylinder Ar concentrations can vary by several orders of magnitude. Preferentially including more Xe from one gas cylinder or another when mixing may affect the concentrations entering the MSS. The refinements to the storage pack mixing procedure likely improved mixing in a batch of gas that would reach the sampling system. The earlier storage pack measurements may be more susceptible to uneven mixing and may be less indicative of the true average Ar concentration in a storage pack. Most gas cylinders in a storage pack have similar Kr concentrations. This mitigates similar concerns for the Kr measurements.

Mixing effects could plausibly account for some non-trivial difference between the measured and true Ar concentrations of a single storage pack. However, it seems unlikely that mixing effects would sufficiently account for an order of magnitude discrepancy after taking a weighted average across all twelve storage packs. Ar preferentially dissolving in the LXe is still the leading theory to explain the difference between the liquid circulation and storage pack measurements.

The reported natural Ar concentration during SR1 is 890 ± 180 ppt (g/g). Like Kr, this concentration is the Ar storage pack weighted average. Ar is approximated to be constant across SR1.

3.9.6 SSS improvements prior to and during LZ’s WIMP search 2024 science run

Before discussing the WIMP Search 2024 science run (WS2024) measurements, several SSS improvements made between SR1 and the end of WS2024 should be noted. In SR1, the SSS exhibited less sensitivity, and its RGA showed more wear than the MSS or its RGA. Changes noted below occurred prior to and during WS2024. The SSS automation, discussed in section 3.8, was also progressively integrated before and during WS2024. The automation will not be discussed further here but likely contributed to improved behavior. Several other minor procedural changes (not discussed) also contributed to the improvements in the SSS behavior.

RGA baseline drift, mentioned in previous sections 3.3.1 and 3.5, is a problem for ultra-high sensitivity measurements. To quickly recap, the term *baseline* refers to a shift in RGA behavior affecting all masses and is probed by measuring the partial pressure of AMU/q 87. A significant rise in baseline indicates that a signal increase in any other isotope can no longer be considered quantitatively reliable. The baseline is directly subtracted from all masses in every measurement, seen in Eq. 3.2 and Eq. 3.3. The correction is considered valid for baseline drift less than one ptorr. Significant baseline drift affected several Kr measurements during WS2024 and prompted some of the changes below.

The most frequent cause for baseline drift is saturation from changes in absolute pressure at the RGA. During WS2024, the pressure gauge intended to measure the RGA pressure was moved closer to the RGA. The change revealed that the pressure seen by the RGA was higher than had been inferred. Higher RGA pressures degrade the RGA CEM faster, and the SSS RGA CEM degraded faster than expected. Impedance valves were adjusted to reduce the pressure in the RGA volume. The CEM’s gain was lowered to reduce wear and tear and improve behavior. The plumbing between the cold trap and the RGA was altered

to reduce mechanical constraints that made the vacuum systems difficult to service. The RGA volume was reduced to increase impurity pressures during flow.

The Xe pre-measurement ice formation process was modified. It was noted that the pressure and temperature in the cold trap during cool down resulted in the formation of a liquid Xe puddle. The puddle froze as the Xe was further cooled. Puddle-like ice formation is not ideal. To remedy this, the cold trap is opened to a large volume during cool down, so the pressure never exceeds Xe's triple point pressure.

Other improvements were made to the cold trap temperature regulation. Better control of the Xe vapor pressure, and therefore the pressure at the RGA, improves RGA systematic behavior. The SSS cold trap has temperature sensors on the trap inlet, middle, and outlet. The cold trap has two heaters near the inlet and outlet that are controlled by PID loops on the respective inlet and outlet temperature transducers.

The PID loops were originally set to regulate to 77 K at both the trap inlet and outlet. The cold trap's coldest point dictates the Xe vapor pressure. Before flow, with both heaters set to 77 K, the middle of the cold trap was colder than the inlet or outlet at equilibrium. This implies the Xe vapor pressure (and the pressure at the RGA) was dictated by the temperature at the center of the trap.

During flow, Xe ice initially forms a sleeve near the trap inlet. The sleeve builds toward the center of the trap as flow continues. At the start of flow in the original configuration, the trap inlet experienced an increased heat load from the incoming Xe. The inlet heater's response to the heat load was delayed, causing the inlet temperature to spike to nearly 81 K. As the sleeve reached the center of the trap, the center temperature rose. The pressure at the RGA rose as well. The pressure continued to increase until the center of the cold trap was hotter than the outlet. The pressure was controlled by the outlet temperature (regulated by the outlet heater) for the remainder of flow.

The ideal place to regulate the Xe pressure is the cold trap outlet. This location expe-

periences the least Xe heat load during flow, and its temperature is regulated by a heater. A temperature gradient must be set across the trap to make the outlet the coldest point. This gradient must be steep enough to prevent the trap center from being the coldest point but cannot be so steep that the heaters are incapable of maintaining it. Further, adding too much heat load to the trap inlet and center, whether via the inlet heater or Xe, will overwhelm the cooling power the pulse tube refrigerator can deliver to the outlet. If the refrigerator is overwhelmed, the outlet temperature will not be controlled.

Two changes were made from these observations. First, the PID loops were tuned to improve the immediate heater response to the sudden heat load at the start of flow. Second, the setpoint temperature at the outlet of the trap was changed to 74 K. Inlet-outlet temperature differences between 2.5 and 3.5 K allow the trap outlet to maintain constant temperature through the duration of flow. None of this is a concern for the MSS liquid N₂ bathed cold trap. Every point within the MSS trap is regulated by the N₂ boiling point.

The final significant change occurred in December 2023 when the RGA CEM was replaced. Many of these improvements, including the SSS automation, made the system more resistant to baseline drift. These changes also made the SSS devices more resistant to degradation, more serviceable, and more durable. There was hope that the modifications would improve the sensitivity of the SSS. Unfortunately, no sensitivity change was noted.

3.9.7 Kr measurements from LZ's WIMP search 2024 science run

LZ WS2024 data was primarily collected from June 22, 2023 until April 1, 2024, with a small portion of data also collected from March and April of 2023. The SSS was exclusively used to make WS2024 cold trap mass spectrometry measurements. The first measurement occurred on July 1, 2023, and measurements continued through April 1, 2024. These are shown in Fig. 3.21. Measurements with baseline drift exceeding the one

ptorr threshold are indicated in red. The baseline drift stabilized significantly following the changes in December 2023.

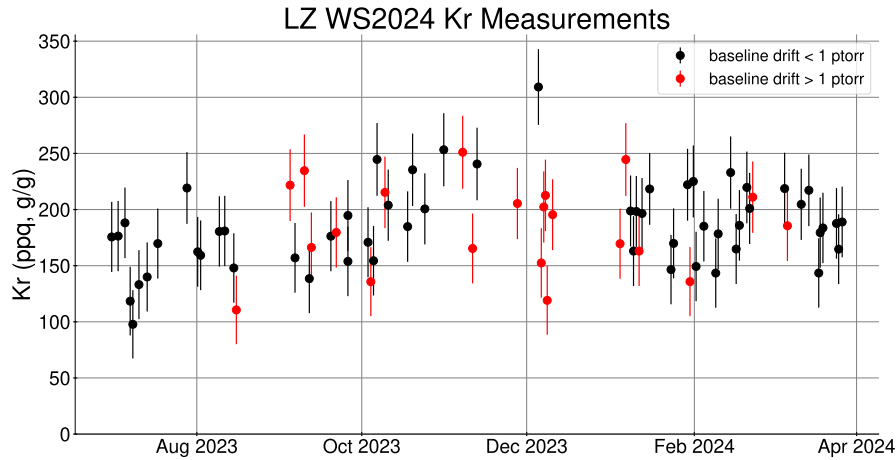


Figure 3.21: WS2024 Kr measurements are shown. These were made from July 1, 2023 until April 1, 2023. Measurements with a "high baseline drift" exceeding one ptorr are plotted in red. High baseline drift measurements are known to be quantitatively unreliable. Part replacements and procedural changes made around January 2024 greatly improved the RGA's worsening baseline behavior.

Setting aside the baseline drift, the projected Kr concentration from the cold gas ingress and storage pack measurements is compared with cold trap mass spectrometry measurements from the start of SR1 until the end of WS2024 in Fig. 3.22.

It is clear that the WS2024 measured Kr concentrations (starting just before August 2023) fall well below the projection from the storage pack and cold gas ingress measurements. This is evidence that the Kr ingress in LZ has decreased, implying the cold gas ingress rate is no longer indicative of LZ's Kr ingress. The reported WS2024 Kr concentration cannot rely on the storage pack and cold gas ingress prediction.

There are several justifiable measurement subsets from Fig. 3.21 that could be used to calculate the WS2024 Kr concentration. It could be argued that all measurements should be included, measurements prior to the hardware changes should be excluded, or measure-

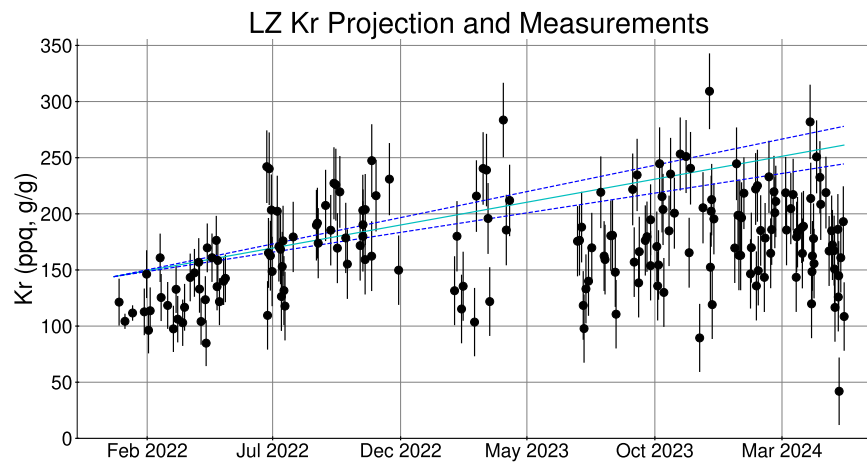


Figure 3.22: All Kr measurements from December 23, 2021 (the start of SR1) through May 15, 2024 are shown. The projected storage pack plus cold gas ingress expectation is shown in cyan. The ± 7 ppq/y uncertainty on the ingress rate is shown by the dashed blue lines. The WS2024 measurements clearly fall below the cold gas ingress projection. No measurements with a bad baseline have been removed from this dataset. This plot indicates that the cold gas Kr ingress rate is no longer a reliable expectation for LZ's Kr ingress.

ments with high baseline drift should be excluded.

The average WS2024 Kr concentration can be quantified using different methods. The simplest option for quantifying the WS2024 concentration is calculating the weighted average of all WS2024 Kr measurements. A linear fit of the measurements by date could also determine the WS2024 Kr concentration. In the case of the linear fit, the average concentration of the fit across WS2024 would be reported. The linear fit would allow for some degree of ingress, avoid over-weighting time periods when the measurement frequency is high, and provide a p-value to assess data quality. Table 3.6 shows the weighted average and the linear fit average of several subsets of WS2024 data.

All combinations of data subsets, baseline inclusion, and calculation type result in similar Kr concentrations. The subset of data chosen (the "Reporting selection" in the table) excludes measurements with a baseline drift greater than one ptorr. The eight measurements immediately before to the SSS CEM replacement and procedural modifications in

Time Window	High BL?	Weighted avg	Linear fit avg	Fit P-value
All WS2024	Yes	182 ± 4	181 ± 4	0.011
All WS2024	No	184 ± 4	183 ± 4	0.217
Jan 2024 to end WS2024	Yes	187 ± 5	187 ± 5	0.565
Exclude Sep - Dec 2023	Yes	177 ± 5	174 ± 5	0.727
Reporting selection	No	182 ± 4	181 ± 4	0.458

Table 3.6: This table shows calculations of the WS2024 Kr concentration using various subsets of data and two different calculation methods. The weighted average and linear fit average columns are listed in ppq (g/g). The quoted uncertainties include only statistical error. The "High BL?" column indicates whether measurements with a baseline drift in excess of one ptorr are included in the selection. High baseline drift measurements are indicated in red in Fig. 3.21. The "Weighted avg" column is the average, weighted by the uncertainty on each individual measurement. The "Linear fit avg" column is the average value of the linear fit to the WS2024 data. The p-value of each linear fit is listed. The "Reporting selection" row indicates the subset of data reported for WS2024. This is identical to including all measurements with baseline drift less than one ptorr and excluding the one measurement that passed the baseline cut in the string of seven of eight measurements that failed the baseline cut. The reported selection is explicitly shown in Fig. 3.23. The values in this table indicate that the many subsets of data and both calculation methods yield very similar results. The reporting selection weighted average WS2024 Kr concentration is $182 \pm 4_{stat}$ ppq (g/g) with the systematic error yet to be applied.

December 2023 are also excluded. Seven of these eight measurements exhibited severe baseline drift and were already excluded by their baseline, effectively removing one additional measurement. This measurement was likely the result of a large downward baseline fluctuation, allowing it to pass the baseline cut and artificially inflate the signal of both ^{84}Kr and ^{83}Kr . The WS2024 data from the reporting selection is shown in Fig. 3.23.

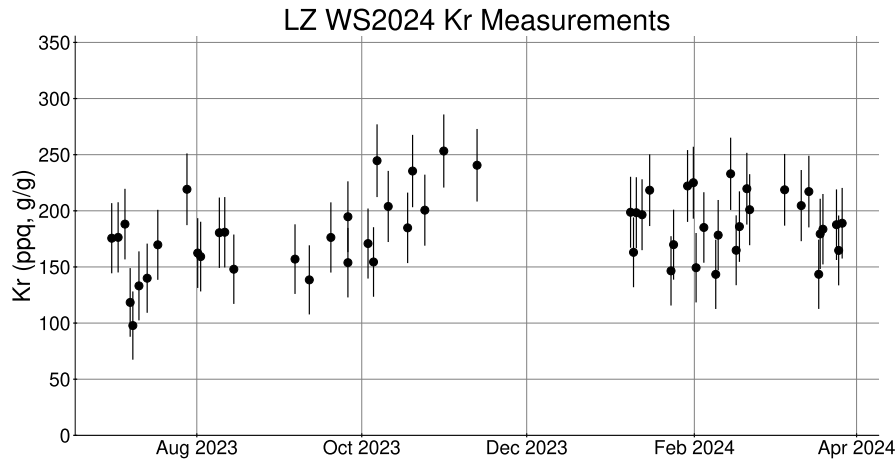


Figure 3.23: LZ WS2024 Kr measurements used to calculate the final weighted average concentration are shown. This selection excludes all measurements with a baseline drift greater than one ptoorr. It also excludes all measurements between November 22, 2023 and December 11, 2023. The RGA exhibited poor behavior over this time period, with seven of eight measurements failing the baseline drift cut. The reported WS2024 Kr concentration is the weighted average of the measurements in this plot. Including the 15% systematic error, the reported WS2024 Kr concentration is 182 ± 26 ppq (g/g).

The weighted mean of the data selection is 182 ± 4 ppq. The average value of the linear fit is 181 ± 4 ppq. The weighted mean is reported as the WS2024 Kr concentration. With the 15% systematic error included, the reported WS2024 Kr concentration is 182 ± 26 ppq (g/g).

3.9.8 Ar measurements from LZ's WIMP search 2024 science run

Similar to Fig. 3.22, the projected Ar concentration, based on the measured cold gas ingress rate, can be plotted from the start of SR1 until May 2024. This is shown in Fig. 3.24. The SR1 average Ar concentration is used as the intercept for the fit projection. If the amount of Ar dissolved in the liquid phase was approximately constant after the start of SR1, Ar measurements would be expected to closely follow the projected ingress. Unfortunately, calibration systematics complicate any conclusions that may be drawn from these measurements.

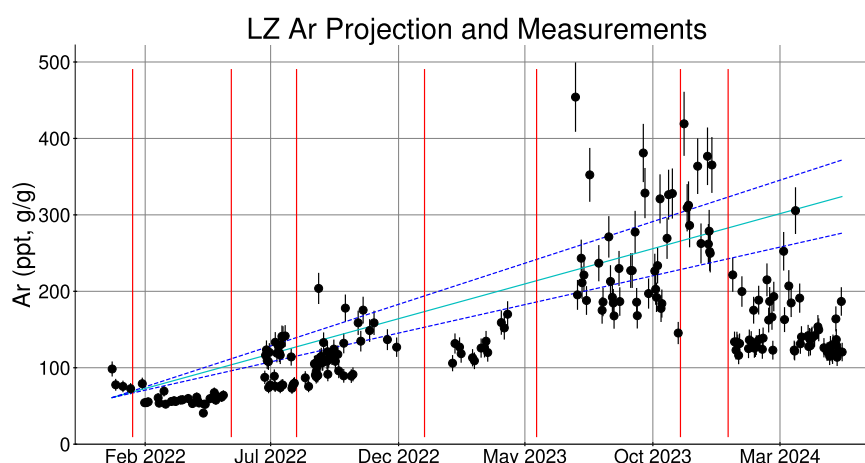


Figure 3.24: The measurements and projection of Ar in LZ from the start of SR1 are shown. The projection in blue is anchored from the average of SR1 Ar measurements (60.8 ppt) as opposed to the storage pack measurements as in Fig 3.22. The dashed blue lines indicate the projection of the uncertainty on the Ar ingress rate. Each red vertical line on this plot indicates a change to the sampling system's Ar systematics. The data between each set of red vertical lines has different calibration related systematics than all measurements outside of the same set of red vertical lines. Calibration related systematics vary far more between subsequent Ar calibrations than between Kr calibrations. The most trustworthy calibration is the final calibration, which took effect in January of 2024. The calibration systematics are discussed in Section 3.6.

The red lines in Fig. 3.24 indicate periods with different calibration related systematics.

Sampling system calibrations must be discussed in more depth to properly explain this plot. Returning to section 3.6, any error on a calibration reference measurement results in systematic error affecting all measurements that use that calibration as a reference. Until January 2024, all Ar calibrations used 100% Ar as their starting impurity. As stated in section 3.6, the ideal calibration concentration is around a factor of five to ten greater than the typical measurement concentration. Measurements in the range of 100 to 200 ppt will ideally use a calibration reference measurement of about one part per billion (ppb). 100 g of cleaned Xe must be mixed with 100 ng of pure Ar to achieve this concentration.

Reducing grams of pure Ar to a 100 ng quantity requires a number of dilution expansions. Referencing Fig. 3.11 and the procedure described in section 3.6, low pressures from the expansions lead to several concerns.

The turbo pumps must be stopped to avoid over-pressure when opening to the expansion volume. Air backflow is possible while the turbo pumps are stopped. Many SSS valves are known to have small leaks across their valve seats. A small leak from the mixing volume to the clean Xe volume or from the impurity volume into the mixing volume (particularly when the mixing volume is near vacuum pressures) could cause a significant discrepancy between the expected and true Ar concentrations. For practical reasons, Ar calibrations prior to 2024 did not reach the desired ppb calibration concentration. The gap between a typical LZ Ar measurement concentration and the typical Ar calibration concentration (for Ar calibrations before 2024) is significant. The RGA response to concentrations that differ by several orders of magnitude is non-linear. Each of these effects will manifest as a calibration systematic in F_{cal} . These are difficult to quantify and are reflected in the conservative 20% systematic on Ar (high sensitivity) measurements.

Ar measurements after the start of 2024 use a calibration impurity mixture of 186 ppb of Ar in Xe. No dilution expansions are required to mix a 1 ppb Ar calibration with 186 ppb Xe-Ar mixture. There is uncertainty on the calculated concentration of the mixture,

but the January 2024 calibration is the most trusted Ar calibration. Future measurements are expected to exhibit less variation between calibrations.

Ar measurements made after the start of 2024 are shown in Fig. 3.25. This selection extends past the end of WS2024 to mid-May of 2024.

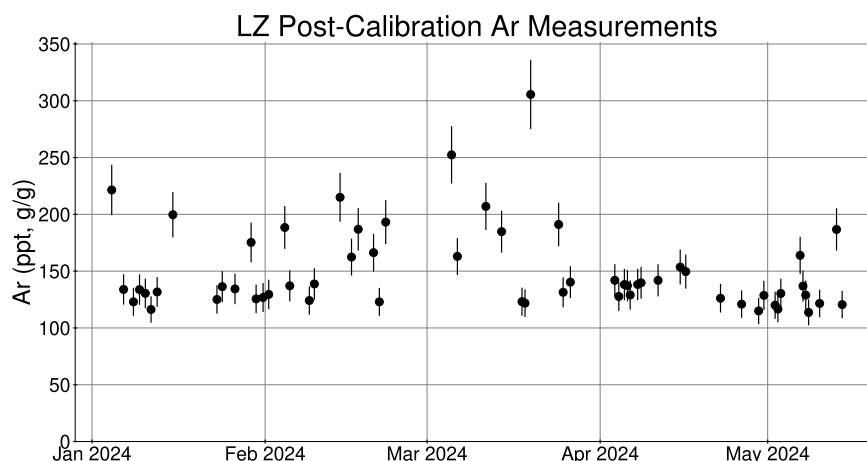


Figure 3.25: Measured Ar concentrations from January 1, 2024 to May 15, 2024 are shown. All measurements use the January 2024 Ar calibration as a calibration reference. The anomalously high Ar concentrations abruptly stop at the beginning of April 2024. This coincides with a Kr calibration.

The error bars appear to be underestimated prior to April 2024. More scrutiny reveals higher Ar concentrations are correlated with higher measured N_2 concentrations. This can be seen in Fig. 3.26. N_2 is removed by the getter and typically should not change between samples.

The N_2 correlation suggests the source of Ar and N_2 may be internal to the SSS. The sudden absence of anomalously high Ar measurements after March 2024 coincides with a Kr calibration. All accessible volumes in the sampling systems are cleaned prior to returning any Xe to LZ after a calibration measurement. The anomalously high Ar measurements could indicate that an infrequently used SSS volume was contaminated with N_2 or Ar following the changes in December of 2023. There is no reason the contamination would

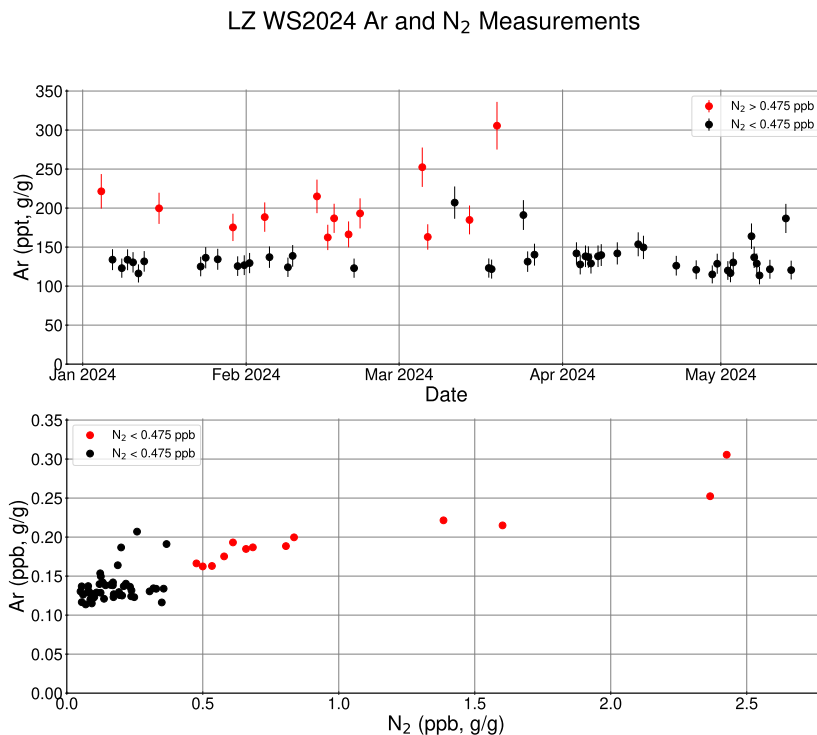


Figure 3.26: Ar and N₂ measurements from January 1, 2024 to May 15, 2024 are shown. The top plot shows Ar measurements over time. Ar measurements with corresponding N₂ measurements greater than 0.475 ppb are indicated in red. The correlation between N₂ and Ar is clear in the bottom plot which shows the same Ar measurements plotted against N₂. The large Ar variation and the high N₂ measurements stop after April 2024. This coincides with the first sampling system Kr calibration. The cause of the high N₂ and Ar measurements is not understood. No data from Fig. 3.25 is excluded from later calculations because of this observation.

only affect certain measurements. With no reason to exclude the high Ar measurements, all WS2024 Ar measurements following the January calibration are included in the WS2024 data set.

The (weighted) average of WS2024 Ar measurements (from January 1, 2024 to April 1, 2024) is $150 \pm 40_{stat} \pm 30_{sys}$ ppt (g/g). This is *not* the reported WS2024 Ar concentration. The quoted statistical uncertainty for this subset of measurements is the full standard deviation as opposed to the standard deviation on the weighted mean. Using the standard deviation reflects ignorance regarding the cause of the higher Ar concentrations.

The observation that Ar preferentially partitions in the Xe liquid and is affected by circulation system thermodynamics implies that the WS2024 Ar measurements are not indicative of the average Ar concentration in LZ. Despite avoiding the cold gas ingress and storage pack measurements when determining the WS2024 Kr concentration, cold gas ingress and storage pack measurements *must* be used to determine the WS2024 Ar concentration.

Measurements presented in sections 3.9.3 and 3.9.5 indicate that the factor $f = C_{Ar}^{SP}/C_{Ar}^{SR1}$ describing the distribution of Ar between the gaseous and liquid phases of Xe is not constant. As a quick exercise, the storage pack plus cold gas Ar estimates can be compared with the selected WS2024 measurements scaled by f , assuming $f = 14.6 \pm 0.8$. Applying the 14.6 factor to the WS2024 weighted average concentration of 150 ± 50 ppt(g/g) yields an expected concentration of 2.2 ± 0.7 ppb in WS2024. The predicted concentration based on storage pack and cold gas ingress measurements is 1.10 ± 0.18 ppb (g/g). The measurements are within two sigma.

The WS2024 scaled measurements provide only a loose constraint on the WS2024 Ar concentration. Regardless, the factor used to describe the distribution of Ar in the circulation system remains questionable. Without better knowledge of the Ar concentration in the Xe liquid, the gaseous WS2024 Ar measurements are not quantitatively useful for con-

straining Ar in LZ. The storage pack and cold gas ingress measurements provide the best estimate of the LZ Ar concentration during WS2024. The reported WS2024 Ar concentration is 1.10 ± 0.18 ppb (g/g).

3.10 Summary of results

All Kr measurements taken since the ICV was integrated into the LZ circulation system are shown in Fig. 3.27.

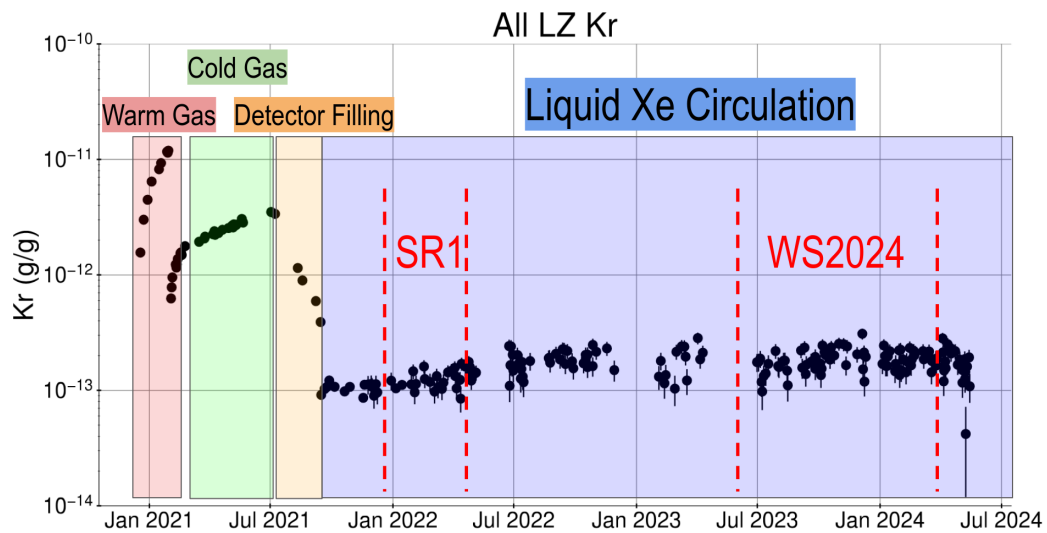


Figure 3.27: A plot of all Kr measurements made with cold trap mass spectrometry across the lifetime of LZ is shown. Measurements begin during warm gas circulation (red) in December of 2020 and end in June of 2024, after WS2024. Cold gas circulation (green) and detector filling (orange) are indicated just before and just after July of 2021 respectively. The remaining measurements were made during LXe circulation (blue). The two science runs discussed in this chapter are indicated by dashed red lines. Gaps in the Kr measurements are the result of periods of sampling system maintenance and modification.

The Kr measurements in this plot tell the story of the detector. Gaseous Xe is first loaded into the detector in December of 2020. The Kr ingress is highest in the room temperature Xe gas circulation period. The detector was emptied and refilled at the start of February 2021 to briefly drop concentrations below a ppt. The ingress rate was reduced in February

and March 2021 as the TPC was cooled. Kr ingress is noticeably lower during the cold gas circulation period. Liquefaction began in July 2021. Xe remaining from the gas circulation period was diluted by cleaner storage pack Xe. As detector filling ended in September 2021, liquid Xe circulation began. Kr concentrations initially rose but eventually flattened as the Kr ingress diminished.

The cold trap mass spectrometry systems have been effectively commissioned and applied to improve knowledge of Kr and Ar within the LZ detector. The MSS is sensitive to 6 ppq (g/g) of Kr and the SSS is sensitive to 20-30 ppq (g/g) of Kr. Both systems meet LZ requirements. The technique and the two systems were used to quantify the Kr and Ar backgrounds in LZ's first and second science runs. There are no mechanisms for quantifying Ar and few mechanisms for quantifying Kr without them.

The two systems have monitored LZ Xe since it arrived at SURF. Both systems were effectively integrated into the LZ control framework, and the SSS now measures impurities in LZ with minimal burden on the user. The long term stability of the SSS is greatly improved. The systems continue to collect valuable results for the experiment. Cold trap mass spectrometry remains critical for monitoring impurities throughout the life of LZ.

Chapter 4: Measurement of the Excited State Decay of ^{85}Kr in LZ's WIMP Search 2024 Science Run

The importance of monitoring ^{85}Kr has been stressed throughout the previous chapter. In addition to using the cold trap mass spectrometry technique, ^{85}Kr can also be tracked using data from the LZ TPC. This technique measures ^{85}Kr using a rare decay branch and is similar to the technique used in [65].

Fig. 4.1 shows the decay scheme for ^{85}Kr . The most common decay branch of ^{85}Kr is through the direct β^- -decay to the ground state, where the electron and anti-neutrino receive the totality of the energy difference between the ^{85}Kr and ^{85}Rb ground states. 0.434% of ^{85}Kr decays to ^{85m}Rb . ^{85m}Rb releases a 514 keV γ to reach the ^{85}Rb ground state with a half-life of 1.015 μs .

In Xe, a decay that proceeds through the ^{85m}Rb state results in prompt scintillation at the time of the β^- -decay, and the production of free charge. The γ from the transition of ^{85m}Rb to its ground state is likely to Compton scatter before being photo-absorbed. Each of the Xe interactions (β , Compton scatter, photo-absorption) produces prompt scintillation and free charge. Signals from both the β and γ from the excited state decay are captured in the same event time window in LZ (provided that both interact in the TPC).

Because the mean free path of a 514 keV γ in LXe is on the order of centimeters, the time between interactions of a Compton scattering γ is less than one nanosecond. Whether the γ compton scatters multiple times or is immediately photo-absorbed, a γ that deposits

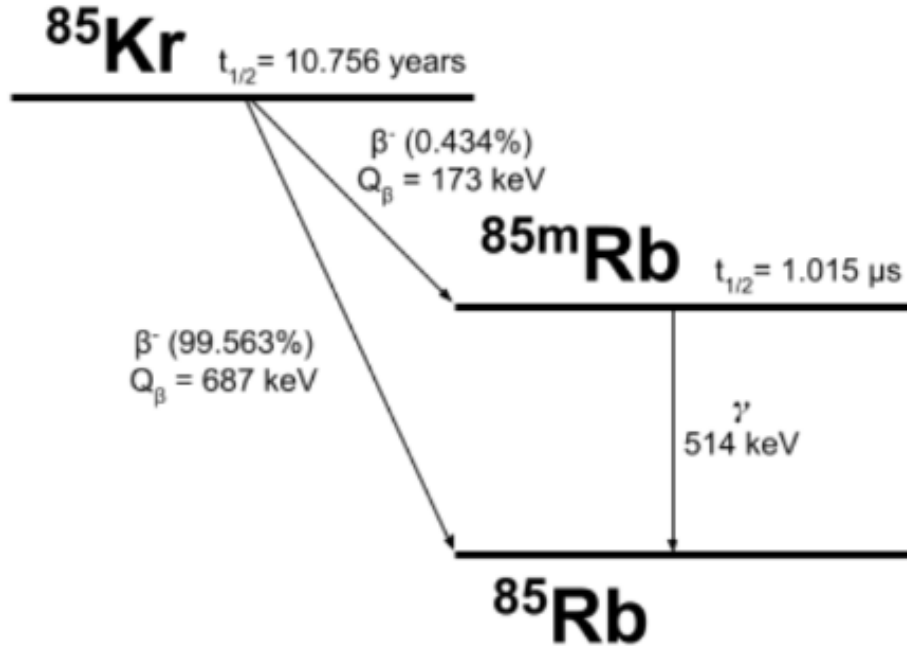


Figure 4.1: The decay scheme for ^{85}Kr is shown. The isotope has a half-life of 10.756 years and a Q-value of 687 keV. The β^- decay to ground state ^{85}Rb is the more common branch, with a branching fraction of 99.56%. This decay is problematic for the LZ WIMP search. The less common branching fraction follows a path through ^{85m}Rb . The decay begins with a 173 keV Q-value β^- decay to ^{85m}Rb . A 514 keV γ decay to ground state ^{85}Rb follows with a half-life of 1.015 μs .

any energy in the TPC produces exactly one S1 signal. The initial β also produces a single S1. If the β and γ are sufficiently separated in time and both deposit energy in the TPC, the ^{85}Kr excited state decay produces two S1s. A pair of S1 waveforms that are consistent with an excited state ^{85}Kr decay are shown in Fig. 4.2.

When the ^{85m}Rb decay occurs in close temporal proximity to the preceding β -decay, the two prompt scintillation signals may not be sufficiently separated for both to be distinguished. Studies show LZ's post-processing software, *LZAP* (LZ Analysis Package), is 100% efficient at resolving two S1s when they are separated by at least 300 ns. Due to the 1.015 μs half-life, only 81.47% of the excited state decays stay in the metastable state for more than 300 ns.

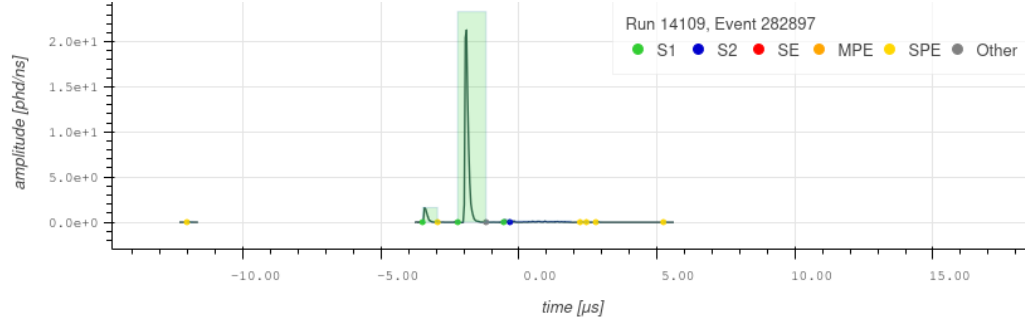


Figure 4.2: A pair of S1 waveforms from a candidate excited state decay are shown. The smaller S1 associated with β decay precedes a larger S1 associated with the γ . The S1s of excited state ^{85}Kr decays are separated by the $1.015\ \mu\text{s}$ half-life of ^{85m}Rb .

The ability to resolve the free charge signals from multiple interactions into individual S2s is limited. The γ may scatter multiple times and create an S2 at each location. The free charge from the β and any γ interactions may merge into a single S2. At least one S2 is expected from the full excited state decay, but multiple S2s are possible.

Section 4.1 gives an overview of the analysis applied to isolate excited state ^{85}Kr candidate events. The initial cuts applied to the data are discussed in section 4.2. Section 4.3 describes the protocol applied to events to correct their S1 areas, S2 areas, and energies. Section 4.4 explains the comparison between data and the simulation framework used to determine cuts and evaluate cut efficiencies in section 4.5. The exclusion cuts and live time calculation for the analysis is discussed in section 4.6. The results of the measurement shown and discussed thoroughly in section 4.7. The chapter concludes with a brief summary in section 4.8.

4.1 Overview

Several cuts are applied to select ^{85}Kr decays that proceed through ^{85m}Rb . The signature of the decay is the $1.015\ \mu\text{s}$ half-life ($1.464\ \mu\text{s}$ mean-life) of ^{85m}Rb that separates the two S1s. No other β -decaying isotopes in LZ are expected to have half-lives on this timescale.

The spatial distribution is expected to be uniform because Kr is thoroughly mixed in the LXe.

LZ detector simulations have been developed to model the detector's response to various backgrounds. The simulations are used to inform the cut boundaries and evaluate the efficiency. Both *fast* simulations and *full chain* simulations are used to evaluate different aspects of the cuts.

Both the fast and full simulations begin by feeding a particle decay generator, a detector geometry, and a conditions setup file to the LZ software package BACCARAT. BACCARAT generates a uniform random spatial particle distribution in the specified volume, then tracks the particle and its decay products using Geant4. Energy deposits from each interaction are recorded. Both flavors of simulation have their *truth* information output from BACCARAT. This truth information includes the initial location of the parent particle, the time at which all parent nuclei decay, the location of each interaction resulting from the β or γ , and how much energy was deposited from each interaction.

The fast simulation deposits are input in the LZLAMA (or simply LAMA) processing framework. LAMA converts the energy depositions into a detector response, including S1 and S2 light output and reconstructed position, then outputs the information in a data-like file. The truth energy depositions can be compared with the reconstructed S1, S2, and position outputs to evaluate the effect of the detector response. The framework is frequently updated to match detector response (in the WIMP search energy range). As its name suggests, it can generate and process many more events in a shorter time than the full simulation chain. The downside is that LAMA does not include individual PMT waveform outputs, is not well tuned to match response in the skin detector, and cannot model outer detector energy deposition or response.

The full simulations take the energy deposits from BACCARAT and convert them to prompt scintillation and free charge according to Noble Element Simulation Technique

(NEST) [66] models implemented in the BACCARAT software. Ray tracing is used to propagate individual photons until they are absorbed or strike a PMT. BACCARAT outputs the PMT photon hits for each PMT and Monte Carlo truth information regarding the energy depositions. The PMT hit information is sent to another LZ software package known as DER (Detector Electronics Response) to simulate PMT response to photons and convert the output to an LZ data-like root file. The DER output is then processed with the same LZAP software that is used to process LZ data.

The full simulation chain is more difficult to tune, not frequently updated, and takes much longer to run than the fast simulation. The full simulation does include individual PMT outputs, which are necessary to evaluate the efficiency of some cuts. The full simulation skin response may be more reliable than the fast simulation response and the full simulations have the outer detector implemented.

Some cuts are developed to exclude periods of low quality data and poor detector behavior during the WIMP search. These cuts may exclude periods of unexplained scintillation light emission or brief time windows following high energy events (like a muon). The exclusion cuts are not evaluated with simulations. Events lost to the exclusion cuts do not manifest themselves as efficiency losses, but as losses to live time.

The goal of the analysis is to convert the observed number of excited state decays to an equivalent concentration of natural Kr in the detector. This is done using Eq. 4.1 where $\Phi_{nat\ Kr}$ is the concentration of natural Kr in LZ, C is the observed number of ^{85}Kr excited state decay events, τ is the mean life of ^{85}Kr , $M_{^{85}\text{Kr}}$ is the mass of a single ^{85}Kr atom, t is the detector's live time, A_n is the natural abundance of ^{85}Kr , f_b is the branching fraction of the ^{85m}Rb excited state decay branch, M_{Xe} is the target Xe mass, $m_{nat\ Kr}$ and $m_{^{85}\text{Kr}}$ are the atomic masses (in AMU) of natural Kr and ^{85}Kr respectively, and ϵ is the cut efficiency.

$$\Phi_{nat_{Kr}}(g/g) = \frac{C * \tau_{85_{Kr}} * M_{85_{Kr}}}{t * A_n * f_b * M_{Xe}} \left(\frac{m_{nat_{Kr}}}{m_{85_{Kr}}} \right) \frac{1}{\epsilon} \quad (4.1)$$

4.1.1 Analysis outline

Processing LZ data with LZAP distills the data down to a number of *RQs* (reduced quantities) of interest. The ALPACA framework efficiently pulls the RQs from the processed files for each event in the specified time window. The main analysis steps are listed below. Steps that cut events are italicized. All events that reach step 11 are exported from the ALPACA framework, allowing later cuts to be evaluated in any order.

1. *Evaluate exclusion cuts (and their effect on live time)*
2. *Check for at least two S1s and one S2*
3. Sort S1 and S2 pulses by size
4. *Remove events failing selection criteria*
5. Identify the S1 from the β , the S1 from the γ , and the largest S2 pulse
6. *Apply S1 δ time (S1 time difference) cut*
7. *Apply fiducial cut*
8. Calculate weighted event position
9. Correct S1 and S2 pulse areas
10. Calculate localization
11. Output important RQs and RQs relevant for subsequent cuts
12. *Apply energy related cuts*
13. *Apply spatial localization related cuts*
14. *Apply cuts related to LZ veto detectors*

4.2 Initial Cuts

Setting aside the exclusion cuts (these are discussed in section 4.6), the first analysis cuts are the *selection criteria* cut, the *S1 δ time* cut, and the *fiducial* cut. These are referred to as the *initial cuts*, and unless otherwise specified, all events from all plots in this chapter pass these three cuts. All events discussed in section 4.4 are an exception.

4.2.1 Selection criteria cut

The selection criteria cut is comprised of several cuts related to the number, timing, and sizes of the S1 and S2 pulses in an event. Events must meet this criteria so certain quantities (like the time between S1s, for instance) can be calculated for the event. The selection criteria requires at least two S1s and one S2 to be present in the event window. This requirement is consistent with the physics of an excited state decay. Next, the S1 pulses and the S2 pulses are sorted by size. The largest S2 is identified.

The largest S1 in the event is expected to be associated with the γ and is labeled as the *S1G*. The S1G must occur before the largest S2. To reduce computing time, any S1G candidate with an area below 10 phd or above 10000 phd is immediately rejected. The S1 associated with the 514 keV γ is expected to be well within this range.

The final requirement for the S1G is that the top-bottom asymmetry (or TBA) is required to be negative. The TBA is a dimensionless quantity describing the relative amount of light detected in the top or bottom PMT array. TBA is described by Eq. 4.2 where A_{top} is the integrated quantity (or area) of light collected by the top PMT array and A_{bottom} is the area of light collected by the bottom PMT array.

$$TBA = \frac{A_{top} - A_{bottom}}{A_{top} + A_{bottom}} \quad (4.2)$$

Recalling discussion from section 2.2.1, S1 light is preferentially collected by the bottom PMT array. The TBA exhibits correlation with drift time: events lower in the detector have more light collected by the bottom PMT array. Nearly all S1s at energies near the γ energy have a negative TBA. Thus, the S1G TBA is restricted to be negative.

Events with a valid S1G are searched for a valid S1 associated with the β . The largest remaining S1 occurring before the S1G, with an area between 10 and 10000 phd and a top bottom asymmetry of less than 0.25, is considered to be the *S1B* candidate. No S1s associated with the β are expected to be above or near 10000 phd, while only a small amount may be below 10 phd. The spread in TBA is wider for lower energy S1s, so the TBA restriction for the S1B candidate is relaxed.

4.2.2 S1 δ time cut

The time between the S1B and S1G (also referred to as the S1 δ time or the S1 delay time) is the strongest identifier of the excited state ^{85}Kr decay. No other isotopes in the LZ detector are expected to exhibit a decay time on the order of single μs . ^{214}Po in the Rn decay chain has a half-life of 164 μs . A small fraction of these relatively common decays may occur on the μs timescale, however, the ^{214}Po α decay produces an S1 area that is too high to pass the selection criteria.

Accidental coincidences between two unrelated interactions in the same event window are expected to be the primary background for this measurement. An accidental coincidence between two interactions is expected to be uniform in S1 δ time. An excited state ^{85}Kr decay would almost never yield an S1 δ time greater than 10 μs . It may be sensible to restrict to only events with delay times less than 5 or 10 μs to minimize the number of accidental coincidences that breach a delay time cut window.

Instead, extending the maximum S1 δ time window well beyond the time when any

excited state ^{85}Kr decays are expected allows the accidental coincidence background events passing all cuts to be quantified at the end of the analysis. The exponential distribution of the excited state signal and the flat distribution of the coincidence background events can be fit together using Eq. 4.3. Integrating the A term across the entire decay time window gives the number of signal counts.

$$f(t) = A * e^{-t/\tau} + B \quad (4.3)$$

A value around $100 \mu\text{s}$ is chosen as the maximum allowed S1 δ time. This provides a wide window for background evaluation, while not extending far enough to invalidate corrections or other cut evaluations. The minimum of the delay time cut is chosen to guarantee any event passing the cut always has two well resolved S1s. As stated at the start of this chapter, the minimum time between two S1s that allows LZAP to resolve both with certainty is 300 ns . This sets the lower bound for the S1 δ time cut. Restricting the minimum delay time results in an efficiency loss ($0.8147 = \epsilon_{0.3\mu\text{s}}$). However, this choice avoids difficulties in evaluating LZAP's ability to resolve individual S1s with a smaller time separation. The maximum delay time is adjusted to $100.3 \mu\text{s}$ to simplify histogram binning.

4.2.3 Fiducial cut

A fiducial (spatial) cut is implemented in the LZ WIMP search to minimize the proportionally higher rate of backgrounds originating from the edges and outside of the TPC. The standard LZ fiducial volume cut consists of a combination of three different spatial cuts: one on the radial position component, one on the Z-position component, and one on the field cage resistors position (effectively two small cylindrical exclusion volumes near the edge of the TPC, infinite in Z). The radial portion of the fiducial cut is divided into 12

azimuthal slices with a slightly different 5th order polynomial (in drift time) dictating the boundary of each slice.

The term M_{Xe} in Eq. 4.1 is the chosen target Xe mass. For the LZ WIMP search, the chosen fiducial cut volume results in a 5.5 ± 0.2 T fiducial mass [67]. The evaluation of the volume and the mass is non-trivial because of local differences in electric field and difficulties reconstructing events near the walls. The volume and mass are studied, set, and evaluated for single scatter events. Redefining and reevaluating the fiducial mass would be a tedious task. There is clear benefit to reapplying the WIMP search fiducial volume to this search.

The exact position of an event with multiple S1s or multiple S2s is ambiguous. The drift time of a single scatter is the time between the S1 and the S2. This cannot be defined in a straightforward manner if multiple S1s are present. For example, in an excited state ^{85}Kr decay, the gamma may travel directly up, Compton scattering several times, while the beta travels downward. The S1B would be seen before the S1G but the S2 from the β would be seen after the (perhaps multiple) S2(s) from the γ . The X-Y position is entirely determined by the S2(s) and does not require pairing with an S1 with an S2, but defining the X-Y position in the presence of multiple S2s is similarly not straightforward.

The most direct way to evaluate an event's Z position is using the time between a single S1 and a single S2. Evaluating the efficiency of the fiducial cut using multiple S1s and S2s is challenging and would invalidate the prior evaluation of the fiducial mass. The simplest S1-S2 pairing in an excited state ^{85}Kr decay is the largest S1 (the S1G) and the largest S2. In a true excited state ^{85}Kr event, at least some fraction of the largest S2 is likely to be the result of a Compton scatter or photo-absorption from the γ . Therefore, the position used for the fiducial evaluation in this study is defined by the largest S1 and S2 and the chosen fiducial volume is the WIMP search fiducial volume. The WIMP search fiducial mass of 5.5 ± 0.2 T is used as the target Xe mass, M_{Xe} in Eq 4.1.

4.3 Position-Based Corrections to S1 and S2 in Multi-Site Events

Reviewing the extensive discussion in section 2.2, both scintillation light collection efficiency and free charge gain depend on position. The values of g_1 (phd/photon) and g_2 (phd/free electron) are defined for energy deposition at the center of the TPC. Depositions occurring elsewhere result in different values of photons detected per scintillation photon or free electron.

Spatial variation in the TPC response must be corrected. LZ uses calibration data to create a map of S1 and S2 corrections, based on the event's X position, Y position, and drift time. These corrections work well for a dark matter search because single scatters have a well defined position.

There is no established protocol for correcting the S1 and S2 areas for events with multiple S1s and S2s. As discussed in section 4.2.3, determining the position of an event with multiple S1s and at least one S2 is non-trivial. A choice could be made to forgo correcting the raw signals. However, correcting the raw S1 and S2 signals is expected to improve S1, S2, and energy resolution (note from Eq. 2.10, $E_c = (S1_c/g_1 + S2_c/g_2) * W_q$). Better resolution allows for the same efficiency with tighter energy cuts, and therefore, improved background reduction.

The single μ s scale decay time is convenient for correcting the raw signals. The window for ambiguity in drift time is only as large as the decay time of the ^{85m}Rb . Because this is small relative to the maximum drift time, even corrections associated with drift times chosen randomly between the S1B and S1G drift times are likely to improve energy resolution. The quantities of interest are the corrected S1G area, the corrected S1B area, the total corrected S2 area, and the corrected energy.

4.3.1 Multi-site corrections procedure

The corrections to the spatial variation in the TPC response are applied after the initial cuts. Limiting to events passing the fiducial cut minimizes the chance a poor correction is applied. Limiting to events with delay times that are 100 μ s at maximum restricts the window for ambiguity in the S1 time.

The correction protocol begins by determining the weighted position of each event. The expression for the (S2) weighted position is given in Eq. 4.4 where $\vec{x}_w$ is the weighted position of the event, $\vec{x}_i$ is the position (x, y, t) of the i th largest S2, and $A_{S2,i}$ is the area of the i th largest S2. Only the five largest S2s are considered in the weighted position calculation. The "Z" component is associated with the time of the S2s.

$$\vec{x}_w = \frac{\sum_{i=1}^{n, n \leq 5} \vec{x}_i * A_{S2,i}}{\sum_{i=1}^{n, n \leq 5} A_{S2,i}} \quad (4.4)$$

Each individual S1 and S2 pulse uses a slightly different position (x, y, and drift) to evaluate its correction factor. The weighted X and Y positions, defined by Eq. 4.4, are used as inputs for both S1 area corrections. The S1G time and S1B time are subtracted from the weighted S2 time to determine the respective drift times of the S1G and S1B. These two drift times and the weighted X and Y positions are used to evaluate the corrections to the S1G and S1B areas.

The positions used to evaluate the S2 corrections are different than the positions used for the S1 corrections. The X and Y positions of individual S2s are well defined and used as the X and Y position input for each S2's correction. The drift time coordinate used for S2 corrections is the difference between the weighted S2 time and the S1G time. This is the same for all S2s. The same drift time is chosen for all S2s to limit calling corrections factors with unphysical drift times. The individual corrected S2 areas in an event are summed to

give the total corrected S2 area.

4.3.2 Results from multi-site corrections

The corrections procedure is applied to fast simulation excited state ^{85}Kr decays that are uniformly distributed in the TPC. The simulated events are required to pass the initial cuts before being corrected. Corrections to the S1B are not shown here, as the S1B is a β -like spectrum with no clear figure of merit for evaluating the benefit of the corrections. The root mean squared (RMS) deviation from the mean is used to quantify the resolution improvement for S1G area, total S2 area, and energy. Corrections to the S1G area are shown in Fig. 4.3.

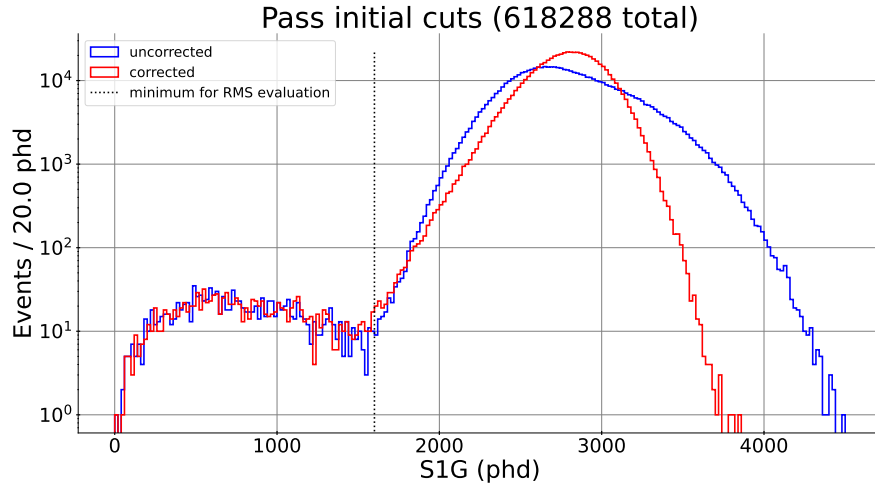


Figure 4.3: Histograms of the S1G area of ^{85}Kr excited state decay events simulated with the fast simulation framework are shown before (blue) and after (red) position corrections are applied. The corrections are intended to counteract the positional variation in scintillation light collection for these events. The S1G is produced by the mono-energetic γ , but is subject to a number of significant smearing effects including recombination and the double photo-electron effect. Only events with S1G areas exceeding the dashed line labeled "minimum for RMS evaluation," are considered in the RMS calculation. The corrected spectrum's improved resolution indicates that the positional corrections are effective.

The corrected S1G distribution has a higher peak event rate. Considering only events

above 1600 phd, the RMS deviation of the uncorrected S1G distribution is 363 phd, and the RMS deviation of the corrected distribution is 235 phd. Some degree of spread is expected to remain after the corrections due to recombination fluctuations. The large improvement in the RMS shows that the S1 corrections improve resolution.

Corrections to the total S2 are shown in Fig. 4.4.

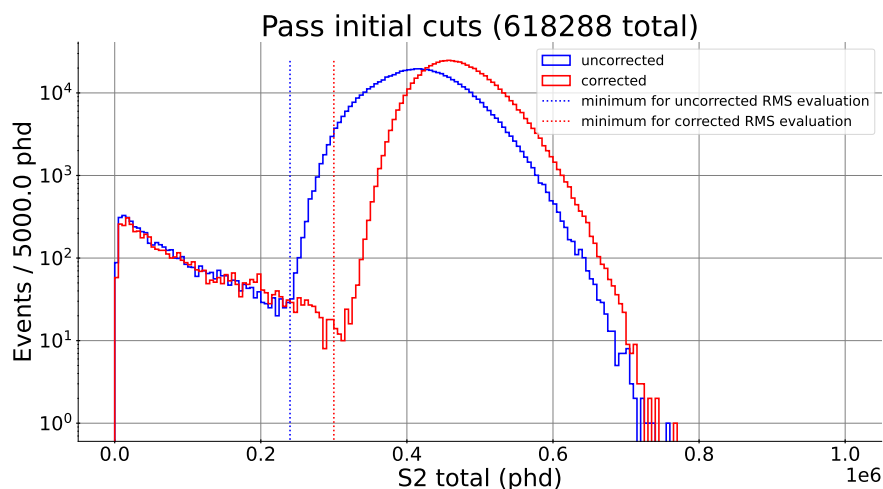


Figure 4.4: Histograms of the S2 total area of ^{85}Kr excited state decay events simulated with the fast simulation framework are shown before (blue) and after (red) position corrections are applied. The total S2 area is not expected to be produced from a mono-energetic source and is also expected to be subject to smearing effects. Events with a β or γ that is not fully contained populate the tail on the left side of the plot. The minimum total S2 used in each RMS calculation is shown by a dotted line with a color corresponding to the color of the respective histograms.

The corrections generally increase the total S2. The RMS deviations are calculated using a different minimum for the uncorrected and corrected spectra. The minimum is changed to selectively remove the low S2 tails of the distribution. These tails are the result of events that are only partially contained in the TPC's active volume. The RMS deviation from uncorrected events exceeding 240000 phd is 62500 phd, and the RMS deviation from corrected events exceeding 300000 phd is 50900 phd. Including all events above 240000 phd in the corrected spectrum only increases the RMS deviation to 51000 phd. The

corrections improve the S2 resolution.

Fig. 4.5 shows the uncorrected and corrected total energy calculated using either uncorrected or corrected S1B, S1G, and total S2.

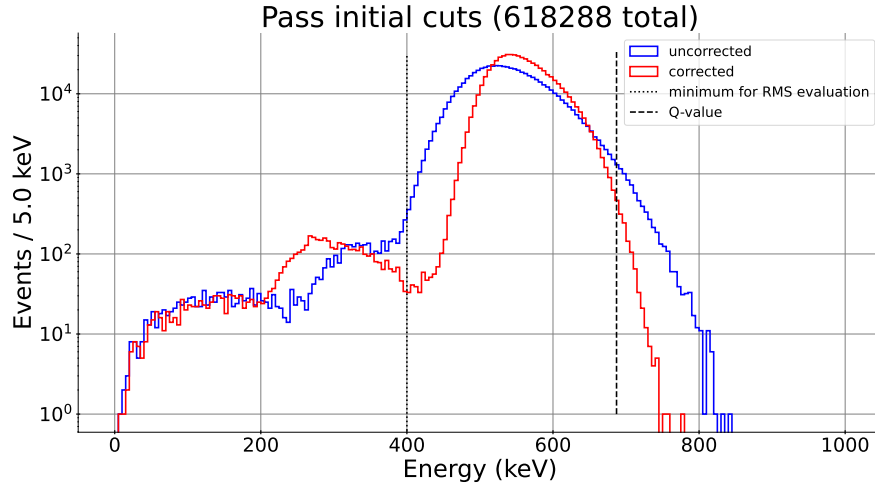


Figure 4.5: Histograms of the total energy of ^{85}Kr excited state decay events simulated with the fast simulation framework are shown before (blue) and after (red) position corrections are applied. The decay Q-value is also indicated by a dashed black line on the plot. As with the S2s, the true energy distribution is not mono-energetic. The energy spectrum of fully contained events should resemble a β spectrum that begins at the γ energy of 514 keV. The total energy is not subject to the same recombination fluctuations that effect the S1s and S2s. The corrected spectrum rises more quickly near the γ energy, and fewer corrected events are seen extending past the Q-value. Only events with energies exceeding the dotted black line (400 keV) are included in the RMS calculation.

The dashed black line shows the Q-value of the decay (687 keV) and the dotted black line shows the minimum event energy used to evaluate the RMS of the energy spectra (400 keV). The low energy portion of the plot primarily includes events where either the β or γ has escaped the detector. There should be a sharp rise at the γ energy (514 keV). The (fully contained) spectrum should appear similar to a 173 keV β spectrum that has been shifted up by the 514 keV γ energy. The corrected energy spectrum better resembles the expected energy distribution. A small number of events have energies exceeding the decay Q-value. The RMS deviation of the uncorrected energy histogram is 57 keV, and the RMS deviation

of the corrected energy histogram is 41 keV.

The RMS deviation of the S1G, total S2, and energy are all improved by the corrections. All further mention of energy, S1 area, or S2 area refers to the corrected values of these quantities unless otherwise specified.

4.4 Simulation-Data Comparison

Simulated data must be validated and compared with real data to ensure its accuracy before cut efficiencies can be evaluated. The goal of this comparison is to understand how the cut values or cut efficiencies may change between simulated and real data. The variables most likely to exhibit simulation inaccuracy are the S1B, S1G, total S2, and energy. The mismatch between simulated and real data must be quantified.

S1 and S2 spectra associated with the continuous β energy spectrum are quite difficult to compare. While the β spectra are easily simulated, identifying a clean selection of S1s and S2s associated with a β source of similar energy in LZ data would be quite difficult. The ^{85}Kr β Q-value is 173 keV. The flat β calibration source used in LZ that is closest in energy is ^{14}C (156 keV Q-value). However, even during the highest activity calibration periods, it is very difficult to confidently assert that a specific event is the result of a ^{14}C decay. Changes in the S1B area cut efficiency are most acute in the lower energy portions of the spectra. The S1B area is assumed to differ from the simulated spectrum by no more than 10%. In most cases, the β contribution to the total S2 is small, so any variation between the real and simulated S2 from the β is considered subdominant.

The mono-energetic γ lines are more easy to identify and compare. An LZ ^{22}Na calibration yields two clean energy lines: one at 511 keV and one at 1275 keV. The 511 keV γ is from electron-positron annihilation following positron emission. The 1275 keV γ is emitted immediately (on the order of picoseconds) after. Three other γ lines from real (not

calibration) data are identified: a 609 keV γ from ^{214}Bi , a 1461 keV γ from ^{40}K , and a 1764 keV γ from ^{214}Bi . The S1 and S2 response to these γ lines are compared in data and simulations.

Unlike the ^{85}Kr excited state analysis, only events with a single S1 are considered for this study. Events with multiple S2s are included. The reconstructed energy is fit to Gaussian, and the S1 and S2 distributions of all events within two σ of the energy centroid are characterized.

The event S1 and S2s are corrected using a procedure that is as similar as possible to the correction procedure for the ^{85}Kr excited state analysis. *Default* corrections are made by LZAP for events with a single S1. The default corrections are likely more accurate because they leave no ambiguity regarding the drift time of an event. The procedure for the ^{85}Kr analysis corrections was validated by comparing with the default corrections for all γ lines. No large deviation was observed between the corrections.

4.4.1 ^{22}Na γ line identification and selection

^{22}Na is placed in the LZ Calibration Source Deployment (CSD) tubes during a calibration. The tubes run vertically at three different X-Y positions in the outer cryostat vessel, centered about 12 cm radially beyond the inner cryostat vessel. Sources are inserted from above and lowered to a chosen Z position.

^{22}Na emits positrons which annihilate and emit back to back γ s. Only one γ can deposit its full energy in the TPC. A 1275 keV γ is emitted in a random direction, effectively coincident to the 511 keV γ s. The probability of two or more of the three emitted γ s entering the TPC is low. However, the the probability of a single γ depositing energy in the TPC while another γ deposits energy in the outer detector is significant. Restricting to events with outer detector energy deposits yields a cleaner ^{22}Na spectrum.

Only calibration data taken when the source's Z-position was between the cathode and the gate grids was analyzed. All calibration data that meets this criteria happens to be from the same X-Y position (same tube, *CSD 2*). The energy spectrum of events from this time period (with no outer detector restriction) is shown in Fig. 4.6 and the spatial positions of the events are shown in Fig. 4.7.

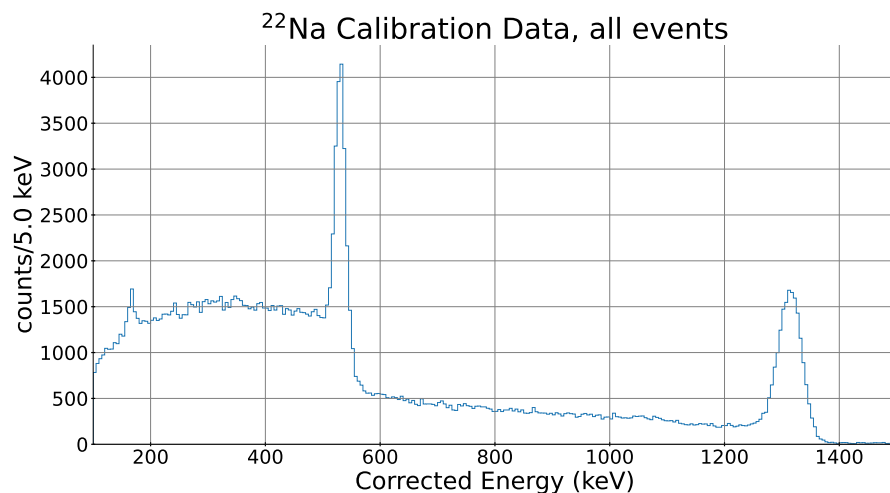


Figure 4.6: An energy histogram of all events with a single S1 and at least one S2 from the ^{22}Na calibration periods in May and June of 2023 is shown. No additional cuts have been applied to this data. Two very clear peaks are noted: one from the 1275 keV γ and one from an annihilation peak at 511 keV. These are both the product of the ^{22}Na decay.

Background can be trimmed to yield a cleaner energy spectrum. Requiring the outer detector energy deposition and restricting to events between 18 cm and 32.5 cm (R^3) from the source position reduces background. Events with energy deposits in the skin detector are likely from skin Compton scatters and imply the full γ energy is not deposited in the TPC. These events are undesirable and are removed. Events failing the Z and field cage resistor components of the fiducial volume cut are removed, but events failing the radial component of the fiducial volume are kept to avoid excessive loss of statistics. Any potential degradation of correction factor quality that results from including events outside the radial portion of the fiducial volume is expected in both simulation and data. This should

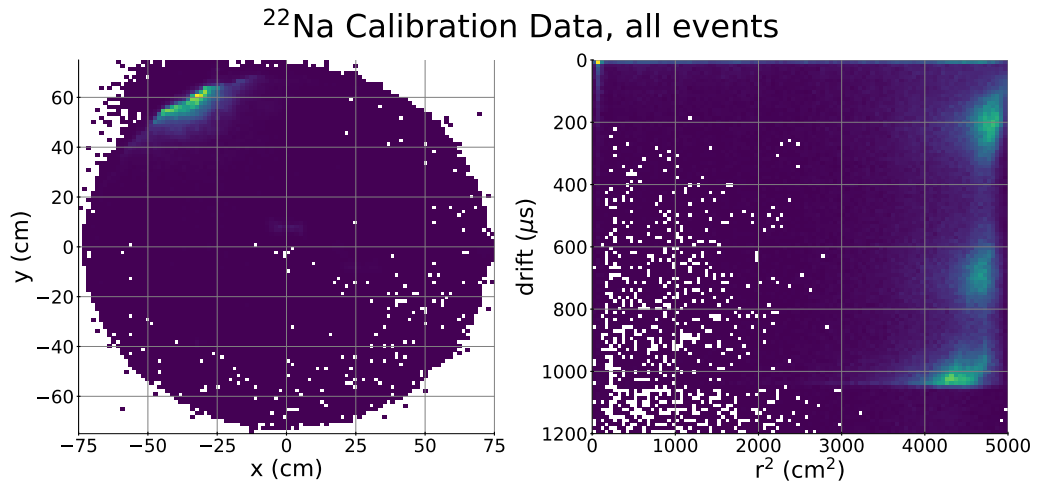


Figure 4.7: The positions of events from the ^{22}Na calibration periods in May and June of 2023 are shown. These events correspond to those shown in the energy spectrum in Fig. 4.6. The left plot shows the X-Y position of events while the right plot shows the r^2 and drift times (Z position) of the events. Note that events with shorter drift times are closer to the top of the detector. The drift time axis has been inverted to reflect this. The position of the azimuthal angle of the CSD tube housing the ^{22}Na source is clear from the high activity region seen in the X-Y plot. The several source heights can be noted in the r^2 -drift plot. Events reconstructed below 1090 μs in drift time or outside of the radius of 73 cm have been reconstructed outside the TPC volume.

not have a large impact on the analysis.

The energy spectrum and spatial positions of events remaining after the cuts discussed above (and limited to energy ranges around the two γ energies) are shown in Fig. 4.8 and Fig. 4.9.

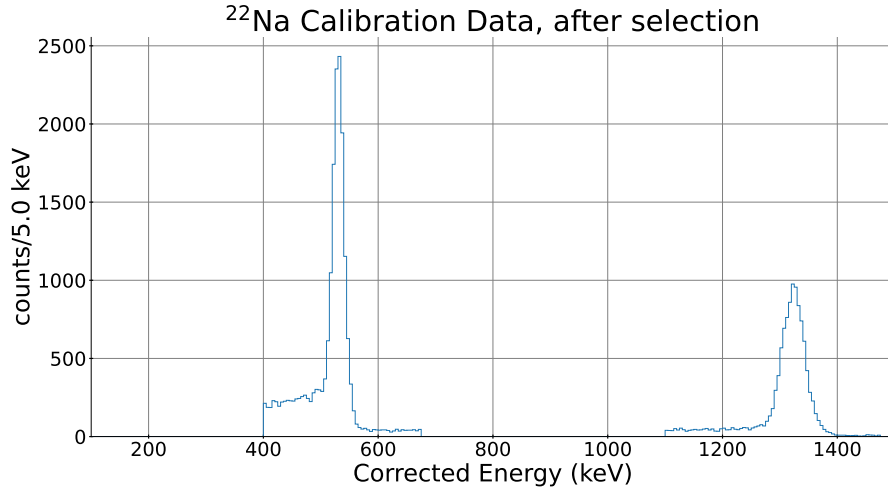


Figure 4.8: An energy histogram of events from the ^{22}Na calibration periods after applying several cuts to remove background is shown. The γ lines of interest are the 511 keV and 1275 keV lines from the ^{22}Na decay is shown. Events reconstructed outside of the Z component of the fiducial volume or in the field cage resistor area are removed. Events with significant skin energy depositions are removed to minimize that events that Compton scatter before reaching the TPC. Only events with energy in the outer detector are kept. The event's largest S2 must be reconstructed between 18 and 32.5 cm (in R^3) from the source location. Finally, events outside of the energy range of interest are excluded. These cuts remove a significant amount of background and isolate the two γ lines.

Outer detector information is not present in the (fast) simulations used for the γ comparison. All events in the simulation are ^{22}Na decays, so an outer detector signal is not necessary to better select ^{22}Na decays. Events with energy depositions in the skin are rejected and the field cage resistor and fiducial Z cuts are applied.

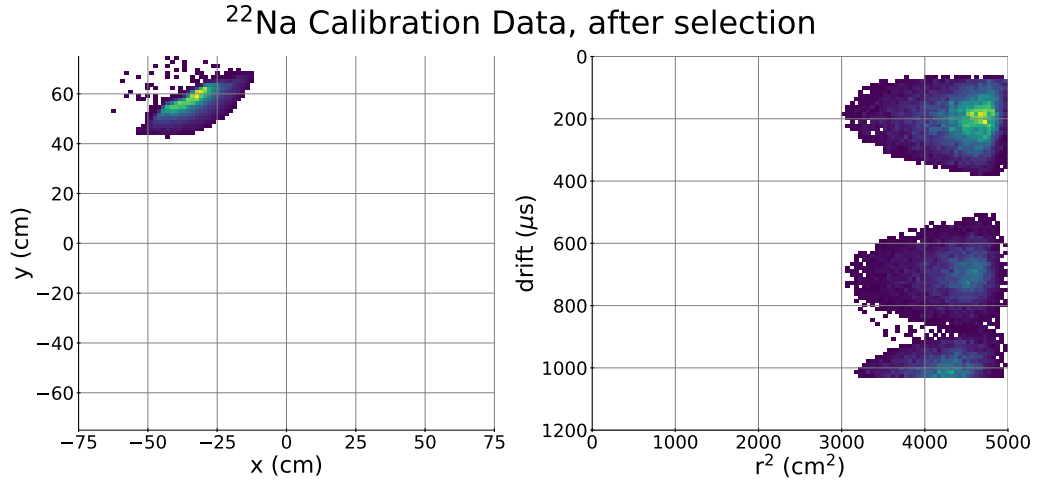


Figure 4.9: The positions of events from the energy histogram in Fig. 4.8 are shown. The left plot again indicates the X-Y position of the events and the right plot indicates the r^2 and drift time positions of the events. A very clear population in X-Y is seen near the CSD position. No events are expected elsewhere due to the source location cut. The event Z positions clearly indicate the various (discrete) source heights.

4.4.2 Other γ line identification and selection

Other gamma lines are prominent enough to be identified in the WIMP search data. The ten days of WIMP search data from June 8, 2023 to June 17, 2023 are used for this analysis. Only events passing the skin cut (implying no energy was deposited in the skin) and all three components of the fiducial cut are selected.

^{214}Bi is a Rn daughter dispersed in the LXe. The majority of ^{214}Bi decays occur within an hour of their Rn parent. Like ^{222}Rn , fewer ^{214}Bi decays happen near the center of the detector when the LXe is in an *isolated*, or low convection, state. The 609 keV ^{214}Bi γ is often accompanied by other (higher energy) γ s, so the selection is limited to events with energy depositions in the outer detector. The 1764 keV γ from ^{214}Bi is also accompanied by other γ s, but those are lower energy and less frequently reach the outer detector. Events in the 1764 keV selection are required to not have significant energy deposits in the outer detector.

^{40}K is found in detector materials. ^{40}K has a half-life on the order of 10^9 years. The majority of ^{40}K events occur near the edges of the detector. ^{40}K can emit positrons, but often emits a 1461 keV γ . This γ is only accompanied by low energy X-rays which cannot consistently reach the fiducial volume. Events with significant energy deposition in the outer detector are rejected.

The ^{214}Bi simulated events are drawn from *late chain* ^{238}U simulations. The parent isotopes are chosen to originate in the TPC walls. Events with deposited energy in the skin are not rejected for the 609 keV γ selection because of loss of statistics. Only the fiducial volume cut is applied to the 609 keV simulations. The 1764 keV γ from simulated ^{214}Bi and the 1461 keV γ from simulated ^{40}K are both identified with the respective cuts applied to select these in data (with the exception of the outer detector). The data energy spectrum after cuts and restricting to energy regions of interest is shown in Fig 4.10.

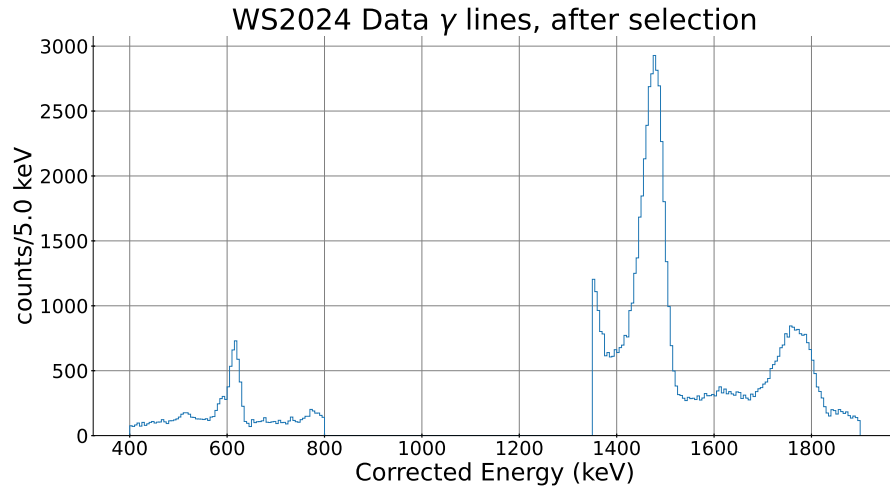


Figure 4.10: An energy histogram of single S1 events with at least one S2 from June 8, 2023 to June 17, 2023 from the LZ WS2024 period is shown. The peaks of interest are the 609 keV ^{214}Bi γ , the 1461 keV ^{40}K γ , and the 1764 keV ^{214}Bi γ . The data selection is restricted to energy regions of interest. Events failing any component of the fiducial cut are rejected. Events in the region below 800 keV are required to deposit energy in the outer detector but not the skin. Events above 1300 keV are required to deposit energy in the skin but not the outer detector. There is fractionally more background in this spectrum than in the ^{22}Na calibration spectrum.

4.4.3 Data-simulation comparison: corrected energy

The data and simulation energy spectra of the five γ lines are compared. The distribution of corrected energy for the 511 keV γ is shown in Fig. 4.11.

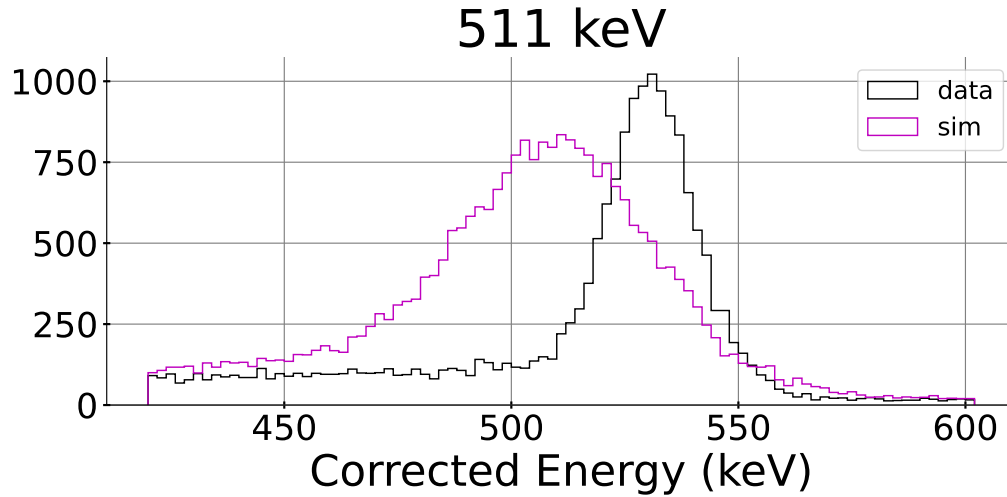


Figure 4.11: Histograms of the data (black) and simulation (magenta) corrected energy spectra for the 511 keV γ produced the decay of ^{22}Na are shown. The simulation spectrum is clearly much wider and lower in energy than the data spectrum.

The data spectrum exhibits better energy resolution and a higher mean. The other γ energy histograms are shown in Fig. 4.12. The simulation appears to consistently overestimate the peak width.

The data spectra have features that complicate their shapes. Different strategies are used to remove some of these undesirable features when fitting. Each spectrum is fit to the sum of a Gaussian and (in almost all cases) another function, intended to capture the asymptotic behavior of the distribution far from the Gaussian center. A maximum likelihood fit is performed. Fits to the 511 keV γ lines are shown in Fig. 4.13 and Fig. 4.14.

The function used to characterize the asymptotic portion of both 511 keV energy fits is a sigmoid. The functional form is given by Eq. 4.5.

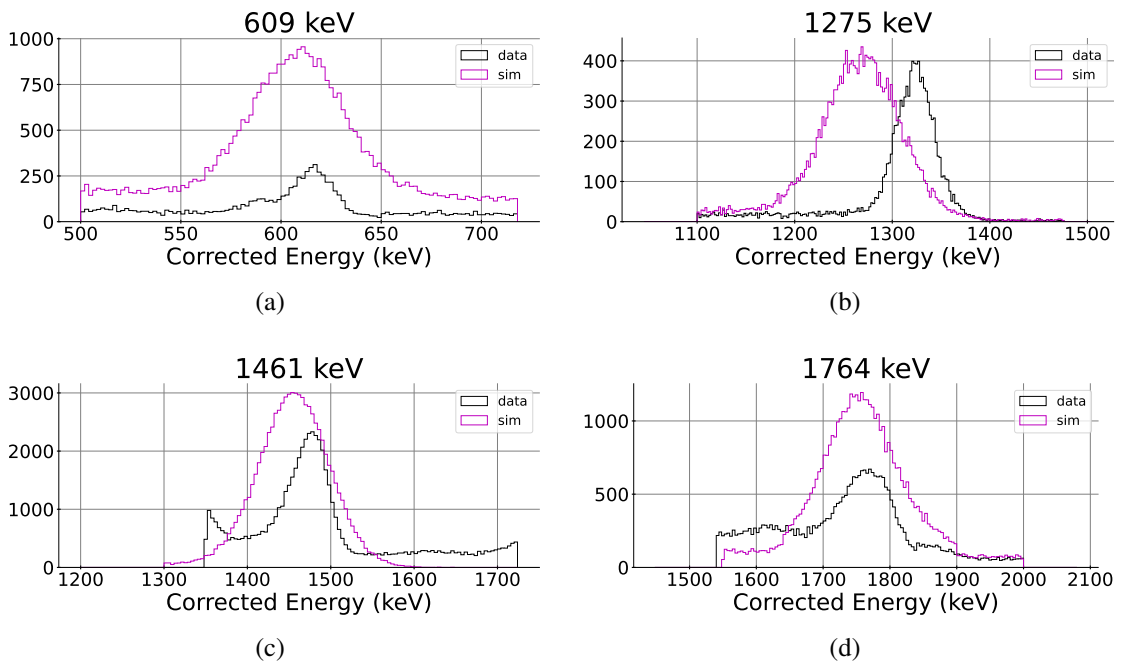


Figure 4.12: Histograms of the data (black) and simulation (magenta) reconstructed corrected energy spectra for the 609 keV (top left), 1275 keV (top right), 1461 keV (bottom left), and 1764 keV (bottom right) γ lines are shown. The peak of all data spectra is higher in energy than the peak of the simulation spectra. The 609 keV data spectrum has fewer statistics than most other displayed spectra.

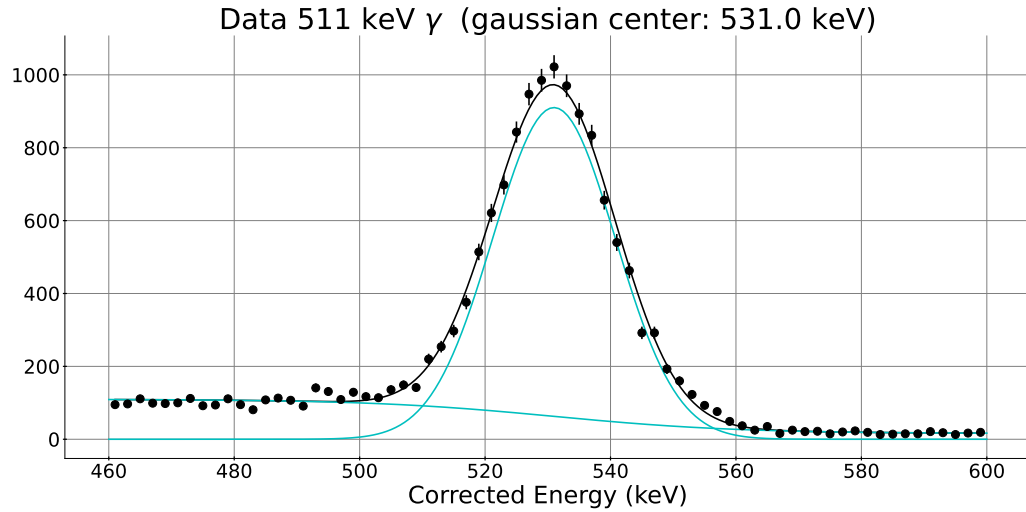


Figure 4.13: A fit to the corrected energy spectrum of ^{22}Na calibration data in the energy range near the 511 keV γ is shown. The Gaussian centroid is 531.0 keV, and the Gaussian width is 9.8 keV. The cyan lines show the individual Gaussian and sigmoid contributions to the fit, and the black line shows the sum of the two components.

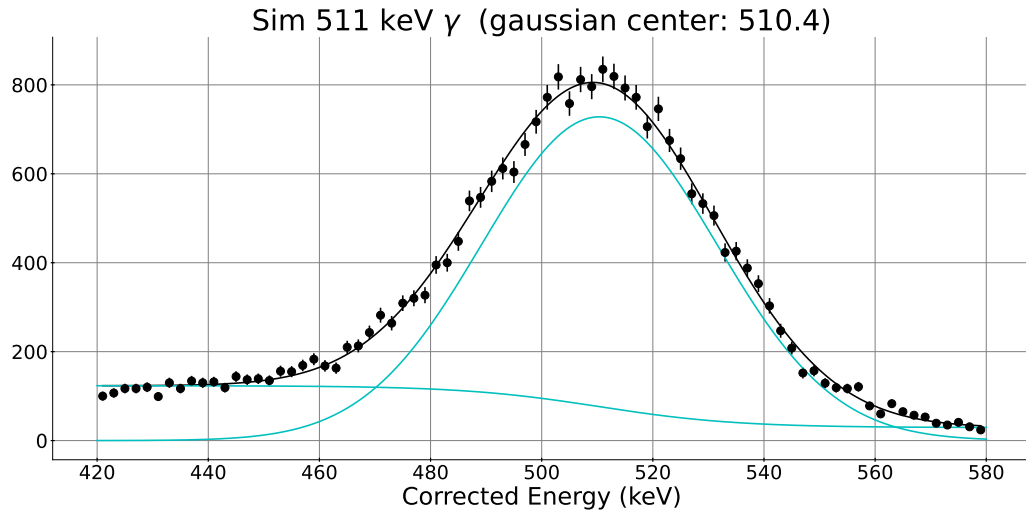


Figure 4.14: A fit to the corrected energy spectrum of ^{22}Na simulations in the energy range near the 511 keV γ is shown. The centroid of the Gaussian is 510.4 keV, and the Gaussian width is 21.2 keV. The cyan lines show the individual Gaussian and sigmoid contributions to the fit, and the black line shows the sum of the two components.

$$f(x) = p_0 / (1 + e^{p_1(x-p_2)}) + p_3 \quad (4.5)$$

The sigmoid center is fixed to the Gaussian center to minimize degeneracy between the two parameters. The contributions of the Gaussian and the sigmoid are shown in the plot. Sigmoids or constants are used as the additional fitting function for all energy fits, with the exception of the data fit to the 609 keV γ . A second Gaussian is used to account for a second peak between 575 and 600 keV. That fit and fits to the data and simulation energy spectra for the remaining gamma lines are shown in section A.1 from Fig. A.1 to Fig. A.8.

All fitted data and simulation Gaussian centroids and widths are summarized by Fig. 4.15. The one and two σ limits around the Gaussian centroids are indicated by the dashed and dotted lines, with the shading indicating regions inside these widths. With the exception of the 1275 keV γ line, the two σ limits of all data energy fits are within the two σ limits of the corresponding simulation fits. This observation confirms that the simulation underestimates the TPC's energy resolution.

4.4.4 Data-simulation comparison: corrected S1 and corrected S2

All events within $\pm 2\sigma$ of each energy peak are used to study the corrected S1 and S2 distributions. Recall that the purpose of the comparison is to understand how the cut values and cut efficiencies may be affected when transitioning from simulation to data. The cut values are intentionally wide to maintain high efficiency for the ^{85}Kr excited state decay. Because of this, disagreement between the simulation and data affects the efficiency most at the *edges* of the distributions. Understanding how the S1 and S2 spectra differ between simulation and data at their edges is more critical than understanding how they shift at their centers.

The edges of S1 and S2 spectra are characterized in two ways. One involves fitting a

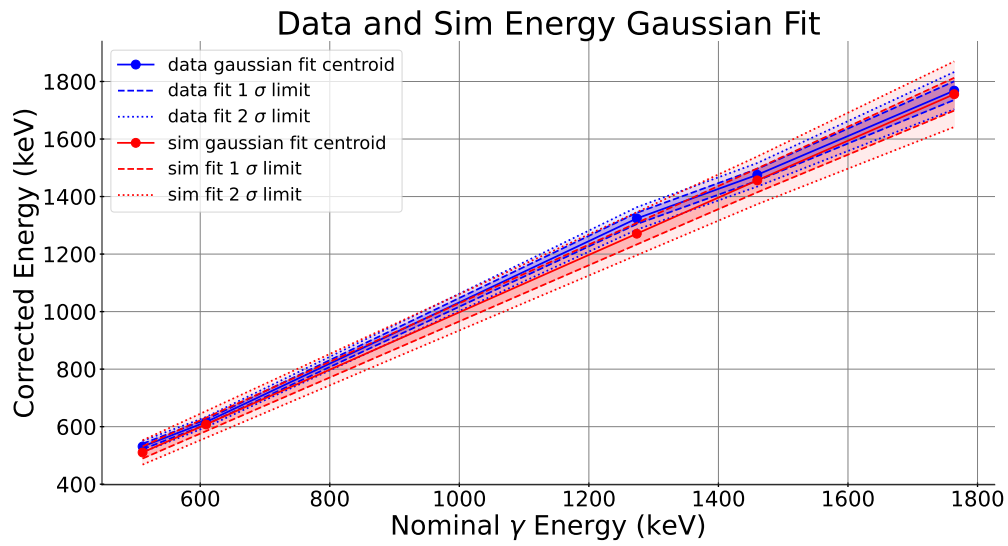


Figure 4.15: The fitted Gaussian centroid and width parameters for the simulation (red) and data (blue) energy spectra for the five γ lines are plotted by their nominal γ energy. The 1 σ and 2 σ bands of the Gaussians are indicated by dotted and dashed lines and shaded in their corresponding color. The simulation 2 σ bands frequently encompass the entire data 2 σ bands, even when their centroids differ significantly. The simulation is underestimating the energy resolution.

Gaussian to the corrected S1 and S2 distributions of events from the $\pm 2\sigma$ energy slice. The gaussian centroid and width of the fit to the S1 and S2 spectra from simulation and data are compared.

The other characterization method simply determines the values of chosen percentiles of the corrected S1 and S2 distributions from the $\pm 2\sigma$ energy slice events. To parallel the Gaussian fits, the 2.5 (-2σ), 16 (-1σ), median (centroid), 84 ($+1\sigma$), and 97.5 ($+2\sigma$) percentiles are assessed for the simulation and data spectra of each γ line. The percentile evaluations are meant to complement the Gaussian fits by accounting for deviation from the normal distribution in the S1 and S2 spectra.

Before characterizing the S1 and S2 distributions individually, the distributions are observed together. The S1 and S2 event distributions in the $\pm 2\sigma$ energy range of both simulation and data for ^{22}Na , ^{40}K , and ^{214}Bi are shown in Fig. 4.16, Fig. 4.17, and Fig. 4.18 respectively.

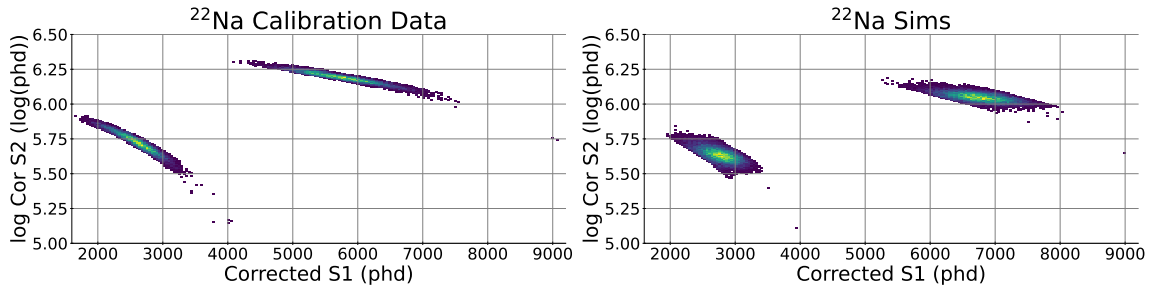


Figure 4.16: The distributions of (log10 of) corrected total S2 and corrected S1 for events within each $\pm 2\sigma$ energy slice of the two (511 and 1275 keV) ^{22}Na γ peaks are shown. Data is shown on the left plot and simulation is shown on the right plot. Slices of constant energy arc from the top left to the bottom right of the plot, along the length of the distributions. Energy increases as the arcs move closer to the top right corner of the plot. The simulation distributions are wider because the 2σ energy bands used to isolate these populations are considerably wider. Each population on each plot is normalized to itself: the color scale for one γ line is not comparable to another.

Lines of constant energy curve out arcs from the top left to the bottom right of each

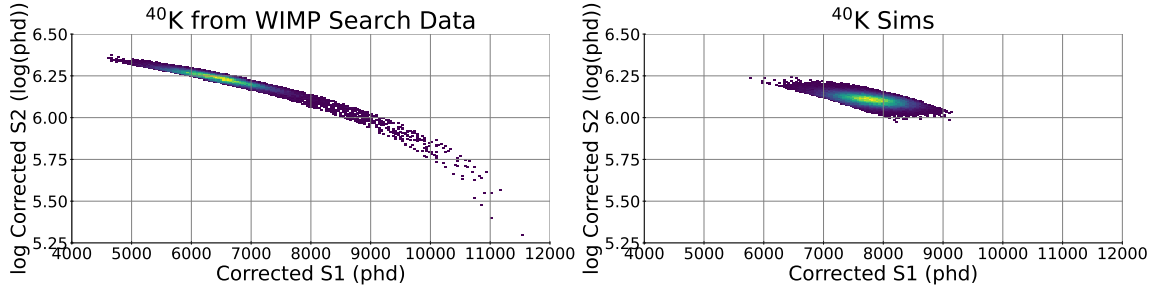


Figure 4.17: The distributions of (log10 of) corrected total S2 and corrected S1 for events within each $\pm 2\sigma$ energy slice of the 1461 keV ^{40}K γ peak are shown. The real data has a surprisingly long high S1-low S2 tail. This is not observed in the simulation plot.

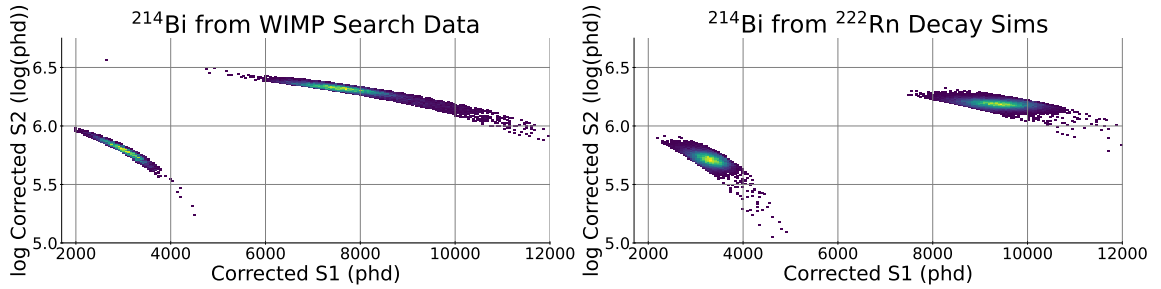


Figure 4.18: The distributions of (log10 of) corrected total S2 and corrected S1 for events within each $\pm 2\sigma$ energy slice of the two (609 and 1764 keV) ^{214}Bi γ peaks are shown. The population associated with the data 1764 keV γ exhibits a very long high S1-low S2 tail, much like the data 1461 keV γ .

plot¹. Despite a larger simulation energy width, the S1 and S2 distributions appear wider in real data. The higher energy γ s in data have a long high S1-low S2 tail.

Corrected S1

The data and simulation distributions of the corrected S1 area of events in the $\pm 2\sigma$ energy slice for the 511 keV γ are shown in Fig. 4.19.

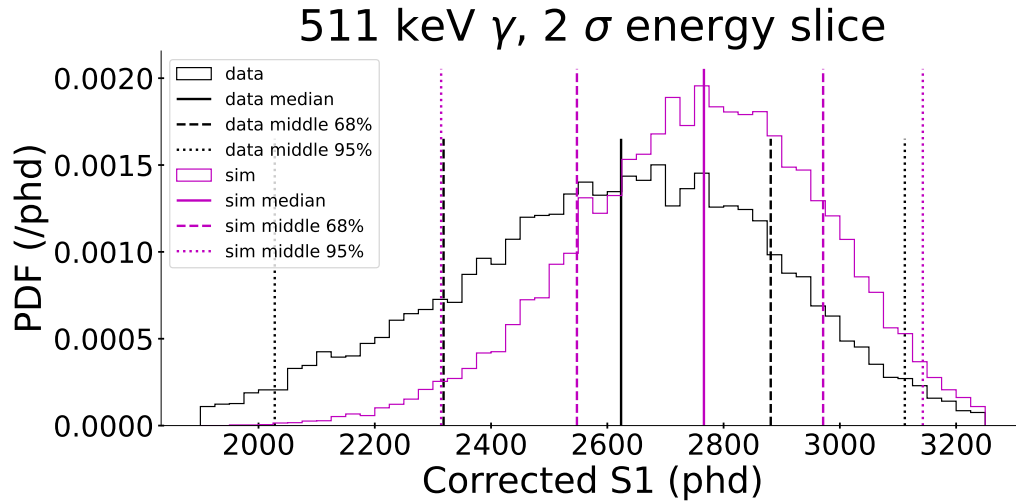


Figure 4.19: Histograms of the corrected S1 of events within the $\pm 2\sigma$ energy slice of the 511 keV γ for the data (black) and simulation (magenta) are shown. The median (solid line), middle 68% (dashed lines), and middle 95% (dotted lines) of each distribution are indicated on the plot. Only the central 99% of the distribution is plotted. The y-axis label indicates the normalization. Data and simulation show stronger disagreement at lower S1 percentiles.

The 97.5 percentile of the corrected S1 distribution shows little change between simulation and data. However, the 2.5 percentile shows significant deviation from simulation to data. The lowest percentiles differ by more than 10%. The remaining γ line S1 histograms are shown in Fig. 4.20. The percentile values of all γ lines are plotted against the nominal γ energy in Fig. 4.21.

¹These arcs would be straight lines on a linear plot.

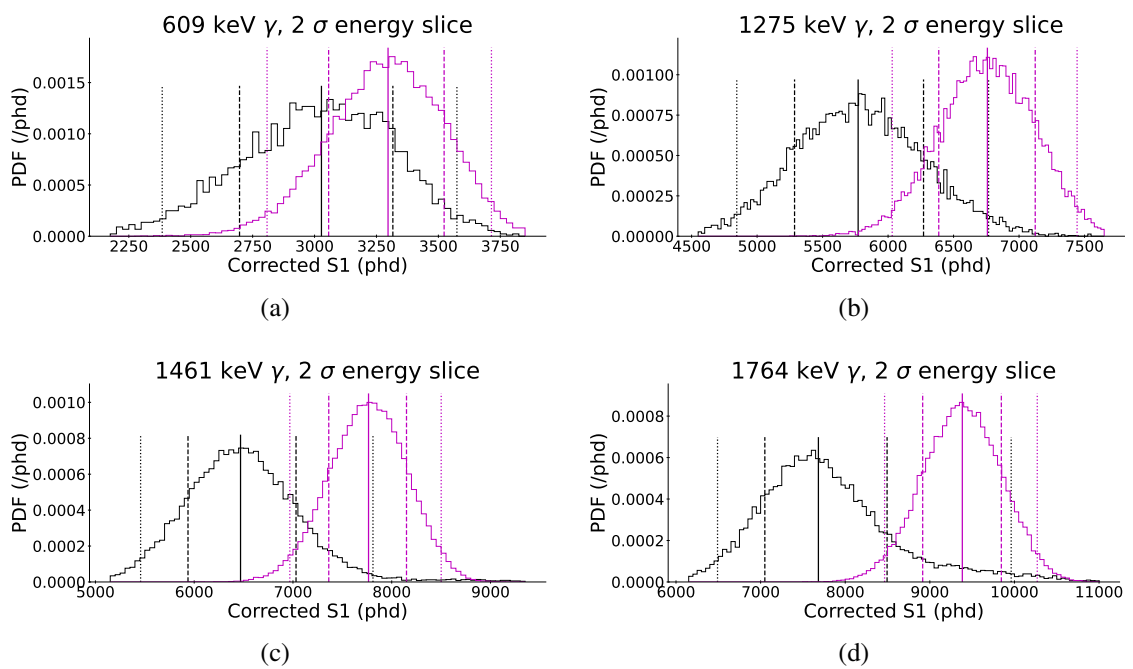


Figure 4.20: Histograms of the corrected S1 of events within the $\pm 2\sigma$ energy slice of the remaining γ s for the data (black) and simulation (magenta) are shown. Each subplot represents a different γ line with the nominal γ energy given in the title. The plots follow the same conventions as Fig. 4.19.

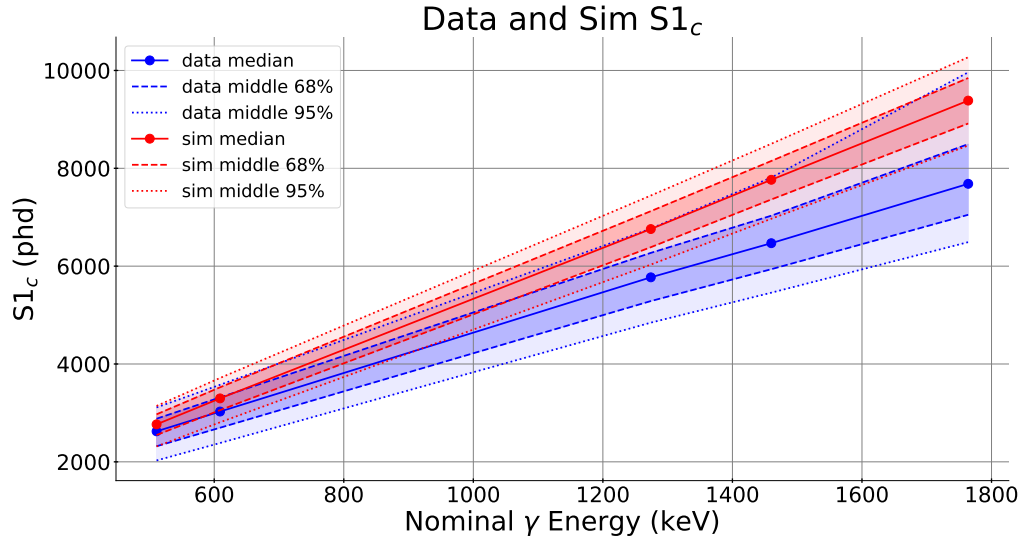


Figure 4.21: A plot summarizing the corrected S1 percentile values in simulation (red) and data (blue) for each γ line is shown. The medians are indicated by filled circles and joined by a solid line. The central 68% of the distribution is denoted by dashed lines, and the central 95% is given by the dotted lines and shaded in the corresponding color.

All percentile values in the data are lower in S1 than their corresponding simulation percentile values. The width of the simulation distribution appears underestimated at all γ energies.

Gaussians are fit to the corrected S1 data and simulation spectra for the 511 keV γ in Fig. 4.22. A maximum likelihood fit is used. Other S1 γ line fits are shown in section A.1 from Fig. A.9 to Fig. A.16. No additional fitting functions are needed to deal with asymptotic behavior. However, certain fit ranges are restricted to handle the non-Gaussian shape of the high S1-low S2 tails in the 1461 and 1764 keV γ s in data. A plot summarizing the S1 fit Gaussian centroids and widths is shown in Fig. 4.23.

The plot is unsurprisingly similar to Fig. 4.21. The simulation S1 means are overestimated, and the simulation S1 widths are underestimated.

The effect of the high S1-low S2 tail, which causes the 97.5 percentile of the 1764 keV γ in data to diverge from the rest of the distribution in Fig. 4.21 is not present in Fig. 4.23.

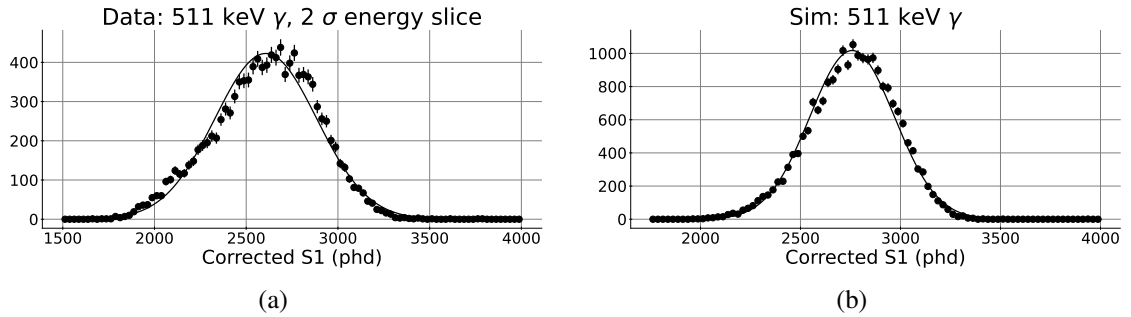


Figure 4.22: Gaussian fits to the corrected S1 distributions of both data (a) and simulation (b) for events in the $\pm 2\sigma$ energy slice associated with the 511 keV γ are shown. No additional fitting functions are needed to address the asymptotic behavior of these distributions. The fitted data centroid and width are 2607 and 277 phd. The fitted simulation centroid and width are 2758 and 212 phd.

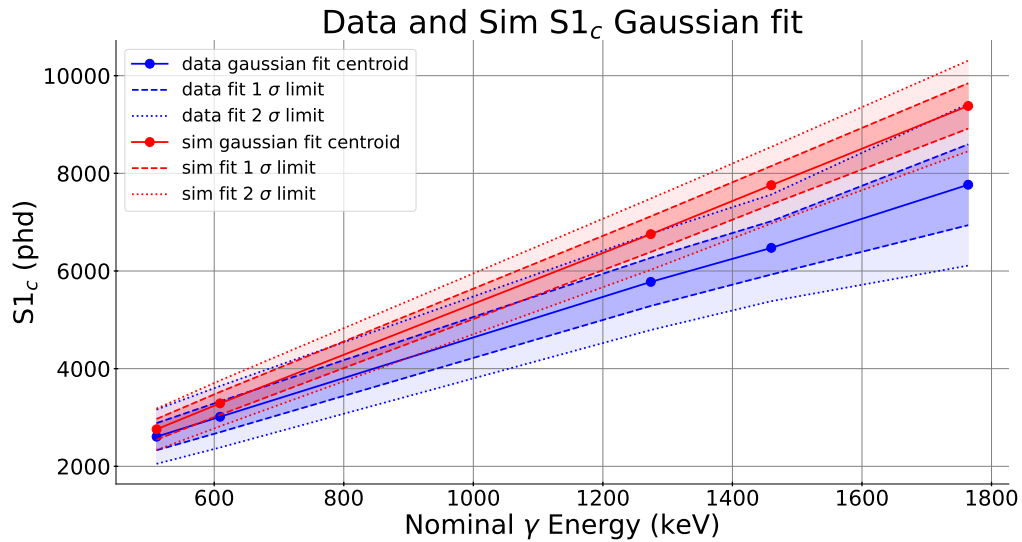


Figure 4.23: A plot summarizing the fitted centroids and widths from S1 distributions of simulation (red) and data (blue) for all γ lines is shown. The fitted centroids are indicated by filled circles and joined by a solid line. The 1σ and 2σ bands of the Gaussians are indicated by dotted and dashed lines and shaded in their corresponding color.

This is primarily because the fit window was truncated to improve the fit quality for the majority of the distribution. Because the energy of interest for a ^{85}Kr excited state decay is 514 keV, ignoring the behavior of this tail (which only presents above 1461 keV) is acceptable.

The data S1 percentile values are plotted against the respective simulation S1 percentile values, and each percentile is least squares fit with a linear function in Fig. 4.24. The corresponding plot using the Gaussian fit centroids and widths is given in Fig. 4.25.

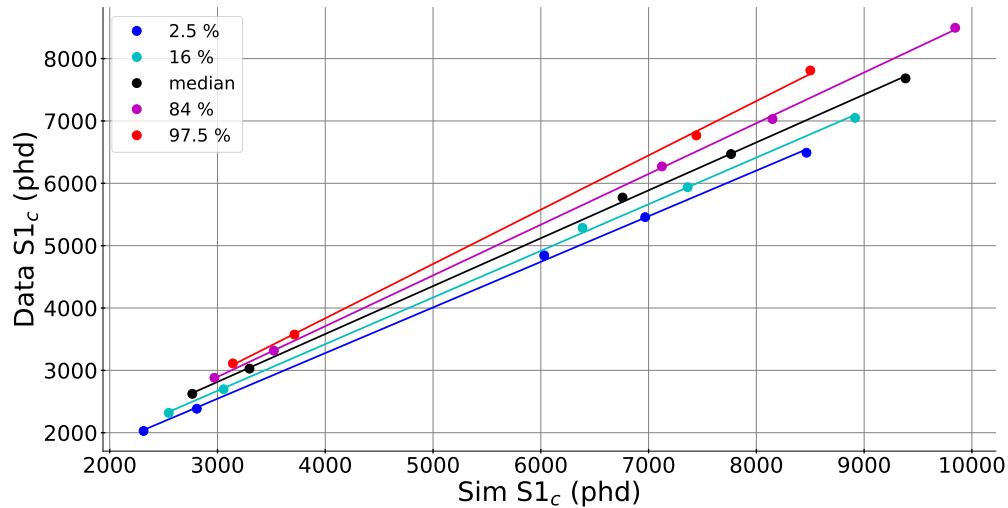


Figure 4.24: The S1 data percentile values are plotted against the simulation percentile values. The 2.5 percentile (blue, analogous to -2σ), 16 percentile (cyan, -1σ), median (black, analogous to the fitted centroid), and 84 percentile (magenta, $+1\sigma$) are plotted for every γ line. The 97.5 percentile (red, analogous to $+2\sigma$) is only plotted for the four lowest γ energies to avoid the high S1 tail seen in the data for the 1764 keV γ . Each percentile group is least squares linear fit (linear plus constant) across all γ lines to obtain the parameters for a conversion between simulation and data. The fit lines for each percentile are shown in the same color as the corresponding percentile markers.

Each color in Fig. 4.24 represents the percentile (or σ deviation in the case of the Gaussian fits from Fig. 4.25) for each of the five γ lines. The left most points in each color represent different percentiles (σ deviation) of the 511 keV γ line, with each successive

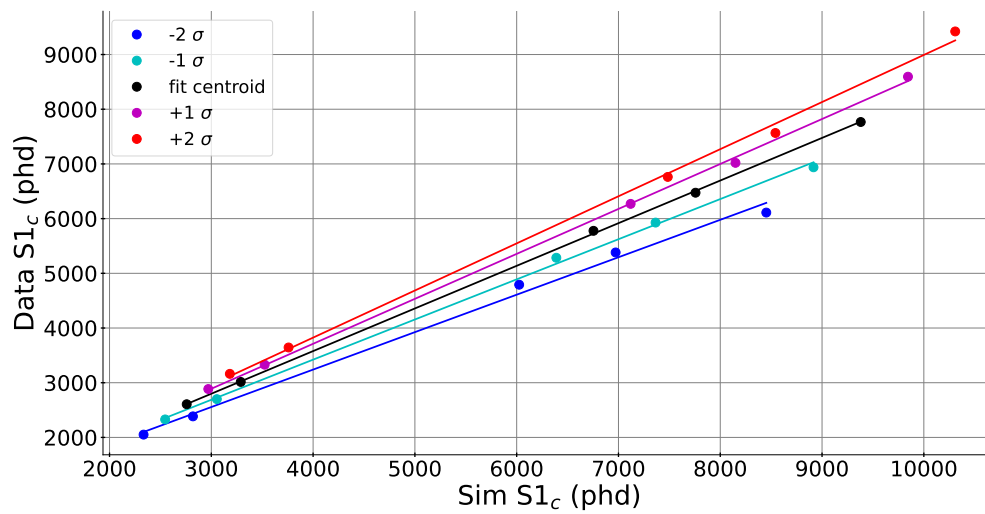


Figure 4.25: The $S1$ Gaussian fit centroids and widths for data are plotted against their simulation counterparts. The -2σ (blue), -1σ (cyan), centroid (black), $+1\sigma$ (magenta), and $+2\sigma$ (red) values are shown for all γ lines. Each standard deviation grouping is least squares linear fit (linear plus constant) across all γ lines to obtain the parameters for a conversion between simulation and data. The fit lines for each standard deviation are shown in the same color as the corresponding standard deviation markers.

series of points moving to the right representing the S1 of the next highest energy γ lines (609, 1275, 1460, 1764). The 97.5 percentile of the 1764 keV γ is not included in the percentile fit plot to avoid biasing the slope of the linear fit.

The percentile linear fits in Fig. 4.24 appear better behaved across all percentiles than the Gaussian derived linear fits in Fig. 4.25. This is especially true of the lowest S1 portion of the spectra (blue) where the most significant disagreement is observed. The error from the linear fit to the 2.5 percentile distribution is also considerably smaller than the error from the -2σ linear fit to the Gaussian centroid and width.

The central values from the 2.5 percentile linear fit from Fig. 4.24 are $m = 0.7317$ and $b = 350.1$. The covariance matrix of the fit is shown in Table 4.1.

$\sigma_{i,j}$	$j = m$	$j = b$
$i = m$	$1.193 * 10^{-4}$	$-6.342 * 10^{-1}$
$i = b$	$-6.342 * 10^{-1}$	$4.051 * 10^3$

Table 4.1: The covariance matrix of the fit to 2.5 percentile S1 distribution data-simulation comparison is shown. The fit to the equation $S1_{data} = m * S1_{sim} + b$ returns central values of $m = 0.7317$ and $b = 350.1$ for the 2.5 percentile fit. The measurements and fit used to obtain the central values and this covariance matrix are shown in Fig. 4.24.

Corrected S2

The corrected total S2 spectra are characterized in a manner that is identical to the S1 spectra. The distribution of the corrected total S2 of the $\pm 2\sigma$ energy slice for the 511 keV γ is shown in Fig. 4.26.

The simulation is greatly underestimates the mean and width of the S2 distribution. This is expected because the S1 was overestimated, and the energies of both simulation and data are similar. The upper percentile value of the spectra disagree by about 20%. The corrected S2 distributions for the other γ lines are shown in Fig. 4.27. Each histogram uses

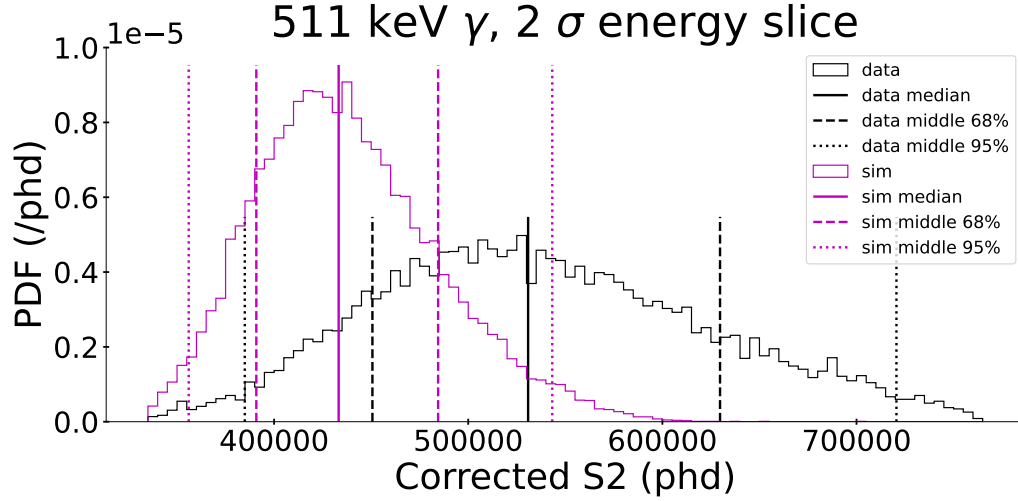


Figure 4.26: Histograms of the corrected total S2 of events within the $\pm 2\sigma$ energy slice of the 511 keV γ for the data (black) and simulation (magenta) are shown. The median (solid line), middle 68% (dashed lines), and middle 95% (dotted lines) of each distribution are indicated on the plot. Only the central 99% of the distribution is plotted. The y-axis label indicates the normalization. Data and simulation show stronger disagreement at higher S2 percentiles.

the same legend convention used in Fig. 4.26. A summary of the percentile distributions for S2 is shown in Fig. 4.28.

Data and simulation show significant disagreement at all γ energies. The disagreement is most pronounced at the higher percentile side of the distribution. The simulation severely underestimates the width of the total S2 distribution. A significant low S2 tail corresponding to the high S1 tail is seen in data for 1461 keV and 1764 keV γ s.

The total S2 Gaussian fits to the data and simulation for the 511 keV γ are shown in Fig. 4.29. Other S2 fits to γ lines are shown in section A.1 from Fig. A.17 to Fig. A.24. A plot summarizing the fit Gaussian centroids and widths for all γ energies is shown in Fig. 4.30

Bins in the low S2 tails of the 1461 and 1764 keV γ s were excluded from the fit windows for the same reasons the tail was excluded from the S1 fits. The difference in the -2σ and 2.5 percentile values in the higher energy γ s is the only qualitative difference between

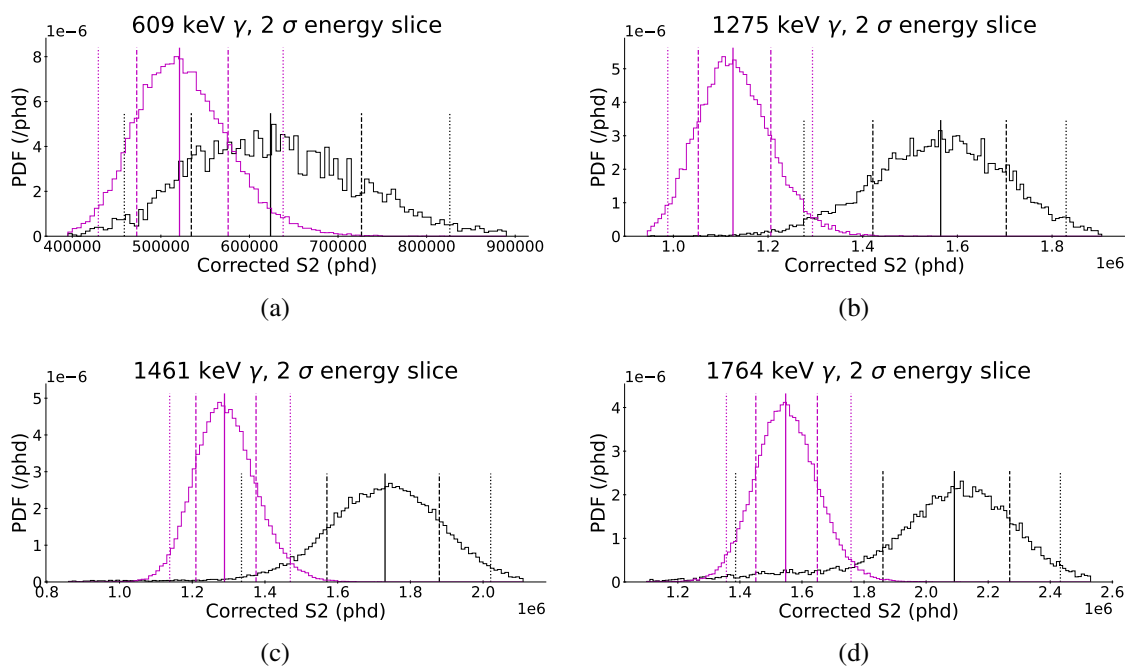


Figure 4.27: Histograms of the corrected total S2 of events within the $\pm 2\sigma$ energy slice of the remaining γ s for the data (black) and simulation (magenta) are shown. Each subplot represents a different γ line with the nominal γ energy given in the title. The plots follow the same conventions as Fig. 4.19.

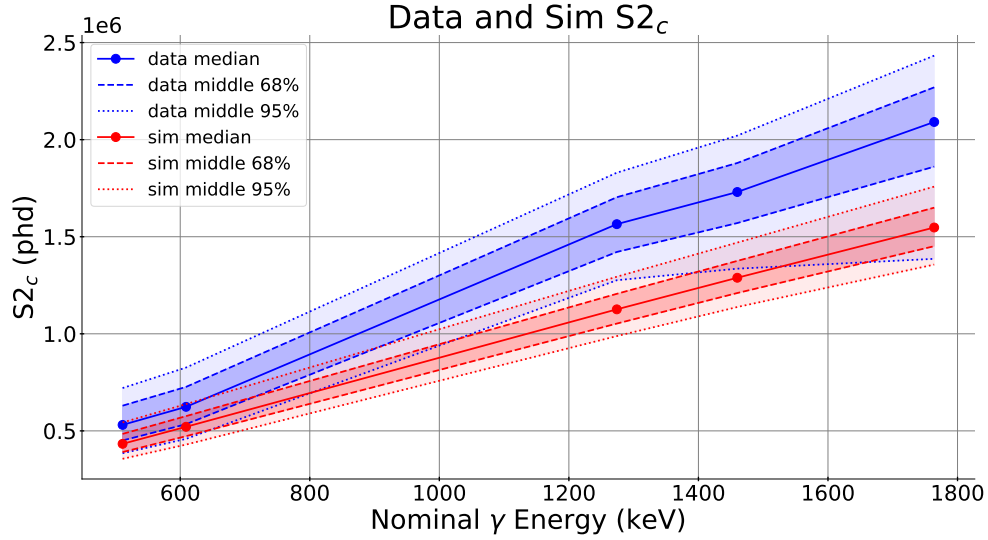


Figure 4.28: A plot summarizing the corrected total S2 percentile values in simulation (red) and data (blue) for each γ line is shown. The medians are indicated by filled circles and joined by a solid line. The central 68% of the distribution is denoted by dashed lines, and the central 95% is given by the dotted lines and shaded in the corresponding color.

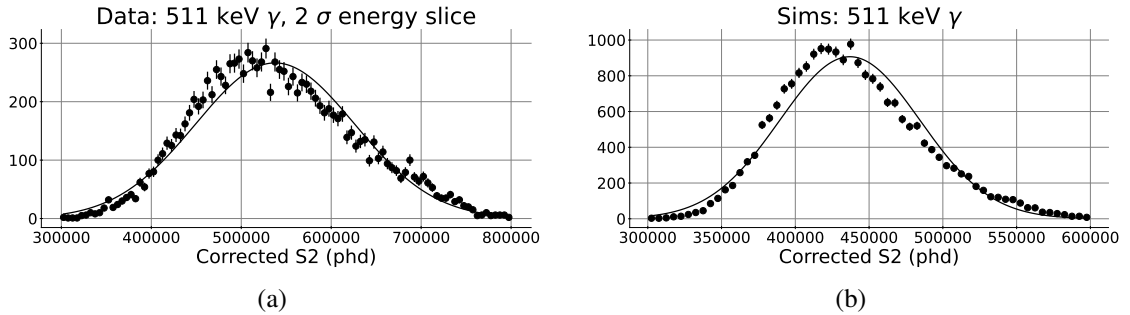


Figure 4.29: Gaussian fits to the corrected total S2 distributions of both data (a) and simulation (b) for a $\pm 2\sigma$ energy slice associated with the 511 keV γ are shown. The distributions show some skew which results in a slight mismatch between the fit and the data around the area of the peak. The distributions match the fit slightly better around the tails, which is generally more important this analysis. The fitted data centroid and width are 537600 and 88500 phd. The fitted simulation centroid and width are 437000 and 47600 phd.

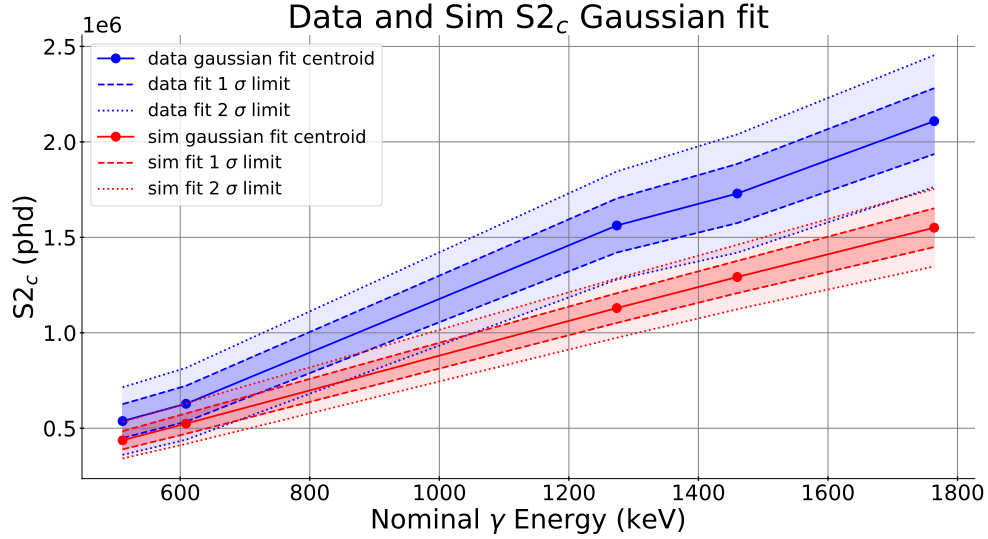


Figure 4.30: A plot summarizing the fitted centroids and widths from total S2 distributions of simulation (red) and data (blue) for all γ lines is shown. The fitted centroids are indicated by filled circles and joined by a solid line. The 1σ and 2σ bands of the Gaussians are indicated by dotted and dashed lines and shaded in their corresponding color.

Fig. 4.28 and Fig. 4.30.

The data S2 percentile values are plotted against the respective simulation S2 percentiles and each percentile is least squares linear fit in Fig. 4.31. The corresponding plot using the Gaussian fit centroids and widths is given in Fig. 4.32.

efficiency loss when transitioning from simulation to data would be most significant at the higher percentiles of the distribution. The percentile linear fits from Fig. 4.31 are generally not as well behaved as the Gaussian derived linear fits in Fig. 4.32.

The central values from the $+2\sigma$ linear fit from Fig. 4.30 are $m = 1.450$ and $b = -67940$. The covariance matrix of the fit is shown in Table 4.2. These parameters are revisited later.

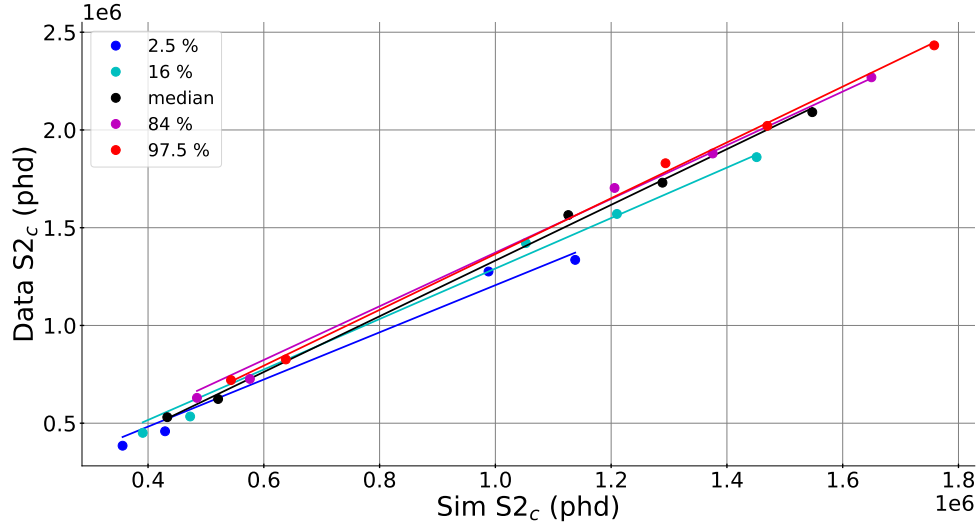


Figure 4.31: The total S2 data percentile values are plotted against the simulation percentile values. The 16 percentile (cyan, analogous to -1σ), median (black, analogous to the fitted centroid), 84 percentile (magenta, $+1\sigma$), and 97.5 percentile (red, $+2\sigma$) are plotted for every γ line. The 2.5 percentile (blue, analogous to -2σ) is only plotted for the four lowest γ energies to avoid the low S2 tail seen in the data for the 1764 keV γ . Each percentile group is least squares linear fit (linear plus constant) across all γ lines to obtain the parameters for a conversion between simulation and data. The fit lines for each percentile are shown in the same color as the corresponding percentile markers.

$\sigma_{i,j}$	$j = m$	$j = b$
$i = m$	$1.201 * 10^{-3}$	$-1.360 * 10^3$
$i = b$	$-1.360 * 10^3$	$1.811 * 10^9$

Table 4.2: The covariance matrix of the fit to the $+2\sigma$ total S2 Gaussian parameter data-simulation comparison is shown. The fit to the equation $S2_{data} = m * S2_{sim} + b$ returns central values of $m = 1.450$ and $b = -67940$ for the $+2\sigma$ fit. The measurements and fit used to obtain the central values and this covariance matrix are shown in Fig. 4.32.

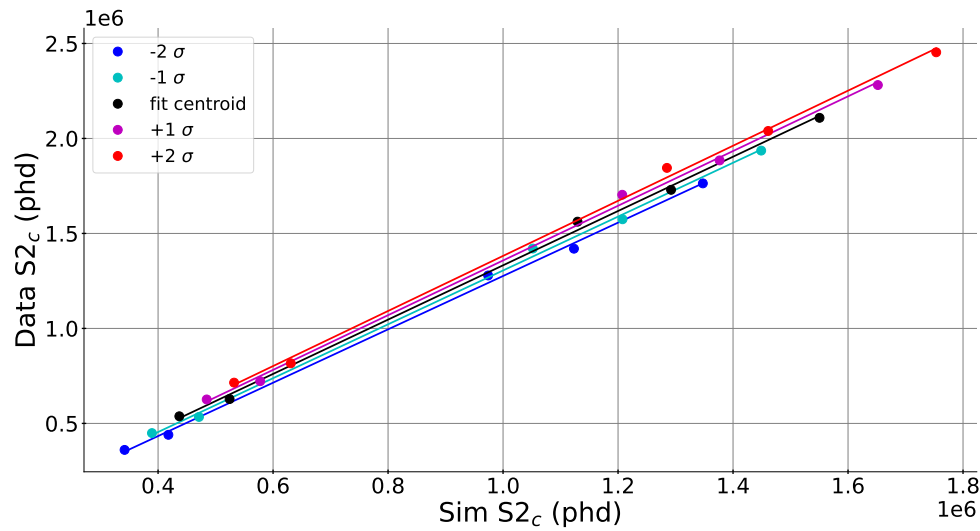


Figure 4.32: The total S2 Gaussian fit centroids and widths for data are plotted against their simulation counterparts. The -2σ (blue), -1σ (cyan), centroid (black), $+1 \sigma$ (magenta), and $+2 \sigma$ (red) values are shown for all γ lines. Each standard deviation grouping is least squares linear fit (linear plus constant) across all γ lines to obtain the parameters for a conversion between simulation and data. The fit lines for each standard deviation are shown in the same color as the corresponding standard deviation markers.

4.5 Cut Description and Efficiency Evaluation

Events undergo a series of cuts following the energy corrections. The cuts can broadly be classified as related to the energy of the event, how localized the event is, or if the event triggers a veto detector. The energy related cuts are on corrected S1B area, corrected S1G area, total corrected S2 area, and corrected energy. Localization related cuts are on S2 localization and δ S1 TBA. Veto cuts are from the coincidence vetoes: the skin veto and outer detector veto.

The efficiency of simulated excited state ^{85}Kr events must be evaluated to determine the efficiency correction factor (ϵ in Eq. 4.1) for real data. The expected number of ^{85}Kr excited state events ranges from 10 and 25 based on the cold trap mass spectrometry measurement. The statistical error on the number of signal events in the excited state measurement is expected to be the dominant uncertainty. The S1 δ time cut is powerful enough to heavily mitigate backgrounds. Because of this, the principle underlying decisions related to setting cut boundaries is to maximize the efficiency for selecting ^{85}Kr excited state events. Maximizing the efficiency increases the number of signal events, reducing the dominant source of error on the number of counts detected. The information gleaned in section 4.4 is used to evaluate the systematic uncertainty on efficiency.

In addition to the cuts listed above, components of the selection criteria must be considered in the efficiency evaluation. The efficiency of the S1 δ time cut, $\epsilon_{0.3\ \mu\text{s}}$, is evaluated numerically by integrating the probability distribution of the decay time of ^{85m}Rb across the range of allowed delay times (from 0.3 to 100.3 μs). The cut efficiency is $\epsilon_{0.3\ \mu\text{s}} = 0.815$. ^{85}Kr excited state decays are recorded only in the WIMP search fiducial volume, where the fiducial cut efficiency is assumed to be unity. The fiducial volume sets the target Xe mass from Eq. 4.1. The statistical uncertainty of the fast simulation cut efficiency is negligible compared to the systematic uncertainty.

As mentioned in the introduction, two flavors of simulation are used to evaluate the cut efficiencies. The *fast* simulations have more statistics and are the preferred evaluation tool when possible. Fast simulations lack individual PMT light collection data and do not simulate the skin and the outer detector so the TBA, the skin, and the outer detector cuts must be modeled with the *full* simulations.

4.5.1 Efficiency of cuts evaluated with the fast simulation

The fast simulation variables are listed below:

1. Basic selection criteria
2. Corrected S1B
3. Corrected S1G
4. Total corrected S2
5. Corrected energy
6. S2 localization

About 1000000 excited state ^{85}Kr decays are simulated with a spatially uniform random distribution in the liquid Xe volume. A fraction of these decays occur in the *reverse field region* of the TPC below the cathode where they do not produce S2s and, therefore, fail the fiducial cut and are not be counted as efficiency losses.

Basic selection criteria

The selection criteria is defined in section 4.2.1. Components of the selection criteria are applied after the S1 δ time and the fiducial cuts for the efficiency evaluation. The TBA is not output by the fast simulations, so no components of the selection criteria related to TBA are used in fast simulations. The S1 δ time cut applied in simulations is not identical to the cut applied in real data. The simulation S1 δ time cut uses truth information from

the output of the LZ BACCARAT file to determine the S1 δ time.

The truth information is recorded independent of whether an event deposits energy in the TPC volume or elsewhere. Events that produce only a single S1 because their delay times are too small to be resolved are removed by this truth delay time cut. The removal occurs prior to the selection criteria evaluation, so these are not counted as fast simulation efficiency losses. An event that has only a single S1, with a β interacting in the TPC volume and decay time greater than 300 ns, but a γ completely escaping the TPC, will not be removed by the S1 δ time cut. An event like this will appropriately be counted as a fast simulation efficiency loss (provided the S1-S2 pair is within the fiducial volume).

The simulation fiducial cut is the same as used in the real data and requires a valid S1 and S2 pair to pass. Events with the β and γ depositing all their energy in the reverse field region produce two S1s but no S2 and appropriately fail the fiducial cut before the selection criteria is evaluated. These events are not counted as fast simulation efficiency losses.

Of the 648748 events passing both the S1 δ time cut and the fiducial cut, 618288 meet the selection criteria. 95.3% of events pass this cut. Fig. 4.33 shows the reconstructed position of the events passing the S1 δ time, fiducial, and selection criteria cuts using both the position of the largest S2 and the weighted position of the event.

Energy cuts

All energy related cut efficiencies are evaluated with the fast simulation framework. The cuts include the corrected S1B, the corrected S1G, the total corrected S2, and the corrected energy cuts. These event losses from these cuts are evaluated both cumulatively and independent of each other.

Fits from section 4.4 prove that there is a significant mismatch between the S1 and S2 areas between data and simulation for γ s near the S1G energy of 514 keV. The cut bound-

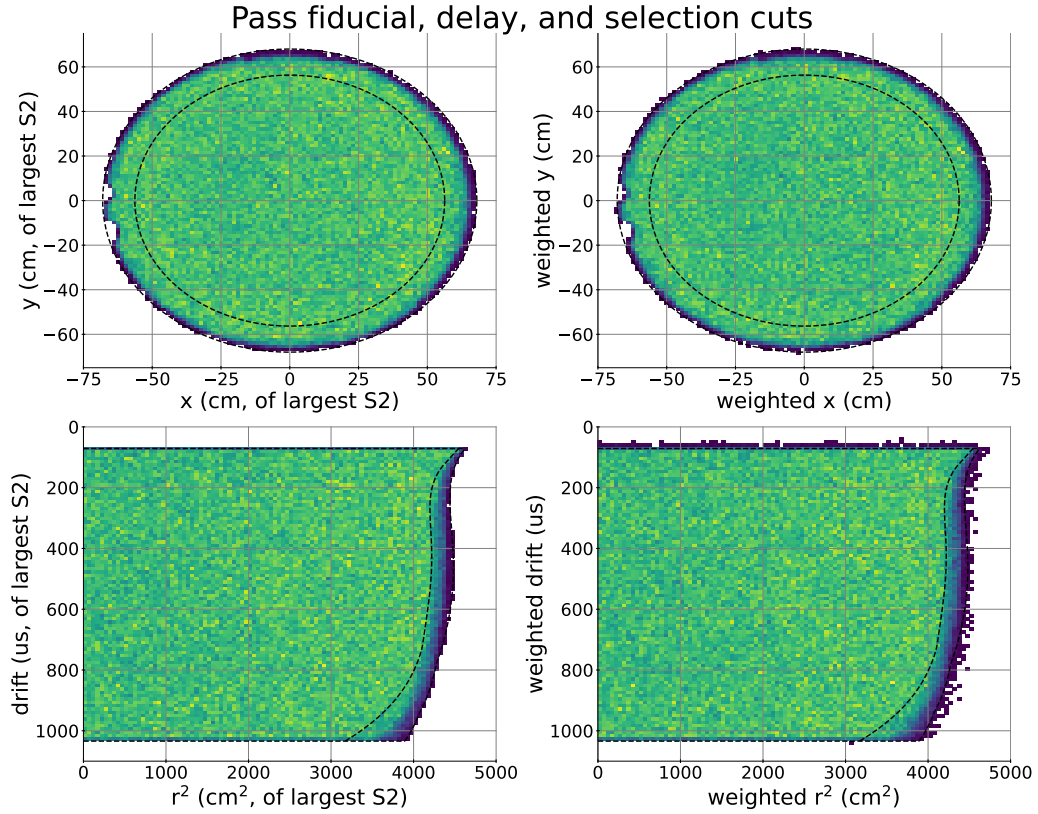


Figure 4.33: The position distribution of 618288 fast simulation events passing the initial cuts is shown. The left plots show the event position given by its largest S2, while the right plots show the event's weighted position. The top plots show the X-Y position of the event, and the bottom plots show the event's r^2 and drift time. The Z and r components of the fiducial boundaries are outlined by dashed lines. The inner-most and outer-most radii of the fiducial volume are shown in the X-Y plots. The inner-most and outer-most radii from the azimuthal slices of the fiducial volume at a particular drift time are shown as dashed lines in the r^2 drift time plots. The subtle cutouts near $X = -70$ cm and $Y = 0$ are from the field cage resistor component of the fiducial volume.

aries are set and efficiencies are evaluated in the fast simulation, then the cut boundaries are scaled to a data equivalent cut boundary value using information from section 4.4.

Some aspects of the systematic uncertainty evaluation rely on the scaling from section 4.4. The fractional uncertainty on the data equivalent cut boundary is applied to the simulation boundary. The simulation boundary is then varied by the fractional uncertainty, and the change in efficiency (after *all* fast simulation cuts, with the remaining cuts fixed to their nominal values) is assessed. This systematic assessment occurs after the fast simulation cut efficiency evaluation. The *uncertainty on a simulation cut boundary* is reflective of the uncertainty on the conversion of that cut boundary from a simulation value to a data equivalent value.

The corrected S1B cut range is 50-1000 phd. Given the (energy) proximity to the well tuned WIMP search region of interest, the data equivalent cut boundaries are the same as the simulation cut boundaries for S1B. The systematic uncertainty on the conversion from simulation to data for S1 areas near the S1B lower bound is very difficult to evaluate, as discussed in section 4.4. The uncertainty on the S1B at this value is unlikely to exceed 10%. Because the S1B is produced by a β spectrum, the density of events with S1Bs near the upper cut boundary is low. Any uncertainty on efficiency due to uncertainty on the upper S1B cut boundary is negligible.

The probability density and cumulative distribution functions for the corrected S1B area of all fast simulation events passing the S1 δ time, fiducial, and selection criteria cuts are displayed in Fig 4.34. The cut boundaries are indicated by dashed lines.

90.3% of events passing previous cuts pass the corrected S1B cut. The lower bound of the S1B cut is the harshest individual cut, aside from the S1 δ time. A plot of the fraction of events passing the S1B cut as a function of the lower bound is shown in Fig. 4.35. The $\pm 10\%$ cut bound uncertainty region is highlighted in yellow.

S1s with no accompanying S2 are referred to as *isolated S1s*. The isolated S1s are more

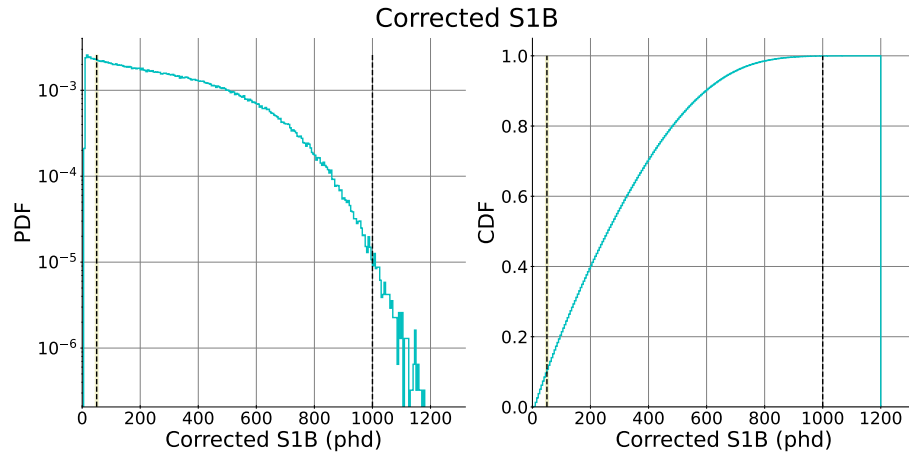


Figure 4.34: The probability density (left) and cumulative distribution (right) of the corrected S1B of fast simulation events passing the initial cuts are shown. This cut is applied identically in simulation and data. The cut boundaries of 50 phd and 1000 phd are indicated by dashed lines. 90.3% of events passing previous cuts pass the S1B cut. The uncertainty region on the lower cut boundary is highlighted in yellow.

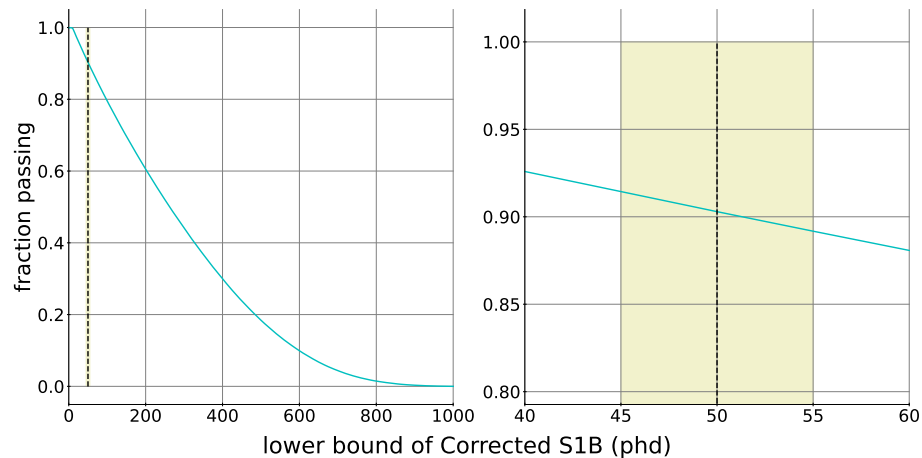


Figure 4.35: The fraction of events passing previous cuts that pass the S1B cut as a function of the specified S1B lower bound is plotted. The fraction is determined using the nominal upper bound value of 1000 phd. The right plot contains the same information as the left plot, but magnifies the region near the cut's lower bound. The yellow region indicates the uncertainty on the cut, based on an assumed 10% uncertainty when converting simulated S1B to a data equivalent value. The fraction of events passing the cut varies by about 0.01 across the region of uncertainty.

prevalent at lower energies. Isolated S1s may form an accidental coincidence pair with an S1G-like S1. Because accidental coincidences are expected to be the primary source of background, the lower bound of the S1B cut is chosen to balance background reduction and high efficiency. Slight efficiency loss is tolerated.

The change in the event fraction passing the cut indicated in Fig 4.35 is not the systematic uncertainty on the fast simulation cut efficiency from the lower bound of the S1B cut. The plotted fraction considers only events passing the prior cuts (S1 δ time, fiducial, and selection criteria) in the denominator. The uncertainty on the fast simulation efficiency from this cut boundary is the change in the number of events passing *all* fast simulation cuts when the S1B lower bound is varied.

The corrected S1G cut range was *initially* chosen to be 2000 phd to 3400 phd in the simulation. The corrected S1G distributions of events passing the selection criteria, the S1 δ time, the fiducial cuts, and the S1B cut are shown in Fig. 4.36.

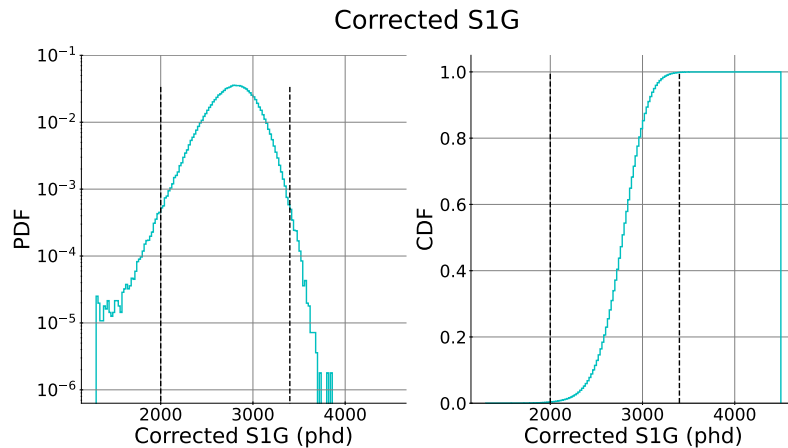


Figure 4.36: The probability density and cumulative distribution of the corrected S1G of fast simulation events passing the prior cuts are shown. The *initial* simulation cut boundaries of 2000 phd and 3400 phd are indicated by dashed lines. The simulation cut boundaries were altered because of the discrepancy between data and simulation discussed in section 4.4.

Given the significant disagreement between simulation and data for S1 areas similar to

most S1Gs, the simulation bounds must be scaled to data equivalent bounds. The fitted parameters $m = 0.7317$ and $b = 350.1$ and the covariance matrix in Table 4.1, taken from the lower 2.5 percentile value fit ($S1_c^{data} = m * S1_c^{sim} + b$) in Fig. 4.24, are applied to the simulation S1G lower bound. The data equivalent lower S1G bound is 1814 ± 45 phd. Applying the fractional uncertainty of the data equivalent bound to the simulation bound, the uncertainty on the S1G lower bound is ± 50 phd.

The initial S1G simulation upper bound of 3400 phd only removes about 0.2% of events. The fraction of events passing the S1G cut as a function of the S1G upper bound is shown in Fig. 4.37.

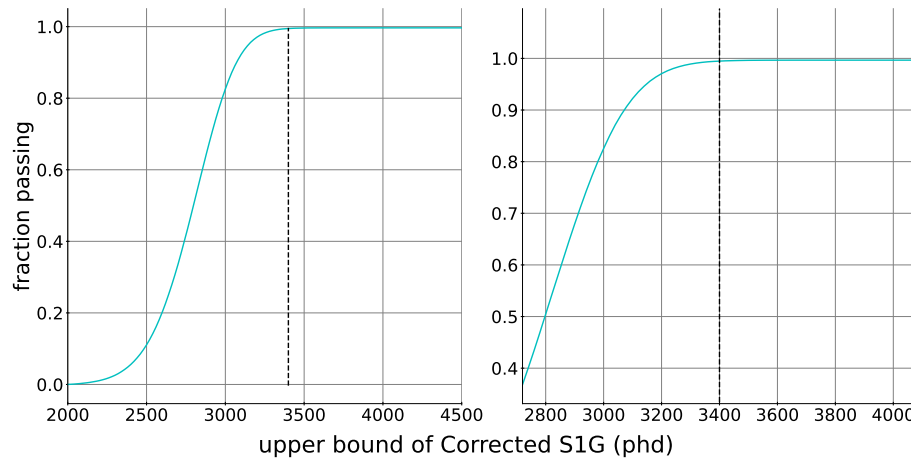


Figure 4.37: The fraction of events passing previous cuts that pass the S1G cut as a function of the specified S1G upper bound is plotted. The fraction is determined using the nominal (simulation) lower bound value of 2000 phd. The right plot contains the same information as the left plot, but magnifies the region near the cut's upper bound. The fraction of events lost from (only) the initial upper bound of the S1G cut about 0.002. This bound is not applied in simulation because of its very small event loss and the simulation's tendency to overestimate S1.

The data S1G distribution is lower in S1 than the simulation S1G distribution. If the S1G upper bound is set to 3400 phd in data, the percentage of events remaining after the cut in data would be between the 99.8% from simulations and unity. It is proposed that the simulation S1G upper bound is removed entirely, increasing the percentage of remaining

events by 0.2%. The data equivalent S1G upper bound is set to 3400 phd. The difference between the cut efficiency with a simulation upper bound of 3400 phd and infinity after all fast simulation cuts have been applied is used as the systematic error on the fast simulation cut efficiency from the S1G upper bound: $\sigma_{\varepsilon_{S1G\uparrow}} = |\varepsilon(S1G \uparrow = 3400) - \varepsilon(S1G \uparrow = \infty)|$.

To review, the revised S1G simulation cut only consists of the lower S1G cut bound of 2000 phd. The *data equivalent* cut boundaries on S1G are 1814 and 3400 phd. Fig. 4.38 shows the PDF and CDF with the revised simulation cut boundary.

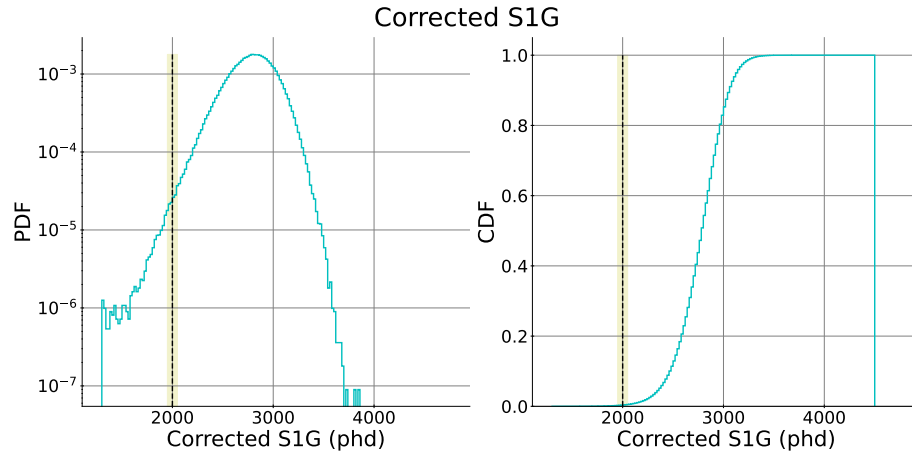


Figure 4.38: The probability density and cumulative distribution of the corrected S1G of fast simulation events passing the prior cuts are shown. This plot contains the same event histogram as Fig. 4.36, with no S1G upper bound. The lower bound is set to 2000 phd, and its region of uncertainty is highlighted. The data equivalent lower bound of the S1G is 1814 phd, and the upper bound is restored to 3400 when the cut is applied in data. 99.5% of events passing previous cuts pass the S1G cut.

99.5% of events passing the selection criteria, S1 δ time, fiducial, and S1B cuts pass the S1G cut. Fig. 4.39 shows fraction of events remaining as a function of the lower bound of the S1G cut.

The total corrected S2 simulation cut range is 350000 to 700000 phd. The total corrected S2 distributions of events passing the former cuts (including S1B and S1G) are shown in Fig. 4.40.

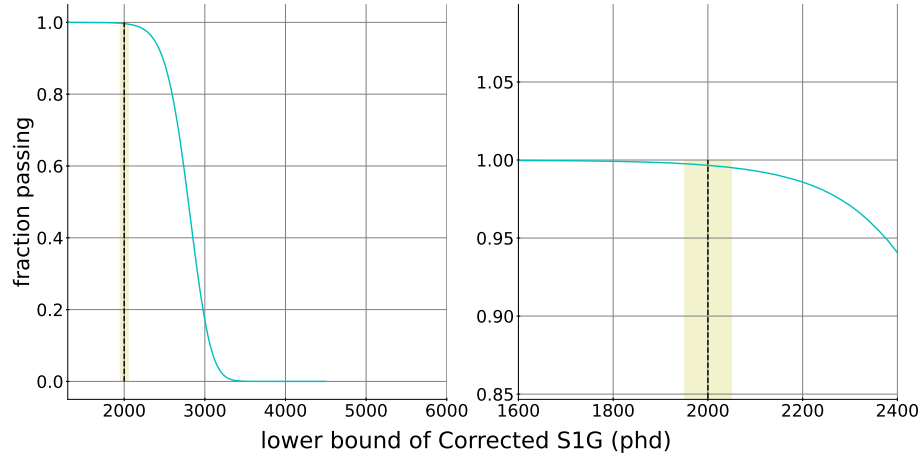


Figure 4.39: The fraction of events passing previous cuts that pass the S1G cut as a function of the specified S1G lower bound is plotted. No S1G upper bound is applied. The right plot contains the same information as the left plot, but magnifies the region near the cut's lower bound. The yellow region indicates the uncertainty on the cut. The event fraction shows little variation across the region of uncertainty.

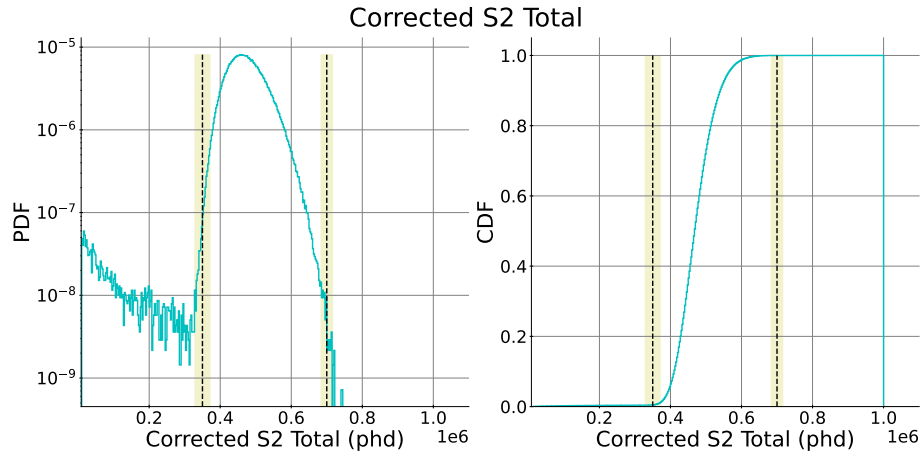


Figure 4.40: The probability density (left) and cumulative distribution (right) of the total corrected S2 of fast simulation events passing all prior cuts are shown. The simulation cut boundaries of 350000 phd and 700000 phd are indicated by dashed lines. The yellow regions indicate the uncertainty on each cut boundary. The data equivalent total S2 bounds differ from the simulation total S2 bounds. 99.5% of events passing previous cuts pass the total S2 cut.

99.5% of events that passed the previous cuts pass the total S2 cut. The uncertainty on the simulation total S2 upper bound is 16300 phd. This is determined with the same procedure used to derive the uncertainty on the S1G lower bound. The fitted parameters $m = 1.450$ and $b = -67940$ and covariance matrix in Table 4.2, taken from the $+2\sigma$ S2 fit ($S2_c^{data} = m * S2_c^{sim} + b$) in Fig. 4.32, are applied to the simulation total S2 upper bound. The data equivalent upper bound of total S2 is 947000 phd. The fraction of events passing the total S2 cut as a function of the total S2 upper bound is shown in Fig. 4.41.

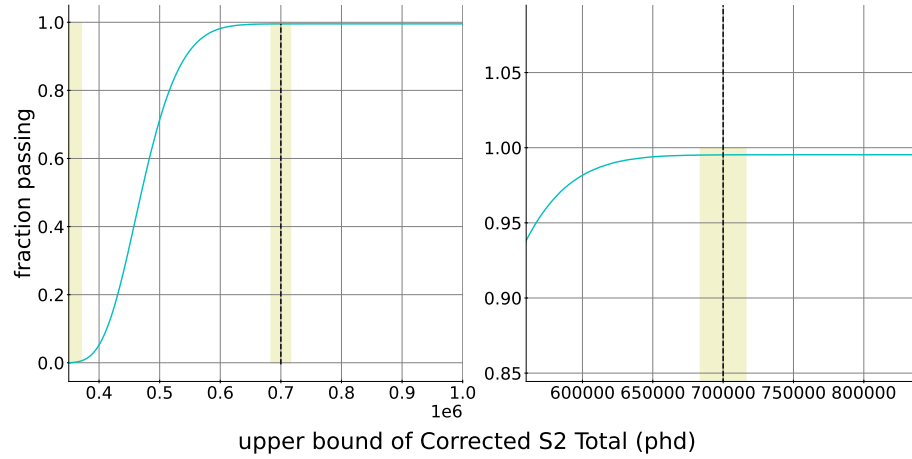


Figure 4.41: The fraction of events passing previous cuts that pass the total S2 cut as a function of the specified total S2 upper bound is plotted. The lower bound maintains its nominal simulation value of 350000 phd. The right plot contains the same information as the left plot, but magnifies the region near the cut's upper bound. The yellow region indicates the uncertainty on the cut. The event fraction shows almost no variation across the region of uncertainty. The data equivalent upper bound of the S2 cut is 947000 phd.

The lower bound total S2 was scaled using the -2σ fit from Fig. 4.32. The data equivalent value of the total S2 lower bound is 363000 phd and the uncertainty on the simulated total S2 lower bound is 21200 phd. The fraction of events passing the total S2 cut as a function of the total S2 lower bound is shown in Fig. 4.42.

The corrected energy cut range is 460 keV to 700 keV. The γ energy is 514 keV and the Q-value of the full decay is 687 keV. The (reconstructed) energy of the vast majority

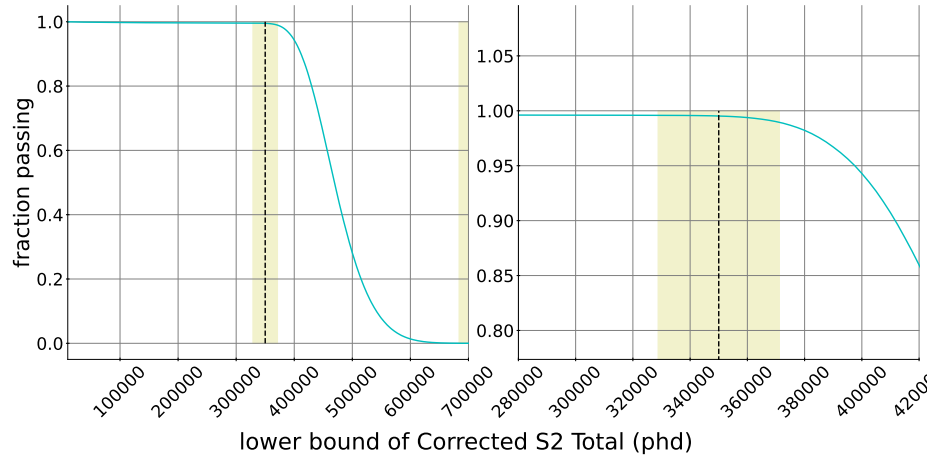


Figure 4.42: The fraction of events passing previous cuts that pass the total S2 cut as a function of the specified total S2 lower bound is plotted. The upper bound maintains its nominal value of 700000 phd. The right plot contains the same information as the left plot, but magnifies the region of the cut's lower bound. The yellow region indicates the uncertainty on the cut. The event fraction shows slight variation, particularly when the cut boundary is raised. The data equivalent lower bound of the S2 cut is 363000 phd.

of fully contained events is between the γ energy and the Q-value. The corrected energy spectrum of events passing all prior cuts is shown in Fig 4.43

99.9% of events passing previous cuts pass the energy cut. From section 4.4.3, the data energy resolution is better than the simulation resolution. Maintaining the same energy bounds between simulation and data should reduce the already minuscule (simulation) event loss when the cut is applied to data. The same energy cut bounds are used in simulation and data. The systematic uncertainty on the fast simulation efficiency from the energy cut is the the full fraction of events that fail the energy cut after all other fast simulation cuts have been applied: $\sigma_{\epsilon_E} = \epsilon(E = (-\infty, \infty)) - \epsilon(E = [460, 700])$.

S2 localization cut

Genuine excited state ^{85}Kr decays have tightly bunched groups of S2s or a single S2. The mean interaction length of a 514 keV γ in liquid Xe is about 3 cm and does not exceed

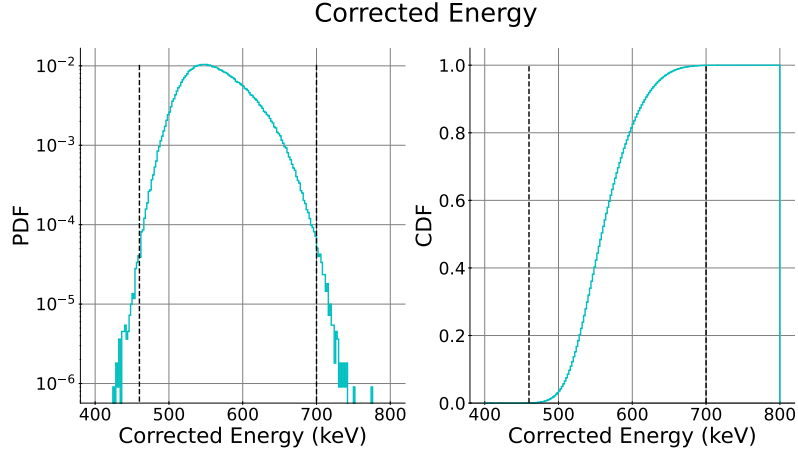


Figure 4.43: The probability density (left) and cumulative distribution (right) of the corrected energy of fast simulation events passing all prior cuts are shown. The cut boundaries of 460 keV and 700 keV are indicated by dashed lines. This cut is applied identically in simulation and data. 99.9% of events passing previous cuts pass the energy cut.

3 cm at any lower energy. Therefore, if an event has two comparably sized S2s over a meter apart, the event is not an excited state ^{85}Kr decay. The S2 localization cut rejects events with clearly unrelated S2s.

Localization is calculated with the weighted position and weighted S2 time in section 4.3.1. The localization variable L is defined in Eq. 4.6, where $\vec{x}_w$ is the weighted (3D) position of the event, $\vec{x}_i$ is the position of the i th largest S2, and $A_{S2,i}$ is the area (energy) of the i th largest S2.

$$L = \frac{\sum_{i=1}^{n, n \leq 5} \|\vec{x}_w - \vec{x}_i\| * A_{S2,i}}{\sum_{i=1}^{n, n \leq 5} A_{S2,i}} \quad (4.6)$$

The time difference between the weighted and individual S2s is converted to a distance (in z) before the magnitude is taken. This is calculated with the equation $dz = dt * h_{LZ} / t_{LZ \text{ max drift}}$, where dz is the distance between the weighted S2 and the individual S2 in the Z direction, dt is the time between the weighted S2 and the individual S2, h_{LZ} is the height of the LZ TPC, and $t_{LZ \text{ max drift}}$ is the maximum drift time of events in LZ.

Like the weighted position, the five largest S2 pulses are used in the localization calculation. The upper bound of the localization cut is 4 cm. The localization of events passing the selection criteria, S1 δ time, fiducial, and energy cuts is shown in Fig. 4.44.

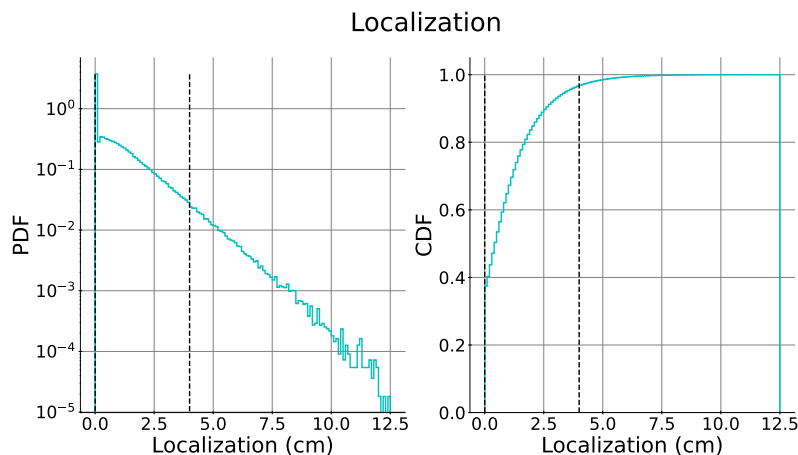


Figure 4.44: The probability density (left) and cumulative distribution (right) of the localization of fast simulation events passing all prior cuts is shown. The upper cut boundary of 4 cm is indicated by a dashed line. Events with a single S2 account for the large spike at a localization of zero. 96.6% of events passing previous cuts pass the localization cut.

96.6% of events passing the previous cuts pass the S2 localization cut. The radiation interaction distances in LXe are well understood. Significant localization mismodeling in the simulation is unlikely. Any systematic error associated with S2 localization is assumed to be negligible.

Efficiency results from the fast simulation

Table 4.3 summarizes the fast simulation evaluated cuts (excluding the selection criteria) and cut boundary values. Table 4.4 provides a summary of the number of fast simulation events passing cuts.

The fast simulation cut efficiency is $\varepsilon_{fast} = 0.822$. The largest efficiency loss is the result of the S1B cut that removes about one tenth of events passing the selection criteria.

Cut variable	Unit	Lower	Upper	Lower (data eq)	Upper (data eq)
Corrected S1B	phd	50	1000	50	1000
Corrected S1G	phd	2000	None	1814	3400
Total Corrected S2	phd	350000	700000	363000	947000
Corrected Energy	keV	460	700	460	700
Localization	cm	None	4	None	4

Table 4.3: A summary of the fast simulation cuts, their bounds, and their data equivalent bounds is shown. The "Lower" and "Upper" columns indicate the values of the lower and upper cut bounds respectively, as they are applied to evaluate the cut efficiency in the simulation framework. The "Lower (data eq)" and "Upper (data eq)" columns show the *data equivalent* lower and upper bound that are used when applying the cuts to real data.

Cut	Total	% (from SC)	Cumulative	% (from prev)	ϵ (cumulative)
FV and S1 δt	648748	N/A	648748	100	1
Sel Criteria	618288	100	618288	95.3	0.953
Cor S1B	558270	90.3	558270	90.3	0.861
Cor S1G	615133	99.5	555422	99.5	0.856
Tot Cor S2	612590	99.1	552730	99.5	0.852
Cor E	612376	99.0	552212	99.9	0.851
Localization	598083	96.7	533458	96.6	0.822

Table 4.4: A summary of the number and percentage of fast simulation events passing each cut is shown. The "FV and S1 δt " row shows the number of events passing the fiducial volume and S1 δ time cuts in both the "Total" and "Cumulative" columns. Events cannot pass the selection criteria cut unless they pass the fiducial and S1 δ time cuts. Events cannot pass any of the cuts listed below the selection criteria cut unless they first pass the fiducial, S1 δ time, and selection criteria cuts. Once an event passes the selection criteria, the number of events passing any cut can be evaluated independent of any of the remaining cuts. For rows below the selection criteria, the number of events independently passing any other cut is the number of events listed in the "Total" column. The corresponding percentage of events that passed the selection criteria passing the cut is listed in the column "% (from SC)". The "Cumulative" column indicates the total number of events passing the cut in that row and in all rows above. The "% (from prev)" column shows the percentage of events passing the cut in that row out of the number of events passing all cuts above the row. The " ϵ (cumulative)" column indicates the cumulative efficiency of events passing the cut in that row and all rows above out of the total number of events passing the fiducial and S1 δ time cut (648748). The total fast simulation cut efficiency is given by the cumulative efficiency after the localization cut: 0.822.

Fig. 4.45 shows the position of events passing all cuts. This can be compared with Fig. 4.33. The spatial distribution of events passing all fast simulation cuts remains uniform in the fiducial volume.

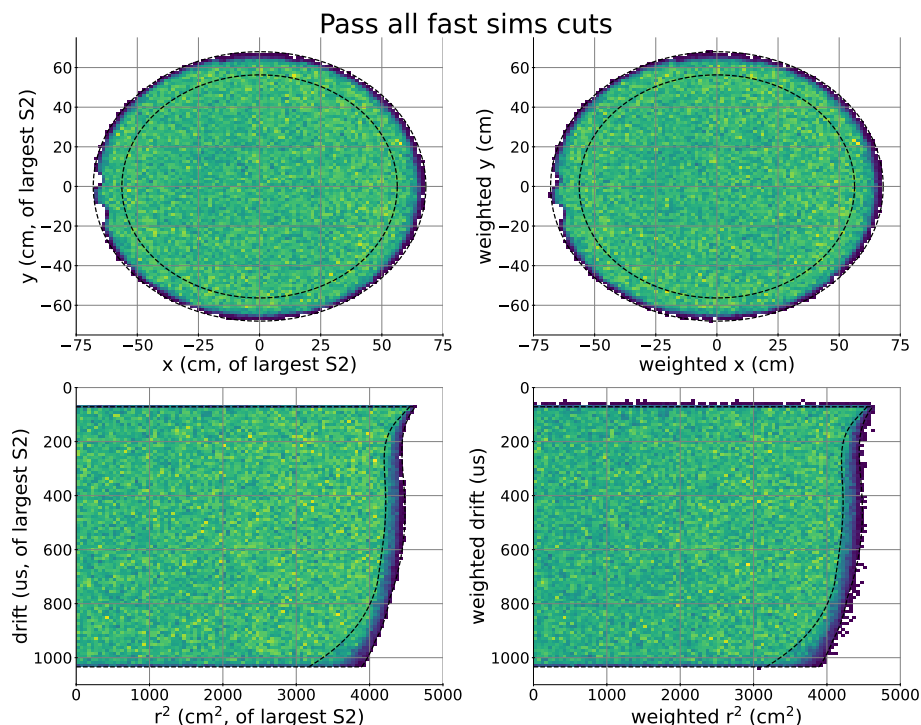


Figure 4.45: The spatial distribution of fast simulation events passing all fast simulation cuts is plotted. This plot follows the same plotting conventions as Fig. 4.33 with the largest S2 position plots on the left and the weighted position plots on the right. The top plots show the X-Y position of events while the bottom plots show the r^2 and drift time. The fiducial boundaries are indicated with dashed lines. There is no evidence that the fast simulation cuts created any spatial bias in the surviving events.

Fig. 4.46 displays all events passing the S1 δ time, fiducial, and selection criteria cuts. Events failing any remaining fast simulation cut are plotted in red, while events passing all are plotted in black.

All simulated events with significant lost charge or light fail the energy cuts, leaving only the population of events in the bulk of the energy distributions. The S1 δ time of events passing the S1 δ time, fiducial, and selection criteria cuts are shown in Fig. 4.47.

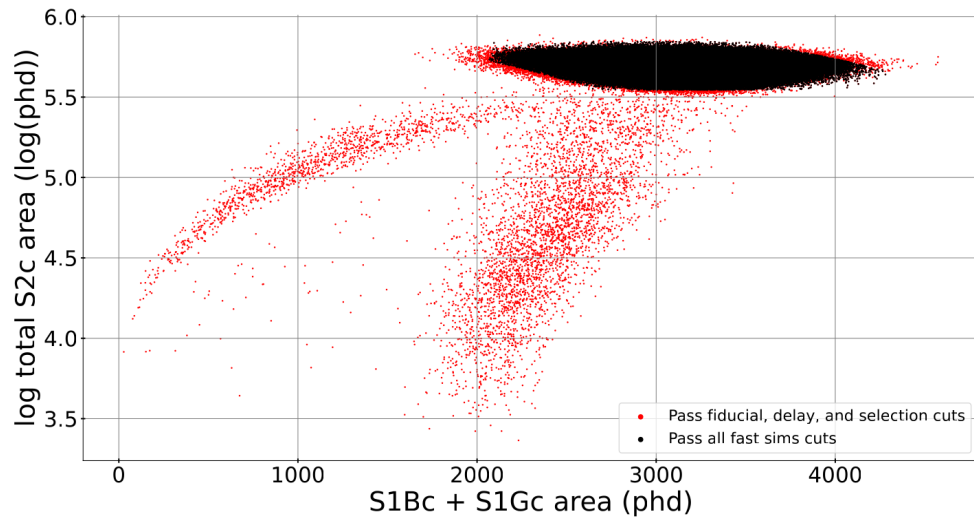


Figure 4.46: The combined S1s (S1B + S1G) and log of the total S2s of fast simulation events that passed the selection criteria but failed any (red) or passed all (black) remaining fast simulation cuts. The cuts isolate the bulk of the distribution. There are two noteworthy bands of failing events. The left lower band exhibits both light loss (S1) and charge loss (S2), indicating that the energy deposited by the decay (likely from the γ) was not fully contained. The right lower band exhibits significant charge loss but no light loss. In these cases, some energy is likely deposited in the reverse field region. The reverse field region lies beneath the cathode where scintillation light is produced but no charge is collected.

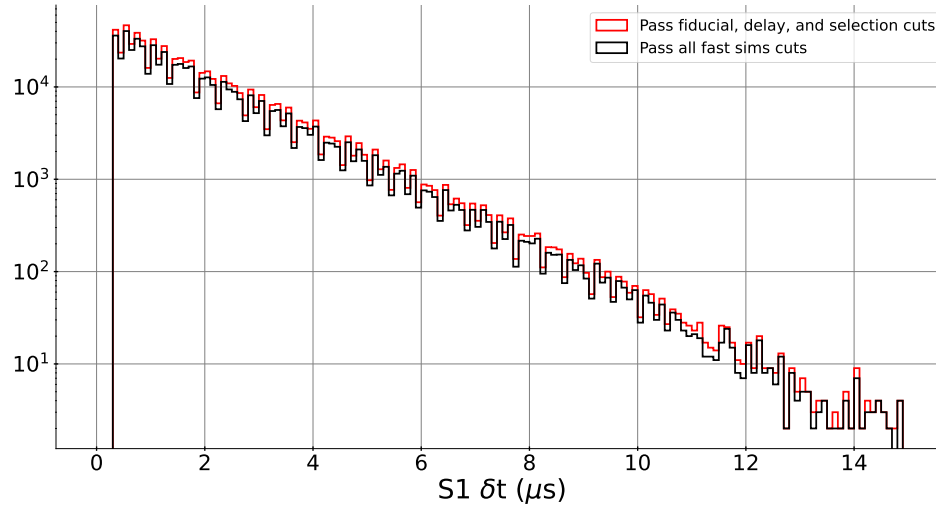


Figure 4.47: A plot of the S1 δ time of fast simulation events that passed the selection criteria (red) and events that passed all fast simulation cuts (black). The fast simulation cuts show no indication of biasing the S1 δ time in a way that would alter the expected exponential distribution of genuine excited state ^{85}Kr signal events.

The ratio of events passing and failing the fast simulation cuts appears constant for all S1 δ time. This indicates that the cuts are not introducing any delay time bias that may affect a fit to the S1 δ time, used to determine the final number of signal counts.

The systematic uncertainty associated with individual cuts is determined by calculating the (absolute) change in efficiency as the cut is varied by its uncertainty, with all other cuts boundaries fixed to their nominal values. Table 4.5 shows the efficiency change for each cut.

Recall that the uncertainty on any given cut bound is intended to represent the uncertainty on the scaling from simulation to data at the simulation cut value. The positive uncertainty on efficiency for the upper bound of S1G is zero because the cut is not applied in the simulation efficiency evaluation; the S1G upper bound (simulation) efficiency is effectively unity and cannot be higher. The right most column of the table shows the efficiency change when the cut boundaries are varied by their uncertainties. The row labeled

Cut Variable	Bound	Nominal	1σ	$\delta\epsilon$
Cor S1B	lower	50	5	$(-)1.03 * 10^{-2} (+)1.05 * 10^{-2}$
Cor S1G	lower	2000	50	$(-)7.41 * 10^{-4} (+)4.23 * 10^{-4}$
Cor S1G	upper	None	–	$(-)1.42 * 10^{-3} (+)0$
Total Cor S2	lower	350000	21200	$(-)4.58 * 10^{-3} (+)4.48 * 10^{-4}$
Total Cor S2	upper	700000	16300	$(-)1.28 * 10^{-4} (+)3.24 * 10^{-5}$
Cor Energy	total	–	–	$(-)7.61 * 10^{-4} (+)7.61 * 10^{-4}$
Total	–	–	–	$(-)1.14 * 10^{-2} (+)1.05 * 10^{-2}$

Table 4.5: Uncertainties on the cut boundaries and efficiency changes associated with the conversion from simulation to data are shown. The cut bound edge is indicated in the "bound" column (either upper or lower). The nominal simulation value of the cut and the uncertainty on the bound are indicated in the "Nominal" and " 1σ " columns respectively. Efficiency changes from varying the cut boundaries by their uncertainty are shown in the $\delta\epsilon$ column. The efficiency changes are used as the uncertainty on the fast simulation efficiency. The efficiency change from both bounds of the energy is the total efficiency loss of the energy cut. The quadrature sum of all efficiency losses or gains is indicated in the "Total" row. The total systematic uncertainty on the fast simulation efficiency is 0.011.

"Total" indicates the quadrature sum of all terms above contributing to either an efficiency loss or an efficiency gain. The positive and negative contributions result in nearly identical efficiency changes. The fast simulation uncertainty is dominated by the efficiency change from the 10% uncertainty related to the lower bound of the S1B. The systematic uncertainty on the fast simulation efficiency is $\sigma_{\epsilon_{fast}} = \pm 0.011$.

4.5.2 Full simulation cuts

Full chain detector simulations are used to evaluate the efficiency of cuts that require information about individual PMTs, the skin veto, or the outer detector veto. These simulations are less frequently relied upon and even less well tuned to detector conditions than the fast simulations. The reconstructed magnitudes of S1s, S2s, and energies from full simulation events may differ significantly from real data events with the same energy.

Energy-related cut efficiency is not evaluated in the full simulation, however, it is nec-

essary to begin the full simulation cut efficiency evaluation with a population of events that is similar to the population passing the fast simulation cuts. Thus, the full simulation events are adjusted to force their S1 and S2 distributions to roughly match the fast simulations. In this way, events that would be removed by the energy cuts are not double counted as efficiency losses if they also fail a veto cut, for instance. Once adjusted, the fast simulation cuts can be applied to the full simulation events before the full simulation efficiency is evaluated. The S1G upper bound is set to the data equivalent value of 3400 phd to mitigate abnormally high S1Gs in the full simulation.

Around 100000 full chain simulation events are generated. The full simulation cuts include the S1G TBA, the S1 δ TBA, the skin veto, and the outer detector veto. The S1G TBA cut is a component of the selection criteria. A cut on S1B TBA is also present in the selection criteria. The S1B TBA cut is fully eclipsed by the S1 δ TBA cut, so the S1B TBA's efficiency is evaluated as a part of the S1 δ TBA cut. All TBA cuts in the selection criteria are removed for the full simulation efficiency evaluation. The spatial position of events passing all fast simulation cuts is given in Fig. 4.48.

Full simulation detector response adjustments

Several aspects of the full simulation spectra may differ from the fast simulation spectra, but the most significant factor is likely to be the g_1 (prompt scintillation light collection efficiency, phd/photon) and g_2 (free charge gain, phd/electron) used to generate the simulations. The fast simulations are generated with LZ's measured WS2024 parameters, $g_{1, WS2024}$ and $g_{2, WS2024}$. The simplest way to adjust the full simulation is to multiply the S1s and S2s by a factor related to the WS2024 and full simulation simulation parameters, $g_{1, full}$ and $g_{2, full}$. This is shown in Eq. 4.7 and Eq. 4.8.

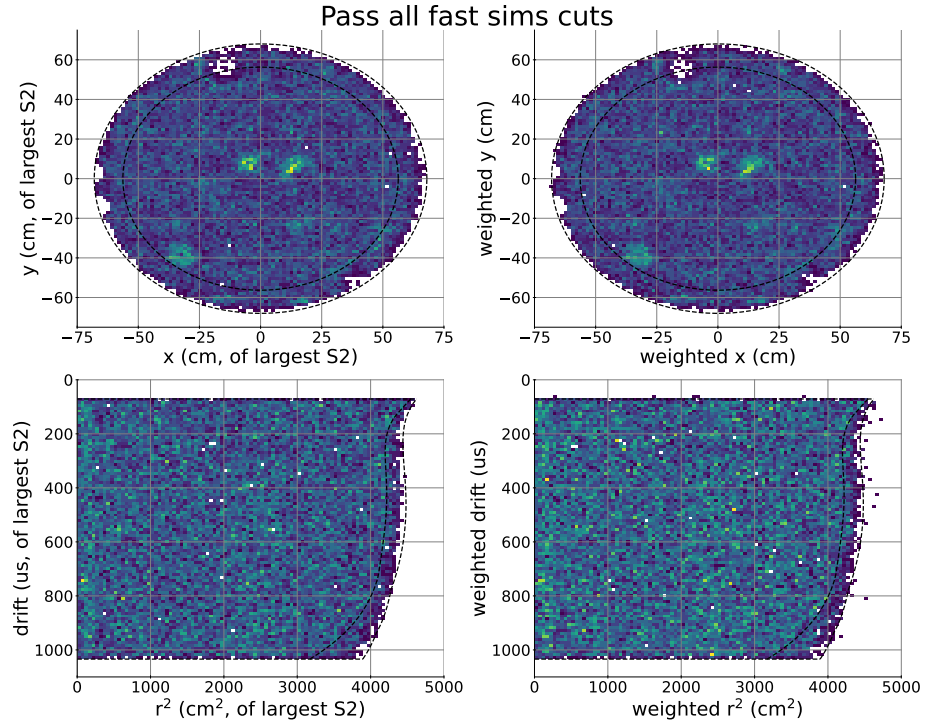


Figure 4.48: The spatial distribution of the 41475 full simulation events passing all fast simulation cuts is shown. This plot follows the same conventions as Fig. 4.33, with the largest S2 position plots on the left and the weighted position plots on the right. The top plots show the X-Y position of events while the bottom plots show the r^2 and drift time. This is the starting distribution for the fast simulation cuts. Certain areas within the X-Y plot appear significantly more populated than others. This is likely the product of imperfect position reconstruction near dead PMTs, not a genuine over-density of events.

$$S1_{adj} = S1_{full} * \frac{g1, WS2024}{g1, full} \quad (4.7)$$

$$S2_{adj} = S2_{full} * \frac{g2, WS2024}{g2, full} \quad (4.8)$$

The adjustments to S1 and S2 are not required to be exact. The full simulation spectra must match only to the degree that a population of events similar to the population passing all fast simulation cuts is used as a starting point for the full simulation efficiency evaluation. The LZ WS2024 g_1 is 0.1122 and g_2 is 34.02. $g1, full$ is set by eye to 0.1045 and yields the spectra shown in Fig. 4.49 and Fig 4.50. Only events passing the S1 δ time, fiducial, and selection criteria cuts are included in the spectra.

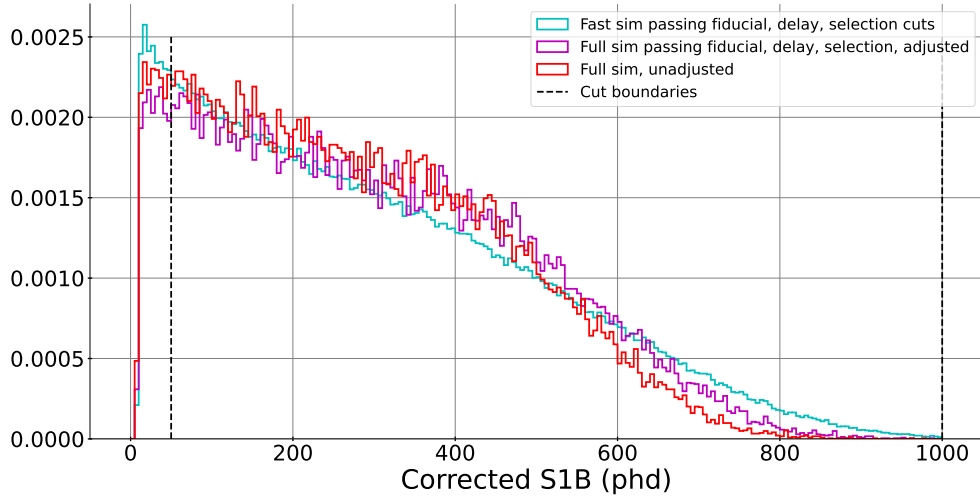


Figure 4.49: The corrected S1B distribution of full simulation events passing the initial cuts before adjustment (red) and after adjustment (magenta) is shown. The corrected S1B distribution of fast simulation events (cyan) passing the same cuts is also displayed. The S1B cut boundaries are indicated.

The cut boundaries on each plot reveal that, even without scaling the S1s, no significant fraction of events was lost or gained between the fast simulation and full simulation. The

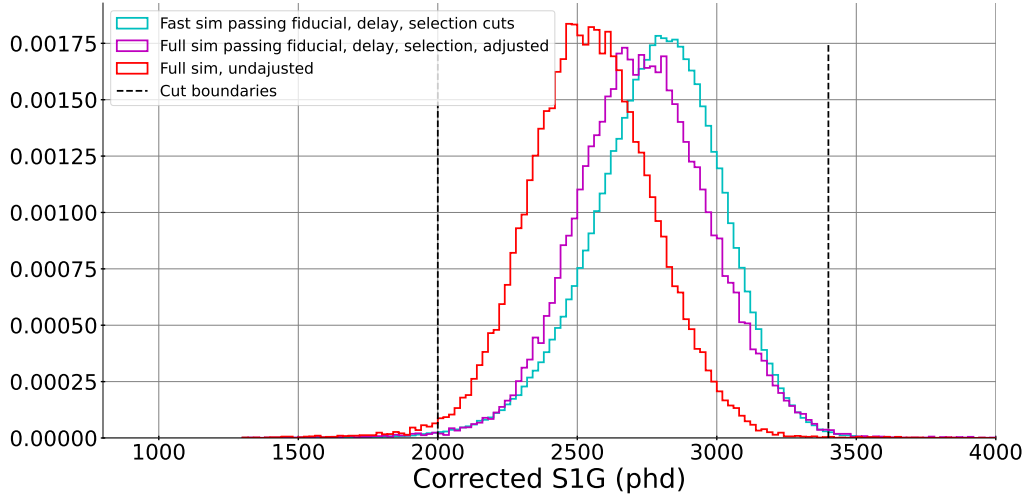


Figure 4.50: The corrected S1G distributions of full simulation events passing the initial cuts before adjustment (red) and after adjustment (magenta) are shown. The corrected S1G distribution of fast simulation events (cyan) passing the same cuts is also displayed. The simulation S1G cut boundaries are indicated. The upper S1G bound of 3400 phd is also included.

g_1 values used in earlier versions of the simulations were expected to be similar to the WS2024. It is unsurprising that only a small change was needed to match the S1s.

The S2 adjustment is far more significant because the charge gain is sensitive to the extraction region voltages. Extraction region voltages changed several times since the detector was first commissioned. The chosen $g_{2, full}$ of 66.0 yields the S2 spectrum shown in Fig. 4.51. The energy spectrum resulting from the combined adjustments is shown in Fig. 4.52.

The fast and unadjusted full simulation S2 spectra disagree by about a factor of two. Both the total corrected S2 and the corrected energy spectra show improved agreement with the fast simulation spectra after adjustment. This is sufficient for performing the full simulation efficiency evaluation.

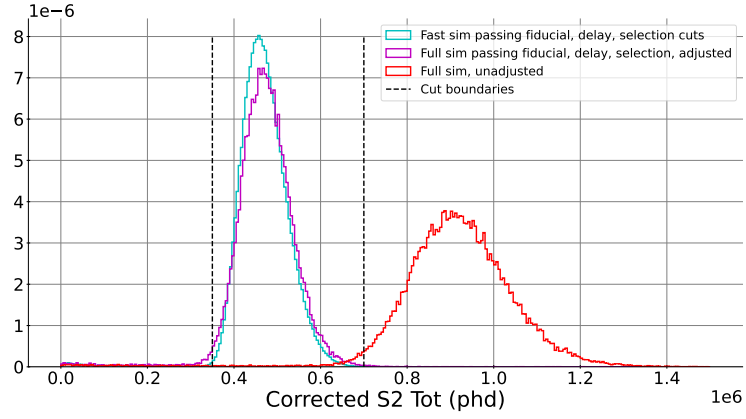


Figure 4.51: The corrected total S2 distributions of full simulation events passing the initial cuts before adjustment (red) and after adjustment (magenta) are shown. The corrected total S2 distribution of fast simulation events (cyan) passing the same cuts is also displayed. The simulation total S2 cut boundaries are indicated.

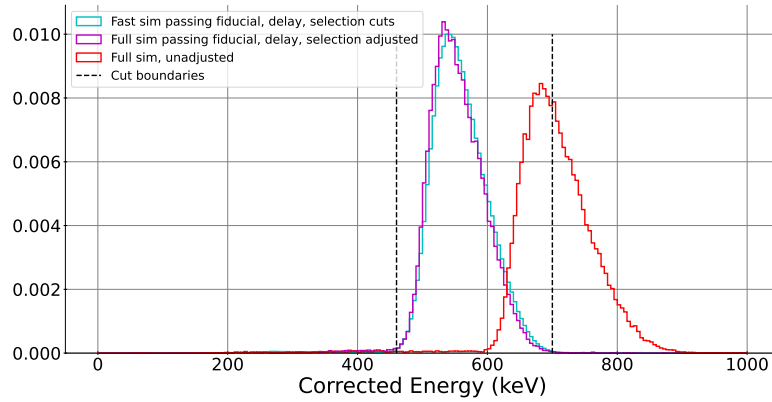


Figure 4.52: The corrected energy distributions of full simulation events passing the initial cuts before adjustment (red) and after adjustment (magenta) are shown. The corrected energy distribution of fast simulation events (cyan) passing the same cuts is also displayed. The energy cut boundaries are indicated.

Top-bottom asymmetry cuts

The two top-bottom asymmetry cuts used in the ^{85}Kr excited state decay measurement are the S1G TBA and the S1 δ TBA. TBA is indicative of the relative amount of light collected by the top and bottom PMT arrays (recall the definition of TBA from Eq. 4.2). An event's S1 TBA is correlated with its drift time: more light is collected in the top PMT array for S1s produced higher in the TPC. The average S1 TBA is preferentially negative, implying more light is collected by the bottom array. This is mostly due to total internal reflection at the Xe liquid surface (see section 2.2.1 for further discussion).

The standard deviation of the S1 TBA for events at a fixed depth decreases as S1 magnitude increases. At S1 sizes in the S1G range, the S1 TBA is almost always negative. A negative S1G TBA is required by the selection criteria to reject decays in the gaseous region. Because the standard deviation of the TBA is larger for the S1B, the S1B TBA upper bound (as a component of the selection criteria) is raised to 0.25.

Fig. 4.53 shows the S1G TBA distribution of all full simulation events passing the fast simulation cuts.

41475 full simulation events pass the selection criteria (excluding TBA cuts), S1 δ time, fiducial, and fast simulation cuts. 40848 events (98.5%) pass the S1G TBA cut. An additional 5% of all events are rejected when the upper bound is lowered to just -0.05. This is seen in Fig. 4.54.

Because the energy deposited by an excited state ^{85}Kr decay is localized to a small volume, the S1B and S1G TBAs should be similar. While the S2 localization variable compares the spatial proximity of S2s in an event, the S1 δ TBA compares the implied relative height of S1s. S1 δ TBA is defined as $\delta TBA = TBA_{S1G} - TBA_{S1B}$. An isolated flash of S1 light near the bottom of the detector paired with a valid S1-S2 pair near the top of the detector would be removed by the S1 δ TBA cut.

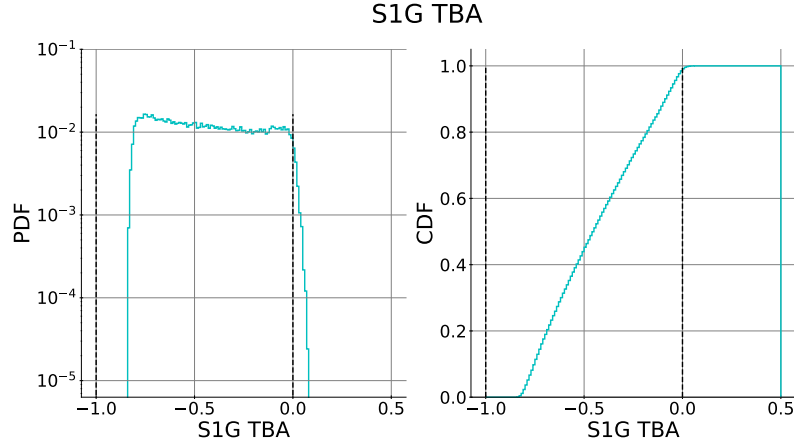


Figure 4.53: The probability density (left) and cumulative distribution (right) of the S1G TBA of full simulation events passing all prior cuts is shown. The cut boundary of 0 is indicated by a dashed line. 98.5% of events passing the previous cuts pass the S1G TBA cut. This cut is implicit in the selection criteria, but cannot be evaluated with the fast simulations.

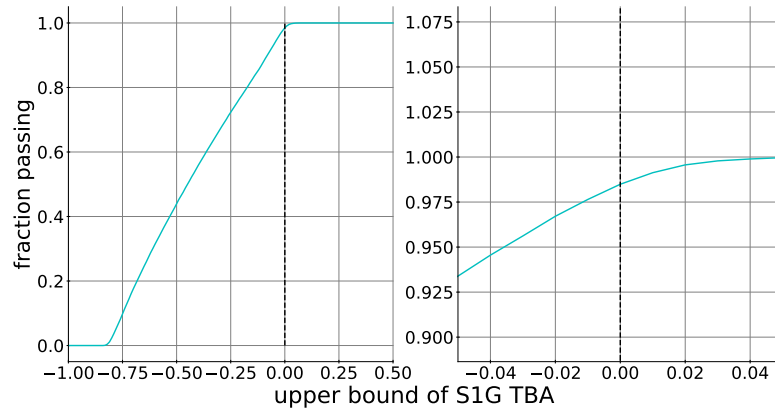


Figure 4.54: The fraction of events passing previous cuts that pass the S1G TBA cut as a function of the specified upper bound is plotted. The right plot contains the same information as the left plot, but is magnified in on the region of the cut's upper bound. A small change in the cut bound significantly changes the fraction of rejected events.

The S1 δ TBA cut range is -0.25 to 0.25. The fraction of events rejected by the S1 δ TBA cut includes the rejected events from the S1B TBA cut ($TBA_{S1B} \leq 0.25$) in the selection criteria. A plot of the S1 δ TBA spectra for events passing all initial cuts, all fast simulation cuts, and the S1G TBA cut is displayed in Fig. 4.55.

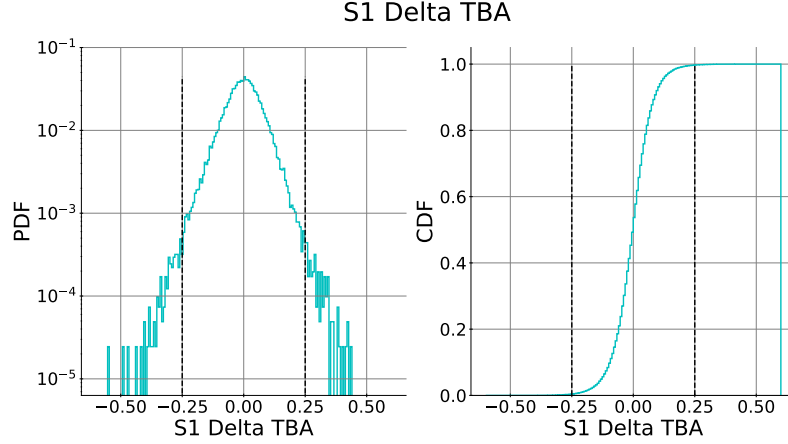


Figure 4.55: The probability density (left) and cumulative distribution (right) of the S1 δ TBA of full simulation events passing all prior cuts is shown. The cut boundaries of -.25 and .25 are indicated by dashed lines. 99.3% of events passing previous cuts pass the S1 δ TBA cut.

The percentage of events passing previous cuts that pass the S1 δ TBA cut is 99.3%. The distribution is fairly symmetric around 0 indicating that neither TBA is preferentially higher than the other. Tightening the cut bound to ± 0.2 does not sharply reduce the passing event fraction. The S1B TBA and S1G TBA distribution of all events passing the fast simulation cuts is shown in Fig. 4.56. The cut boundaries are indicated on the plot.

Veto Cuts

The two veto detectors, the Xe skin and the outer detector, are intended to reject events entering or exiting the TPC. The skin veto detector is discussed further in section 2.3. A γ entering the TPC may pair with an independent interaction inside the TPC to create an

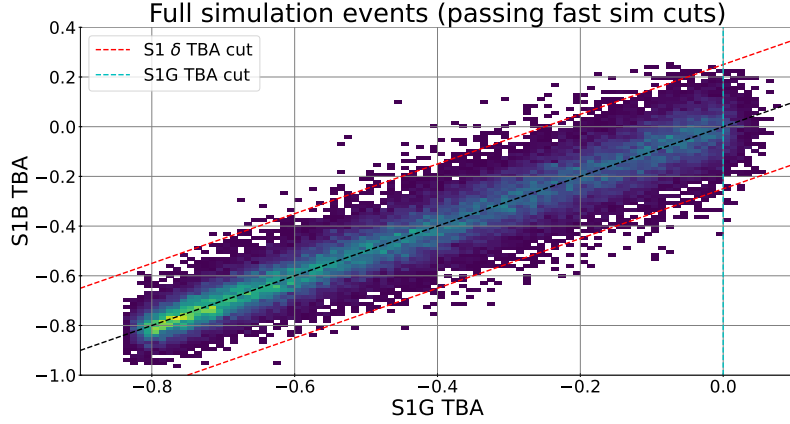


Figure 4.56: The S1B TBA and S1G TBA distribution of fast simulation events that pass all cuts (before the TBA cuts) is shown. The S1G TBA cut bound is indicated by a dashed cyan line and the S1 δ TBA is indicated by dashed red lines. The S1B TBA = S1G TBA line is plotted in dashed black. The majority of events are clustered around this line.

excited state ^{85}Kr -like event. The skin may capture scintillation light from the γ as it enters to tag and reject the event. Between the skin veto and the fiducial volume cut, most γ s entering the TPC are rejected or not observed in the search. A legitimate excited state ^{85}Kr event may partially escape the TPC and deposit energy in the skin, so an efficiency evaluation is still necessary.

The outer detector is discussed in section 2.4. The outer detector can detect γ s entering or exiting the TPC as well. Backgrounds interact in the outer detector, causing it to trigger at a given rate. Because the outer detector veto cut is used, legitimate ^{85}Kr events falling in the veto window cannot be captured. This manifests as a live time loss for the study. This is discussed further in section 4.6.2.

The skin and outer detector veto cuts used in this analysis are identical to those used in the LZ WS2024 science run. The cuts search for a veto detector pulse in a specified time window around the S1 arrival time of each event. In this case, both S1s are considered. The pulse in this window must meet specified magnitude, coincidence, and other requirements to reject the event. Both vetoes have a *prompt* and *delayed* component with different pulse

area requirements.

The efficiency of the skin and veto cuts is evaluated for full simulation events passing the initial, fast simulation, and TBA cuts. Both cuts are 100% efficient. The initial and fast simulation cuts remove all events that fail either veto cut.

Full simulation cut results

Table 4.6 summarizes the number of events passing the full simulation cuts.

	Total	% (after fast cut)	Cumulative	% (from prev)	ϵ (cumulative)
Fast Sims	41475	100	41475	100	1
S1G TBA	40848	98.5	40848	98.5	0.985
S1 δ TBA	41189	99.3	40571	99.3	0.978
Skin Veto	41475	100	40571	100	0.978
OD veto	41475	100	40571	100	0.978

Table 4.6: A summary of the number and percentage of full simulation events passing each cut is shown. All events are required to pass the initial and fast simulation cuts to be considered. After, all cuts can be evaluated independently of one another. The "Total" column indicates the number of events passing each cut independently. The "% (after fast cut)" column indicates the percentage of events passing the cut in that row out of the total number of events passing the fast simulation cuts. The "Cumulative" column indicates the total number of events passing the cut in that row and in all rows above. The "% (from prev)" column indicates the percentage of events passing the cut in that row out of the number of events passing all cuts in the rows above. The " ϵ (cumulative)" column indicates the cumulative efficiency of the cut in that row and all rows above. The full simulation cut efficiency is the cumulative efficiency after the outer detector veto cut: 0.978.

The 97.8% of events passing the initial and fast simulation cuts also pass the full simulation cuts. No events passing the initial and fast simulation cuts are removed by the vetoes. Fig. 4.57 shows the spatial position of events passing all cuts. This should be compared with Fig. 4.48.

There is no clear spatial bias present in the remaining events compared to the starting population of events. The distribution of event S1 δ time before and after the full simulation

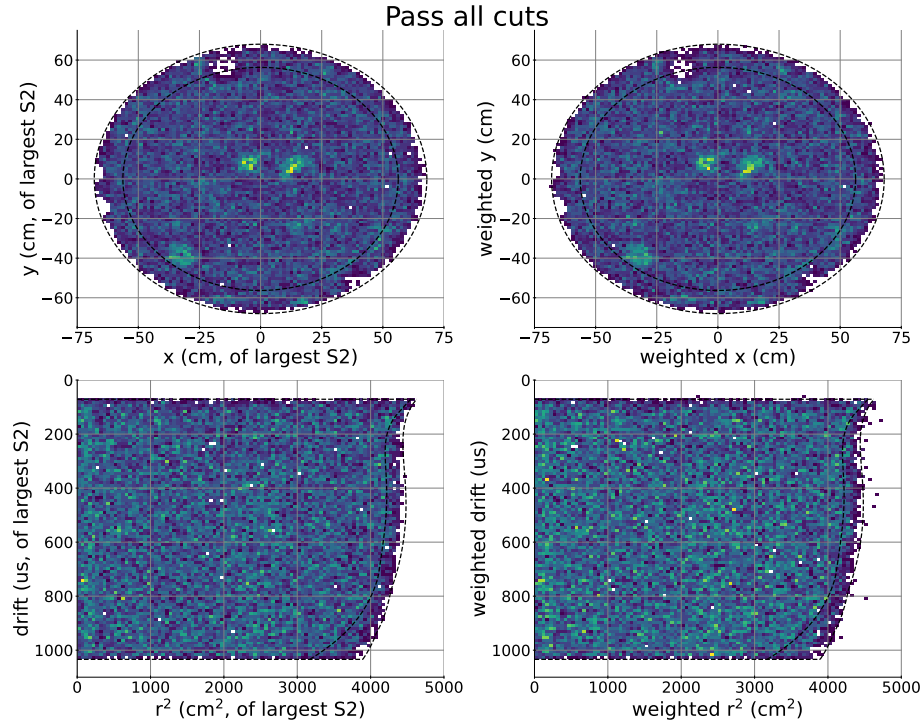


Figure 4.57: The spatial distribution of full simulation events passing all cuts is plotted. This plot follows the same plotting conventions as Fig. 4.48 with the largest S2 position plots on the left and the weighted position plots on the right. The top plots show the X-Y position of events while the bottom plots show the r^2 and drift time. The fiducial boundaries are again indicated with dashed lines. The final fast simulation distributions show no evidence of spatial bias relative to their initial distribution from Fig. 4.48.

cuts is shown in Fig. 4.58

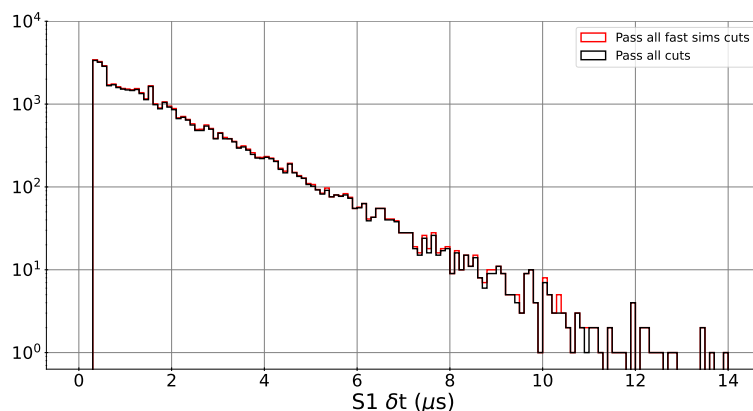


Figure 4.58: The S1 δ time distribution of full simulation events passing the fast simulation cuts (red) and events that passed all full simulation cuts (black) is shown. The full simulation cuts show no indication of biasing the S1 δ time in a way that would change the expected exponential distribution of candidate ^{85}Kr events.

The events failing the fast simulation cuts do not appear to exhibit any significant bias in S1 δ time. This is another indication that fitting to an exponential in S1 δ time is still a valid way to assess the number of signal counts in real data.

S1 TBA vs drift model toy Monte Carlo and systematic evaluation

The TBA cut event loss evaluations are entirely reliant on the full simulation framework to accurately model the TBA. When initially implemented, the full simulation TBA output was tuned using calibration data. The TBA is not likely to have changed much between SR1 and WS2024, but small factors like (recently) deactivated PMTs could affect TBA. An updated, calibration-informed verification of the TBA from the full simulations is desirable.

A cut comparing the drift time and S1 TBA was developed to exclude accidental events in the LZ WIMP search. This model was informed by CH_3T calibration data from April and May 2023, discussed in section 5.4.3. This calibration dataset includes both ^3H and

^{14}C decays, extending to the ^{14}C Q-value of 156 keV in energy.

The cut receives a drift time and a *raw* (or uncorrected) S1 area as an input before determining the expected mean TBA (via a 4th order polynomial fit) and standard deviation of the TBA. The cut then verifies the measured TBA is within three sigma of the expected TBA. Events with measured S1 TBAs exceeding three standard deviations from the mean S1 TBA given the event's drift time and raw S1 area are removed. The cut itself is not applied to the excited state ^{85}Kr search, however the estimated mean TBA and standard deviation of the TBA calculated within the cut can be useful for crosschecking the TBA efficiency loss evaluations of the full simulation framework.

The crosscheck is a toy Monte Carlo simulation that is applied outside of the full simulation and fast simulation frameworks. It uses the raw S1 areas and drift times from events surviving the fast simulation as a starting point. The general procedure is given below.

1. Begin with raw S1G, raw S1B, and drift time output of fast simulation
2. Transport the β a distance that is determined by an exponential distribution with a mean of 3 cm
3. Determine the Z projection of the transport distance using a cosine distribution and convert to a new temporary S1B drift time
4. Feed the raw S1B area and temporary S1B drift time to the functions used to calculate the expected mean and standard deviation of the S1B TBA
5. Repeat the previous step for the S1G using the raw S1G area and recorded event drift time
6. Generate TBAs from a normal distribution using the respective calculated mean and standard deviation for each S1

The recorded drift time of an event is the time between the largest (corrected) S1 and the largest S2 of the event. This time is most likely associated with the (first) γ interaction, so the toy Monte Carlo displaces the β by a distance drawn from an exponential distribution

with a mean corresponding to the mean γ travel distance of about 3 cm. This is projected in the Z direction and converted to a drift time.

The mean TBA for an event with a given raw S1 magnitude and drift time is modeled using the 4th order polynomial. The standard deviation of the TBA is determined by the mean TBA, the raw S1 area, and several parameters obtained by fitting to ^3H and ^{14}C calibration data. Both S1 TBAs are drawn from a Gaussian random variable dictated by each S1's respective mean TBA and expected standard deviation.

533458 events passed the fast simulation cuts and were delivered to the toy Monte Carlo. The S1B TBA is plotted against the S1G TBA in Fig. 4.59.

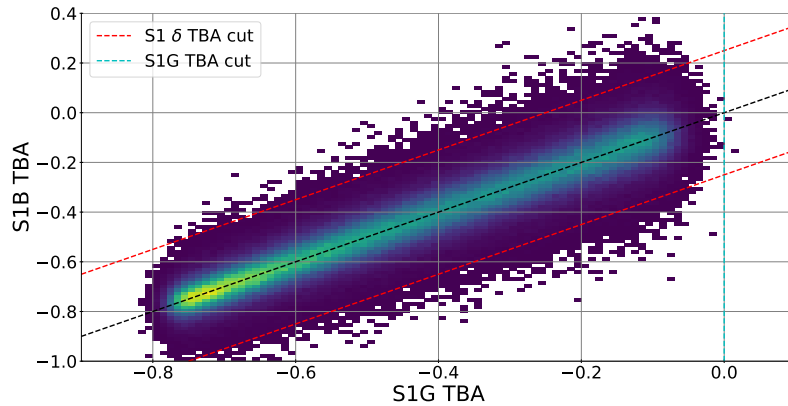


Figure 4.59: The distribution of the S1B TBAs and S1G TBAs generated by the toy Monte Carlo simulation is shown. The initial positions and S1 areas are drawn from fast simulation events passing all fast simulation cuts. This histogram can be compared with Fig. 4.56. This histogram has noticeably fewer events with S1G TBAs that exceed 0 but otherwise looks similar.

Of the initial 533458 events simulated with this method, 99.50% passed the S1 δ TBA cut, compared to 99.31% for the full simulation. The most glaring difference between the toy Monte Carlo and the full simulation is the absence of events with S1G TBAs exceeding 0. The S1G TBA cut removes 1.5% of events in the full simulation but removes only three in the toy Monte Carlo. Otherwise, the general shape of the distributions is similar. The

toy Monte Carlo S1 δ TBA and drift time distribution is shown in Fig. 4.60.

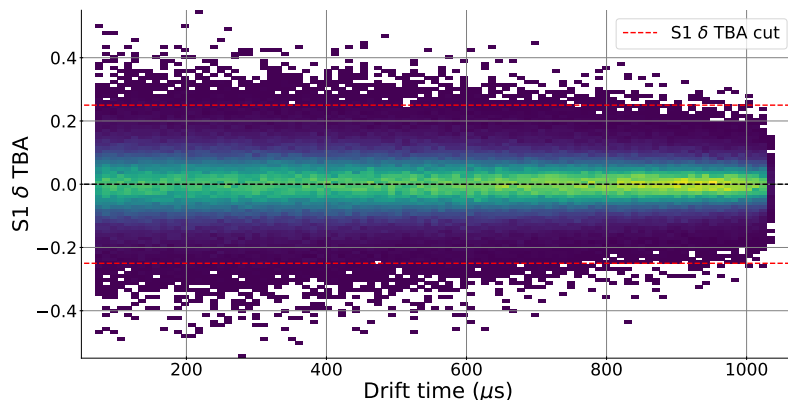


Figure 4.60: The distribution of the S1 δ TBAs generated by the toy Monte Carlo and the drift time from the fast simulation output is shown. The S1 δ TBA cut bounds are indicated in red. The distribution is wider near the top of the detector.

The toy Monte Carlo is limited in several respects. For simplicity, the γ is assumed to interact just once. In reality, the γ may Compton scatter multiple times before being photo-absorbed. However, each successive scatter lowers the photon's energy and reduces its mean travel distance. Though it is an underestimate, the approximately 3 cm mean distance between the β and (single) γ interactions should be sufficient to crosscheck the full simulations. This approximation would likely result in a slight overestimate of efficiency.

The γ is more likely to be associated with the (largest) S2 used to determine the drift time than the β . However, the choice to always displace the β neglects the instances where the largest S2 includes all the β energy and some fraction of the γ energy, perhaps its second or third largest energy deposit. The uncertainty in drift time is an unavoidable problem for both the toy Monte Carlo and the main analysis.

The function used to calculate the spread in TBA for a depth and S1 area is validated by calibration data that only extends to energies reaching the ^{14}C Q-value of 156 keV. The modeled TBA may not accurately extrapolate to S1s produced by 514 keV γ s. Less

significant shortcomings of the simulation include the lack of consideration given to the radial position of events and the non-Gaussian nature of the TBA distribution when the mean TBA is near ± 1 (its physical boundary).

The full simulation and the toy Monte Carlo are not in perfect agreement. However, both suggest the TBA related efficiency loss is quite small. There are questions regarding both estimations of TBA efficiency loss. The difference between the cut efficiency of the toy Monte Carlo and the full simulation is the systematic uncertainty on the full simulation efficiency: $\sigma_{\epsilon_{full}} = 0.0177$. The statistical uncertainty is negligible.

4.5.3 Simulation efficiency summary

The efficiencies of the fast simulation cuts ϵ_{fast} (0.822), the full simulation cuts ϵ_{full} (0.978), and the S1 δ time cut $\epsilon_{0.3\mu s}$ (0.815) are assumed to be independent and are multiplied to determine the final efficiency, ϵ , using Eq. 4.9.

$$\epsilon = \epsilon_{fast} * \epsilon_{full} * \epsilon_{0.3\mu s} \quad (4.9)$$

The total efficiency of all cuts, ϵ from Eq. 4.1, is 0.655. The statistical uncertainties on the efficiencies are negligible compared to the systematics. The systematic uncertainty on the fast simulation cut efficiency $\sigma_{\epsilon_{fast}}$ (0.011) and the systematic uncertainty on the full simulation cut efficiency $\sigma_{\epsilon_{full}}$ (0.017) are propagated to determine the uncertainty on the efficiency, $\sigma_{\epsilon} = 0.014$.

4.6 Data exclusion and live time evaluation

A number of pathologies in data are not present in simulations. Periods of low quality detector behavior, external interference (from muons, for instance), or intentional changes

to the detector are identified in LZ. The pathology or change associated with each period is determined to be either disruptive or benign for properly identifying excited state ^{85}Kr decays and must be removed from the analysis if necessary. This removal represents a live time loss. The proper live time associated with the search can be computed after the appropriate periods are removed.

4.6.1 Detector time window and event exclusion cuts

The cuts applied to the search include cuts on time periods of elevated single electron and S2 rates, elevated single photoelectron and S1 rates, PMT trips, muon energy depositions, TPC burst noise, outer detector burst noise, poor PMT behavior, and poor event start DAQ buffer quality. All of these cuts are identical to those used in the LZ WIMP search. Several more exclusion cuts from the LZ WIMP search are not used in this analysis. The absent cuts are primarily optimized for single scatter searches at lower energies.

Large S2s, like those following a muon event, may bury or obscure an excited state ^{85}Kr decay in LZ. Alternatively, a pathological source of S1 light may pair with a real decay to mimic an excited state ^{85}Kr event. The muon cut, TPC burst noise cut, elevated single electron and S2 rate cut, and elevated single photoelectron and S1 rate cut are intended to remove periods when an excited state Kr event may be lost within a larger signal or may be fabricated by an accidental coincidence.

Muons entering the TPC are often followed by elevated S2, electron, and photoelectron rates. The *muon cut* excludes all events occurring in the 20 seconds that follow. Occasionally, and often following a muon, large bursts of S2s occur in the TPC. These bursts may happen milliseconds to 100's of seconds after the muon. All events during the bursts are removed by the *TPC burst noise cut*. Periods of high S1, S2, electron, and photoelectron rates can present without a muon. The *elevated single electron and S2 rate cut* removes pe-

riods of abnormally high electron emission. Sustained rates of electron emission are often localized to specific X-Y positions. These are referred to as *hot spots*. The *elevated single photoelectron and S1 rate cut* removes periods with excessively high rates of scintillation light.

The outer detector is known to observe large, sudden bursts of energy, similar to the TPC. These are not correlated with muons. Though signals in the TPC may not be affected by an outer detector noise burst, the presence of the burst may hide an outer detector veto signal that would otherwise reject the event. The *outer detector burst noise cut* is implemented to remove time periods when the outer detector is unable to detect potential veto signals.

The DAQ buffers can occasionally be filled at the start of an event. There may be information lost from individual PMTs when this happens, resulting in artificially smaller summed waveforms. The *DAQ buffer start cut* rejects events which have their buffers filled at the start (the time of the S1) of an event. Time periods when individual PMTs were functioning improperly are removed by the *PMT trip cut*.

4.6.2 Live time evaluation

A proper evaluation of the ^{85}Kr excited state measurement live time is non-trivial. The total number of calendar days spanned by the WS2024 period is 370.1 days. Of this, 265.5 days of WIMP search data are used for the excited state decay measurement. The data acquisition system (DAQ) is limited in its ability to collect and digitize all signals. Once an event window ends, a hold off is imposed before the DAQ can collect more data, allowing the buffers time to unload. The *physics live time* in which the DAQ could record an event if it had occurred is estimated to be 252.4 days. A complete application of all WIMP search exclusion and live time influencing cuts reduces live time for the LZ WIMP search in the

WS2024 period to 220.0 days [67].²

The live time for the WS2024 excited state ^{85}Kr measurement is expected to be somewhere between the 220.0 days quoted for the WIMP search and the 252.4 days when a WIMP event could be captured by the DAQ. The absence of several WIMP search exclusion and live time influencing cuts allows for more excited state decay measurement live time. The most significant live time reduction in the WIMP search is the result of the *electron train* veto, removing nearly 10% of the physics live time. This veto is intended to reject events with long tails of single electrons and small S2s that follow the primary S2(s). These tails may bleed into subsequent events which are also vetoed. These electron trains are rarely caused by events in the WIMP energy range but are more common for higher energy events. Many excited state decay candidates were found to cause electron trains, requiring that the cut not be applied. Thus, the live time for this search is expected to be closer to 252.4 days than 220.0 days.

Several of the discussed exclusion cuts simply block out macroscopic windows of time related to degraded detector performance. These are simple to handle: no live time is accrued when the exclusion cuts are active because legitimate excited state decays are rejected when the exclusion cuts are active. Any legitimate excited state decays with an S1 occurring during the skin and outer detector veto windows are rejected. The outer detector veto and skin veto reduce the measurement live time.

The largest live time loss for this search is due to the outer detector veto. The outer detector's background rate, discussed in section 2.4, is primarily to blame for this. The dead time of this cut in isolation was extensively studied and determined to be 2.50% for the WS2024 period. Combining this with the skin veto results in a live time of about 97% between the two vetoes.

²It should be noted that the WS2024 WIMP search period includes a small number of additional data files that are not in the excited state ^{85}Kr decay measurement period. The WIMP search physics live time is about three days greater than the excited state ^{85}Kr decay measurement live time.

A summary of the live time losses accrued during the WS2024 period is given in Table 4.7. The live time of the WS2024 excited state ^{85}Kr decay search is 242.5 days. This is the value of t in Eq. 4.1.

	Time (d)	% of physics live time
Total time elapsed	265.5	N/A
Physics live time	252.4	100
High single photoelectron / S1	252.0	99.86
High single electron / S2	251.3	99.58
PMT trip	252.0	99.86
Muon	251.9	99.79
TPC burst	252.2	99.91
OD burst	252.4	>99.99
Buffer start	252.3	99.95
Veto detectors	244.8	97.00
All exclusion cuts	242.5	96.08

Table 4.7: The live time losses from all exclusion cuts are summarized. All events following the physics live time can have their live times evaluated independently of each other. The physics live time retained by each cut independent of the others is indicated in the "Time (d)" column. The percentage of physics live time retained by each cut is noted in the column "% of physics live time". The total live time for the WS2024 excited state ^{85}Kr decay is given in the "All exclusion cuts" row: 242.5 days. Note that adding the losses from each cut does not sum to the total lost percentage of physics live time in the "All exclusion cuts" row because some periods of time are affected by multiple exclusion cuts.

4.7 Results and Discussion

The S1 δ time distribution of real WS2024 events passing all ^{85}Kr excited state decay cuts is shown in Fig. 4.61. Event S1 δ times are fitted to Eq. 4.3 using an unbinned maximum likelihood fit with τ fixed to the ^{85m}Rb excited state mean life, $\tau = 1.464\mu\text{s}$. The fit is shown in the plot.

27 events pass all cuts and appear in the plot. A very clear signal is seen in the low S1 δ time region. Seven events have S1 delay times between 0.3 and 1.3 μs and are in the

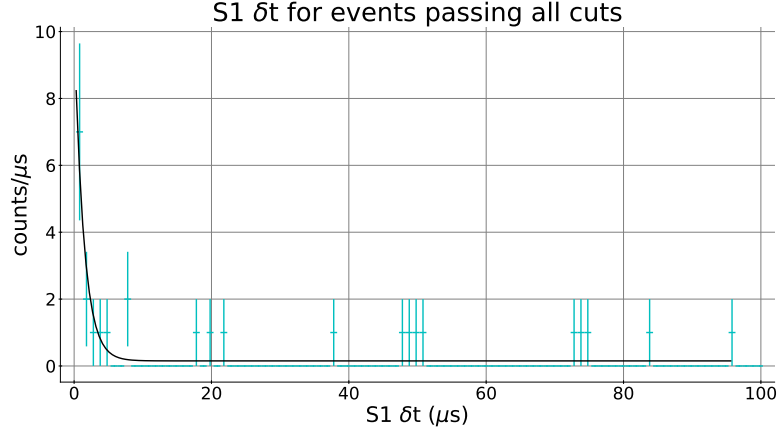


Figure 4.61: The S1 δt of the 27 WS2024 events passing all cuts are histogrammed and maximum likelihood fit (unbinned) to an exponential plus constant. The fitting window extends from $0.3 \mu s$ to $100.3 \mu s$. The mean life of the decay term is fixed to $\tau = 1.464 \mu s$. The fit parameters are $A = 9.91^{+3.32}_{-2.74}$ (amplitude of the exponential) and $B = 0.15 \pm 0.04$ (value of the constant). Each bin is $1 \mu s$ wide. The error bars on the plot are not used in any calculations and are for display only.

first bin. An additional five events are in the next four $1 \mu s$ time bins. The fitted amplitude of the exponential (signal) term A is $9.91^{+3.32}_{-2.74}$ and the constant (background) term B is 0.15 ± 0.04 . Fig. 4.62 focuses tighter on the signal region, displaying only the first $20 \mu s$ with finer binning.

The data and fit appear to be in good agreement, providing clear evidence that the signal is consistent with the excited state decay of ^{85}Kr . This is further confirmed by floating τ in the fit: $\tau_{\text{floated}} = 1.31^{+0.83}_{-0.51} \mu s$. τ_{floated} is consistent with the known mean decay time.

The exponential term of Eq. 4.3 is inserted into Eq. 4.10 and integrated across the delay time window, $t_{\min} = 0.3 \mu s$ to $t_{\max} = 100.3 \mu s$ to get the number of signal counts, C from Eq. 4.1.

$$C = \int_{t_{\min}}^{t_{\max}} A * e^{-t/\tau} dt \quad (4.10)$$

The number of signal counts is $C = 11.83^{+3.96}_{-3.27}$. Eq. 4.1 is revisited to convert the num-

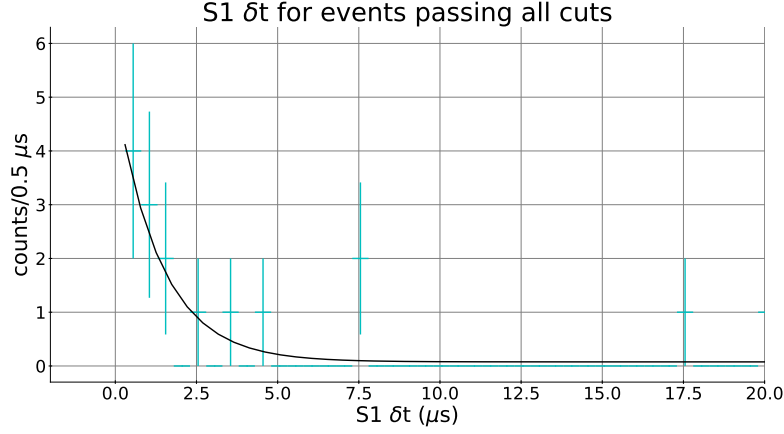


Figure 4.62: This plot contains the same data as Fig. 4.61 but magnifies the first 20 μs . The bin width is 0.5 μs . The binning and the error bars are, again, for display only and not used in any calculations. The fit and data agree across the low delay time period.

ber of signal counts, C , to a ^{nat}Kr concentration in LZ, $\Phi_{nat\text{Kr}}$, where $\tau_{85\text{Kr}} = 15.66\text{ y}$ is the mean life of ^{85}Kr , $M_{85\text{Kr}} = 1.41 \times 10^{-25}\text{ kg}$ is the mass of a ^{85}Kr atom, $t = 242.5/365.25\text{ y}$ is the detector live time during the search, $A_n = (2.0 \pm 0.2) \times 10^{-11}$ is the natural abundance of ^{85}Kr [57][58], $f_b = 0.0043$ is the decay branching fraction through ^{85m}Rb , $M_{Xe} = 5500 \pm 200\text{ kg}$ is the target mass (fiducial mass) of Xe, $m_{nat\text{Kr}} = 83.80\text{ amu}$ is the atomic mass of ^{nat}Kr , $m_{85\text{Kr}} = 84.91\text{ amu}$ is the atomic mass of ^{85}Kr , and $\epsilon = 0.655 \pm 0.014$ is the efficiency of all cuts.

$$\Phi_{nat\text{Kr}} = \frac{C * \tau_{85\text{Kr}} * M_{85\text{Kr}}}{t * A_n * f_b * M_{Xe}} \left(\frac{m_{nat\text{Kr}}}{m_{85\text{Kr}}} \right) \frac{1}{\epsilon} \quad (4.1)$$

The LZ WS2024 ^{nat}Kr concentration measured with the ^{85}Kr excited state decay is $\Phi_{nat\text{Kr}} = 124_{-37}^{+44}\text{ ppq (g/g)}$. This is less than, but consistent with, ^{nat}Kr concentration from the cold trap mass spectrometry measurements: $182 \pm 26\text{ ppq (g/g)}$. The measurements differ by 1.13σ .

4.7.1 Prompt and delayed event comparison

Events with an S1 δ time of less than $5 \mu\text{s}$ are more likely to be signal events, while events with an S1 δ time exceeding $10 \mu\text{s}$ are overwhelmingly expected to be backgrounds. The events are classified by their delay times. *Prompt* events have an S1 δ time of less than $5 \mu\text{s}$, and *delayed* events have an S1 δ time that exceeds $5 \mu\text{s}$. There are 12 prompt events and 15 delayed events. The number of integrated signal counts, $C = 11.83^{+3.96}_{-3.27}$, suggests that most, if not all, of the prompt events are excited state decays. Prompt events in the following plots are indicated in cyan, and delayed events are indicated in red. The corrected S1B histogram of events passing all cuts is shown in Fig. 4.63.

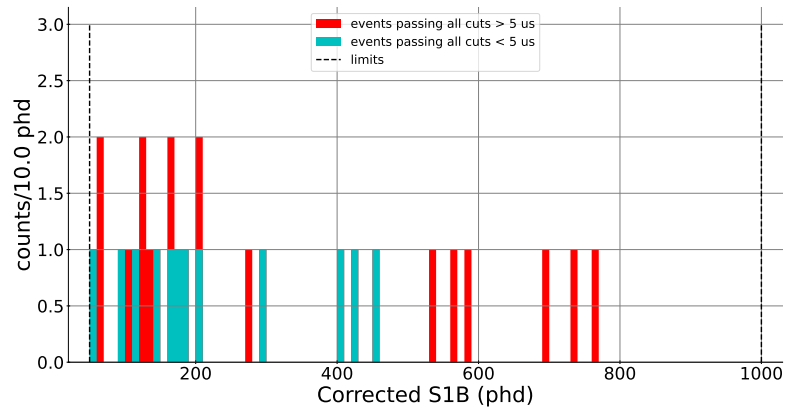


Figure 4.63: The corrected S1B histogram of events passing all cuts in the WS2024 period is shown. Prompt events are shown in cyan, and delayed events are shown in red. The cut bounds are drawn in black dashed lines. The histograms are stacked, meaning that a delayed events in the same bin as prompt events are placed on top of the prompt events. The bin width is 10 phd.

Prompt events are more dense at lower S1B areas. The expected distribution of true excited state decays is β -like. The fast simulation S1B probability density function is seen in Fig. 4.34, for comparison. The density function is plotted with a log scale, and only events inside of the cut boundaries should be considered. The prompt event distribution

appears consistent with the simulation distribution³. Background events are spread wider across the cut window but are most dense at low S1B areas.

The corrected S1G histogram of events passing all cuts is shown in Fig. 4.64.

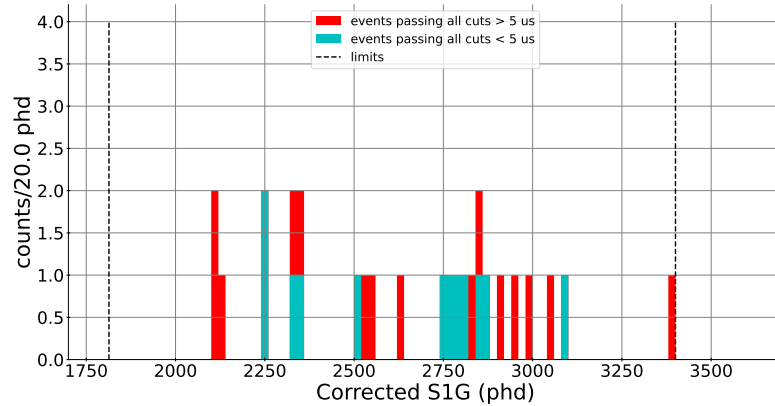


Figure 4.64: The corrected S1G histogram of events passing all cuts in the WS2024 period is shown. Prompt events are shown in cyan, and delayed events are shown in red. The (data equivalent) cut bounds are drawn in black dashed lines. The bin width is 20 phd.

The γ that produces the prompt scintillation light in an excited state decay is mono-energetic, but the γ energy deposit is subject to recombination that widens the S1G distribution. Poisson fluctuations on the number of scintillation photons reaching the PMTs, the PMT quantum efficiency, and double photo-electron effect contribute to additional smear in the S1G distribution. The fast simulation S1G probability density function is shown in Fig. 4.38. Comparing the prompt event distribution to the simulation density function is difficult due to low statistics, but no prompt events are within 300 phd of the cut boundaries, as expected.

The corrected total S2 histogram of events passing all cuts is shown in Fig. 4.65.

The corrected total S2 distribution for prompt events appears more Gaussian and has a

³Note, the probability density functions in section 4.5 display the density of events that pass only the cuts prior to the cut being discussed. For S1B, only the initial cuts have been applied. Cuts discussed after a given density plot in section 4.5 have not been applied. The density function changes slightly for events passing *all* cuts. This is true of all the probability density functions from section 4.5 that are referenced in this section.

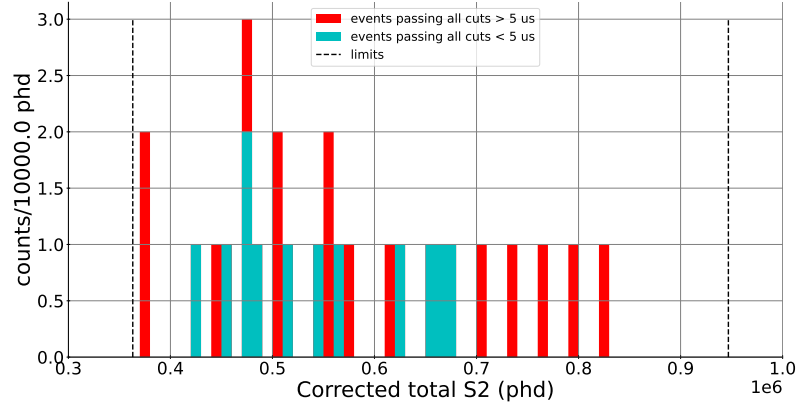


Figure 4.65: The corrected total S2 histogram of events passing all cuts in the WS2024 period is shown. Prompt events are shown in cyan, and delayed events are shown in red. The (data equivalent) cut bounds are drawn in black dashed lines. The bin width is 10000 phd.

smaller standard deviation than delayed events. This distribution is also subject to recombination fluctuations that smear the other distributions, and contains contributions from both the β and the γ . The corresponding probability density function is shown in Fig. 4.40. Recall from section 4.4 that the S2 distribution is observed to be wider in data than in simulation, which is why the cut boundaries differ. By eye, the prompt event distribution appears to be consistent with the simulation probability density function.

The corrected energy histogram of events passing all cuts is shown in Fig. 4.66.

Prompt events passing all cuts are clustered between 530 and 610 keV. Unlike the S1s and S2s, the energy distribution is not widened by recombination fluctuations. Fig. 4.43 shows the fast simulation energy probability density function (this can also be seen on a linear scale for all events passing initial cuts in Fig. 4.52). The prompt event distribution is consistent with the simulated distribution. No prompt events are measured with an energy below the γ energy or above the full decay Q-value (687 keV). The observed energy distribution strengthens the assertion that the prompt events are genuine excited state ^{85}Kr decays. Delayed events seem uniformly distributed throughout the full cut window.

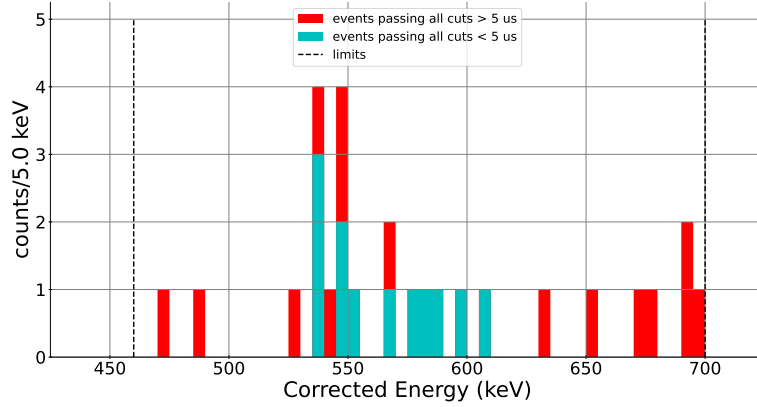


Figure 4.66: The corrected energy histogram of events passing all cuts in the WS2024 period is shown. Prompt events are shown in cyan, and delayed events are shown in red. The cut bounds are drawn in black dashed lines. The bin width is 5 keV.

The log of the corrected total S2 is plotted against the sum of the corrected S1 for events passing all cuts in Fig 4.67. The events are placed on top of the fast simulation total S2 vs total S1 efficiency plot.

Data and fast simulation events have different energy (S1 and S2) scales and, therefore, different cut values, as discussed in section 4.5.1. The prompt events carve out a narrow slice in energy and all fall on the bulk of the simulation events passing all cuts. The slight top left bias of the prompt events relative to the majority of the passing simulation events is consistent with the observations from section 4.4 regarding the underestimation of S2 and overestimation of S1 in the simulations.

The localization histogram of events passing all cuts is shown in Fig. 4.68.

The density function of localization of simulated events in Fig. 4.44 indicates that the majority of true excited state ^{85}Kr decays should at low localizations. The prompt events are consistent with that expectation. The delayed events are also found more often at low localizations.

The S1 δ TBA histogram of events passing all cuts is shown in Fig. 4.69.

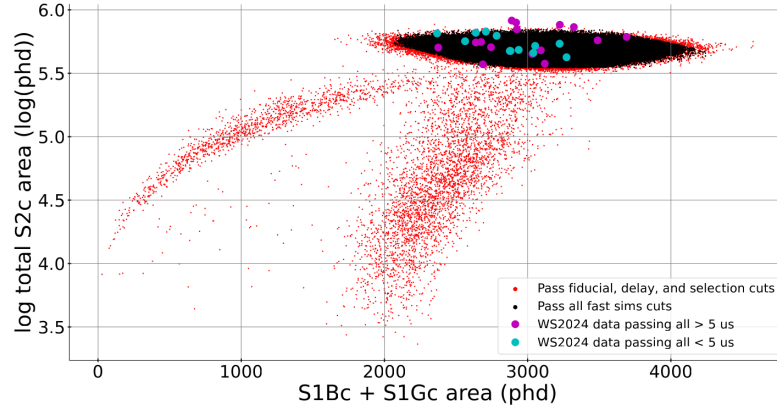


Figure 4.67: WS2024 events passing all ^{85}Kr excited state cuts are plotted by the $\log_{10}$ of total corrected S2 and sum of corrected S1B and corrected S1G. They are overlayed on the fast simulation events passing (black) and failing (red) the fast simulation cuts, as seen in Fig. 4.46. Prompt events are marked in cyan, but delayed events are marked in magenta. The simulation and data cut boundaries in both S1G and total S2 are different, which is why several WS2024 events are outside of the simulation cut region.

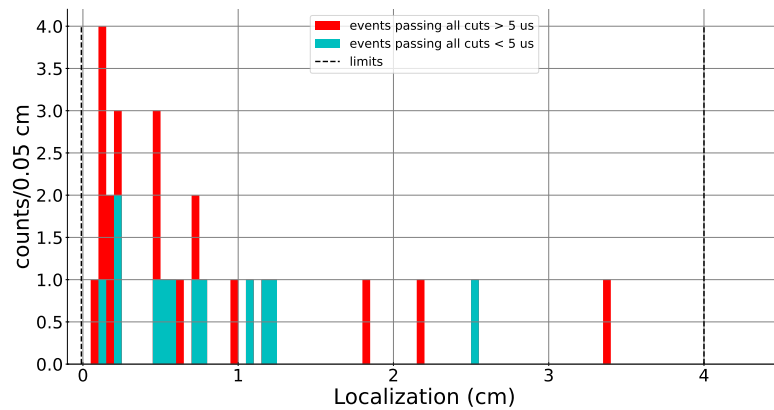


Figure 4.68: The localization histogram of events passing all cuts in the WS2024 period is shown. Prompt events are shown in cyan, and delayed events are shown in red. The cut bounds are drawn in black dashed lines. The bin width is 0.05 cm.

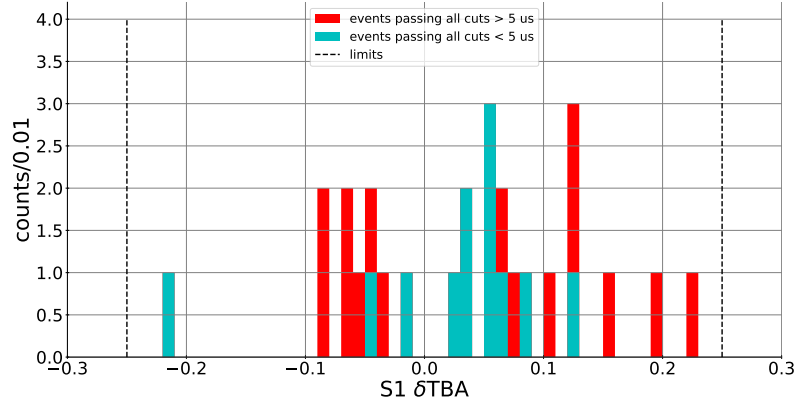


Figure 4.69: The S1 δ TBA histogram of events passing all cuts in the WS2024 period is shown. Prompt events are shown in cyan, and delayed events are shown in red. The cut bounds are drawn in black dashed lines. The bin width is 0.01. True excited state ^{85}Kr decays are expected to be symmetric about 0 based on the full simulation distribution. Statistics are low, but it appears there is a slight positive bias ($S1G > S1B$) in the S1 δ TBA of prompt events. The majority of prompt events still have TBAs near 0, as expected.

The S1 δ TBA distribution shows a clear bias to higher δ TBAs. The variable is defined as $\delta TBA = TBA_{S1G} - TBA_{S1B}$. This implies the prompt event S1Gs create more light in the top array than their counterpart S1Bs. The density function of S1 δ TBA of simulated events in Fig. 4.55 suggests no bias should be expected. The majority of prompt events have δ TBAs near 0, as is expected from the density function. The delayed events are generally further from 0.

The locations of events passing all cuts are plotted in Fig. 4.70. The marker color conventions are the same as those used throughout this section.

The most striking aspect of the spatial event distributions is the dearth of prompt events in the top $350 \mu\text{s}$ of the detector. The relative absence of backgrounds in this region is also noteworthy. No simulation plots have indicated that any degree of spatial bias should be expected. The positive-Y half of the detector also contains a large fraction of the prompt events, but this is not nearly as glaring because of the two prompt events well below the

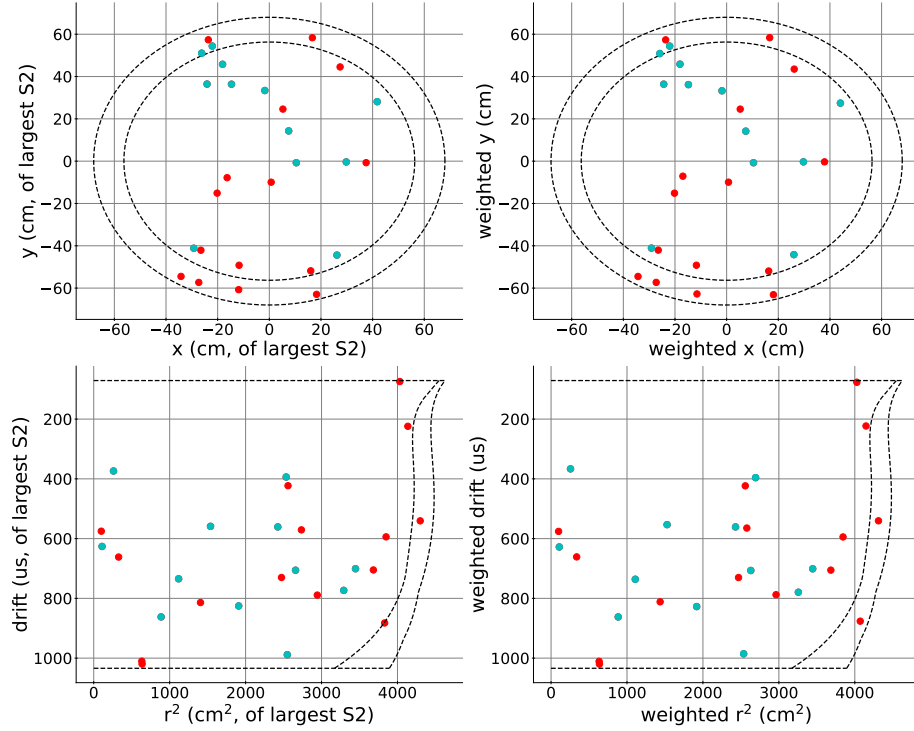


Figure 4.70: The locations of events passing all cuts in the WS2024 period are shown. Prompt events are shown in cyan, and delayed events are shown in red. This plot follows the same conventions as the previous spatial plots with the largest S2 positions plotted on the left, weighted positions plotted on the right, X-Y positions plotted on the top, and r^2 and drift time plotted on the bottom. The fiducial boundaries are outlined. There is a noticeable absence of prompt events at drift times of less than $380 \mu\text{s}$, and a glaring disparity in the total number of events between the top and bottom halves of the detector. This is discussed further in section 4.7.4.

detector's X axis. This is revisited in section 4.7.4.

The calendar date of events passing all cuts is shown in Fig. 4.71. The live time fraction is indicated by the histogram in the background.

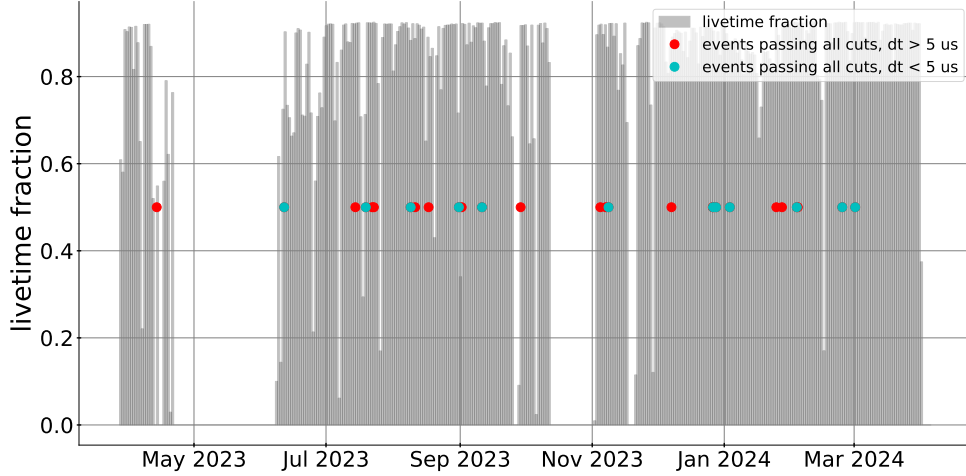


Figure 4.71: The calendar dates of events passing all cuts in the WS2024 period are shown. Prompt events are shown in cyan, and delayed events are shown in red. A histogram of the live time fraction from each calendar day is shown behind the events. The maximum live time fraction rarely exceeds 92%. Days when calibrations occur have less live time. Calibrations are responsible for the two wide gaps in data taking. The prompt events appear evenly distributed in the accumulated live time.

The prompt events appear evenly distributed across periods when live time was accrued. No significant temporal bias is expected among genuine excited state ^{85}Kr decays. It is difficult to draw any firm conclusions about the delayed events from this plot.

4.7.2 Handscan

Waveforms and PMT hit maps of events passing all cuts are observed to verify their quality and ensure their general behavior appears as expected. A subset of prompt signal candidates and delayed events are chosen for this section. The remaining prompt and

delayed waveforms and PMT hit maps are included in appendix section A.1.

Run 13579, event 195234 is a prompt candidate shown in Fig. 4.72. This event looks like a prototypical excited state ^{85}Kr candidate. The top left plot shows the summed PMT waveforms of two clear, well-resolved S1s (their windows are highlighted in green). These occur within one μs of each other.

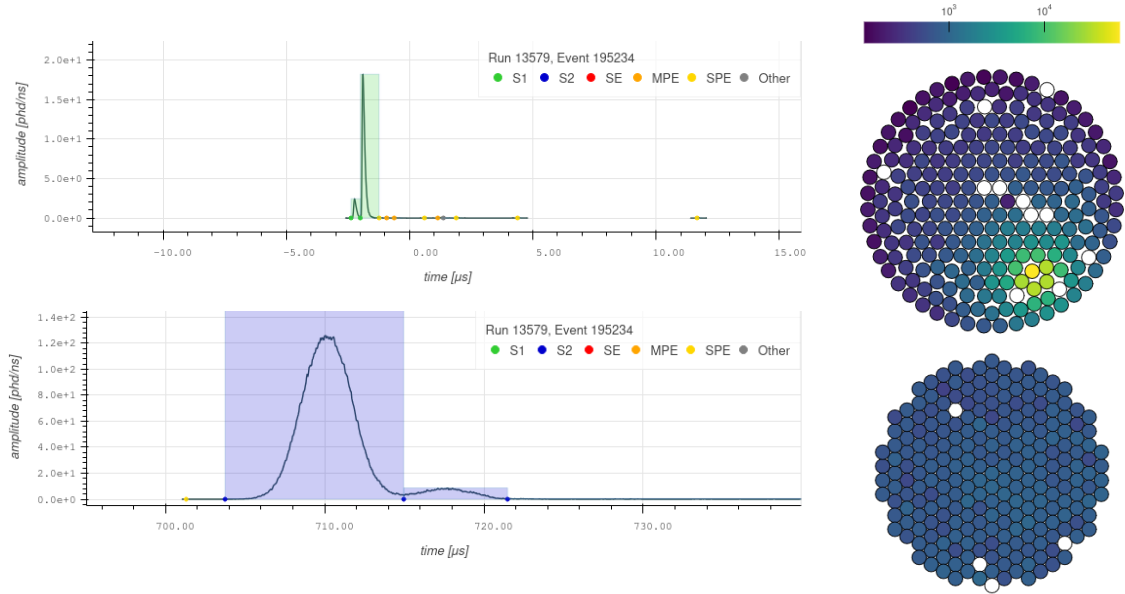


Figure 4.72: Waveforms and PMT hit maps are shown for the prompt candidate: run 13579, event 195234. The top left plot shows the two S1 waveforms highlighted in green. The bottom left plot shows the S2 waveforms highlighted in blue. The time and amplitude axes of the waveform plots have different scaling. The event's PMT hit map is shown on the right with the hit map for the top array at the top and the bottom array at the bottom. The PMT hit map is dominated by the S2s because their magnitude is much larger. The top array indicates the event's X-Y position. No light is collected by several inactive PMTs. The delay time of this event is less than a μs , and the drift time is about 700 μs .

The lower left plot shows the summed PMT waveforms of the two S2s (their windows are highlighted in blue). The S2s are relatively close in time (about 9 μs between their peaks) as expected. The amplitude axis is scaled to show the full (larger) S2 area. If plotted on the same scale as the S1, the second smaller S2 would appear comparable in height to the S1G, with a much wider pulse width. The time between the S1s and S2s is slightly

more than $700\ \mu\text{s}$, indicating that the event occurred about 45 cm above the cathode.

The PMT hit maps are shown in the right diagram for the top array (top) and the bottom array (bottom). The yellow cluster of PMTs in the top array indicates the event's X-Y position. This event occurred at the five o'clock azimuthal position, slightly more than halfway from the detector center to the TPC wall.

Run 14366, event 255010 is a prompt candidate shown in Fig. 4.73. This event has two S1s, separated by about $1.5\ \mu\text{s}$. Three partially overlapping S2s occur about $400\ \mu\text{s}$ later. The event occurred about 85-90 cm above the cathode at the two o'clock azimuthal position.

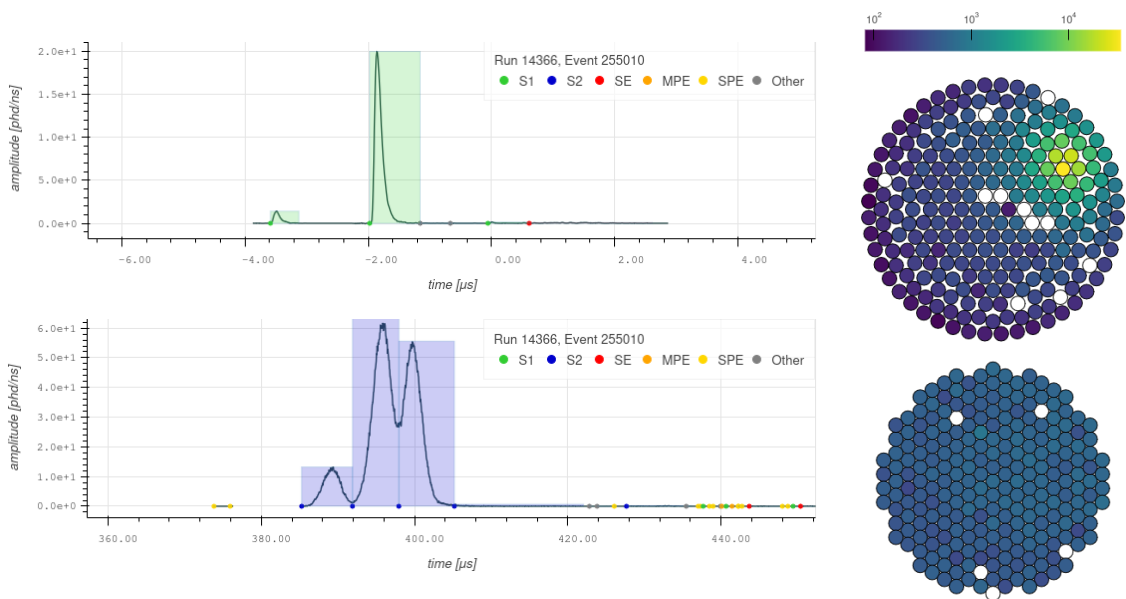


Figure 4.73: Waveforms and PMT hit maps are shown for the prompt candidate: run 14366, event 255010. The top left plot shows the two S1 waveforms, and the bottom left plot shows the S2 waveforms. The event's PMT hit map is shown on the right for the top array (top) and the bottom array (bottom). The delay time of this event is about $1.5\ \mu\text{s}$, and the drift time is just under $400\ \mu\text{s}$.

Run 15242, event 260404 is a prompt candidate shown in Fig. 4.74. This event has a candidate S1B that appears very small. Its (raw) pulse area of about 110 phd and is well within the cut boundary. The delay time of the event is about $2\ \mu\text{s}$. Two S2s are observed,

with a drift time of about $860 \mu\text{s}$.

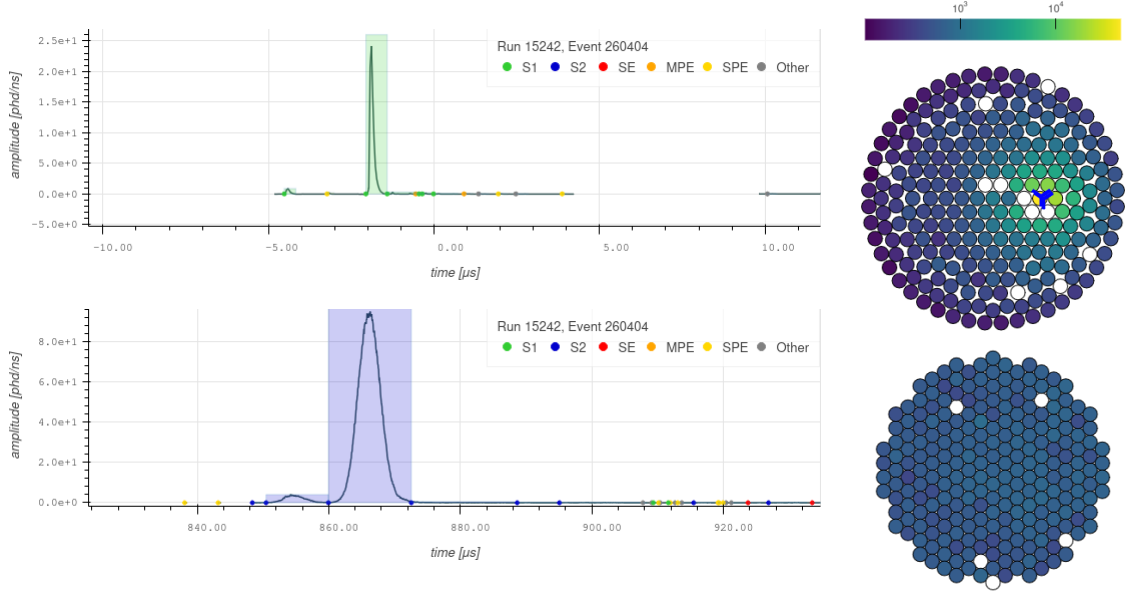


Figure 4.74: Waveforms and PMT hit maps are shown for the prompt candidate: Run 15242, event 260404. The top left plot shows the two S1 waveforms, and the bottom left plot shows the S2 waveforms. The event's PMT hit map is shown on the right for the top array (top) and the bottom array (bottom). The two blue "Y" shaped markers in the top array diagram mark the centroid position of each S2. The centroids are in nearly the same position for this event. The delay time of this event is about $2 \mu\text{s}$, and the drift time is about $860 \mu\text{s}$.

Prompt candidate event waveforms and PMT hit maps show no evidence that would suggest the prompt events are not ^{85}Kr excited state decays. The remaining prompt candidate waveforms and PMT traces are shown from Fig. A.25 to Fig. A.33 in appendix section A.1.

Run 13980, event 257977 is a delayed event shown in Fig. 4.75. The S1s in this event are quite far apart in time, with a delay time of about $90 \mu\text{s}$. Only a single S2 is present and the drift time exceeds $1000 \mu\text{s}$.

This event is narrowly not rejected by both the fiducial and S1 δ time cuts. The time between the S1B candidate and the only prominent S2 is about $1100 \mu\text{s}$. This is longer than the maximum drift time and implies that the S1B cannot be related to the S2. The S1B

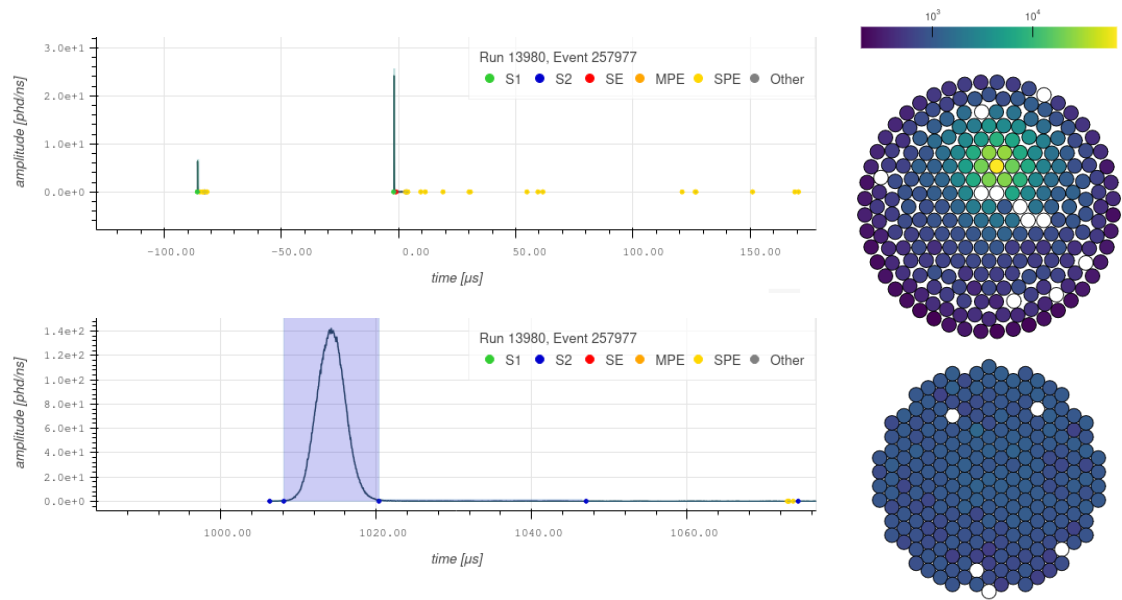


Figure 4.75: Waveforms and PMT hit maps are shown for the delayed event: run 13980, event 257977. The top left plot shows the two S1 waveforms, and the bottom left plot shows the S2 waveform. The event's PMT hit map is shown on the right for the top array (top) and the bottom array (bottom). The delay time of this event is about $90 \mu\text{s}$, and the drift time is about $1020 \mu\text{s}$.

candidate may be the product of an energy deposition in the reverse field region (RFR) below the cathode, where no charge is collected. The event is plausibly a coincidence pairing of an energy deposition in the RFR with another larger energy deposition just above the cathode.

Because the S1B and S2 cannot be related, this event is definitively not an excited state ^{85}Kr decay. However, if the energy deposition contributing to the S2 and candidate S1G happened about $90\ \mu\text{s}$ earlier, this event may have been considered a prompt ^{85}Kr excited state decay candidate. This is a reminder of the value in keeping events with delay times up to $100\ \mu\text{s}$, allowing coincidence backgrounds to be fit and quantified.

Run 14305, event 150309 is a delayed event shown in Fig. 4.76. The delay time of the event is about $50\ \mu\text{s}$.

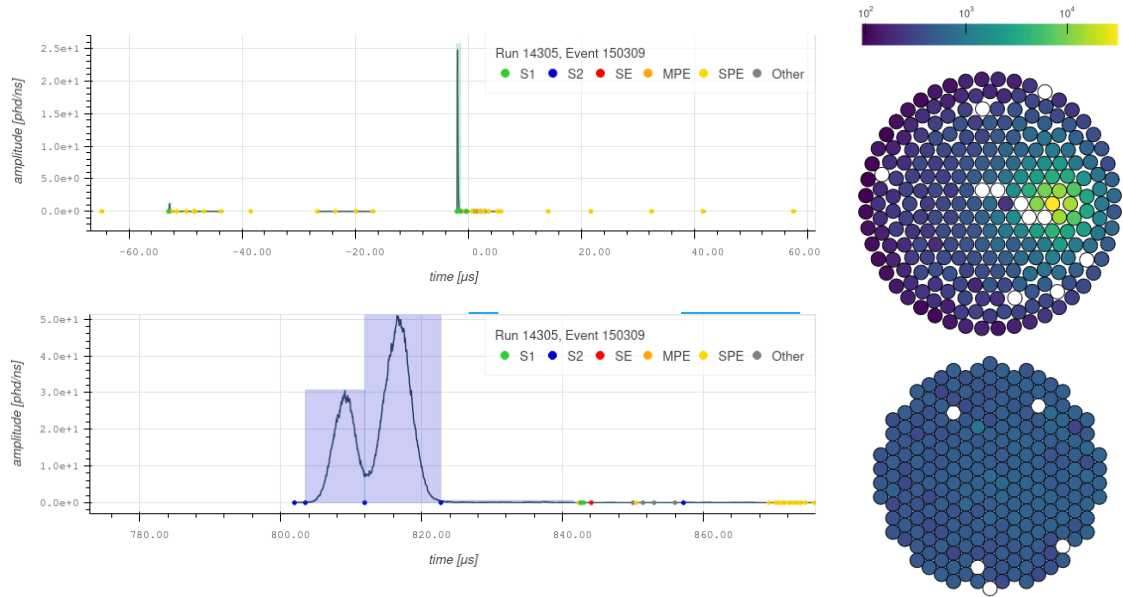


Figure 4.76: Waveforms and PMT hit maps are shown for the delayed event: run 14305, event 150309. The top left plot shows the two S1 waveforms, and the bottom left plot shows the S2 waveforms. The event's PMT hit map is shown on the right for the top array (top) and the bottom array (bottom). The delay time of this event is about $50\ \mu\text{s}$, and the drift time is slightly more than $800\ \mu\text{s}$.

Both S2s are relatively close in X-Y and drift time. It is unlikely that the energy deposi-

tion causing the S1B candidate could produce an S2 as large as either of the prominent S2s alone. This implies that the energy deposition producing the S1G candidate is responsible for at least a fraction of both S2s. The energy deposition causing the S1B either did not result in free charge (in an area where charge could be collected) or its free charge merged into the S2s from the energy deposition producing the S1G candidate. The PMT hit map shows the event is quite localized in X-Y, meaning that the S1B energy deposition would have to occur directly below the S1G energy deposition if it produced detectable charge.

Run 15182, event 291534 is a delayed event shown in Fig. 4.77. This event has a delay time of about $7.5 \mu\text{s}$.

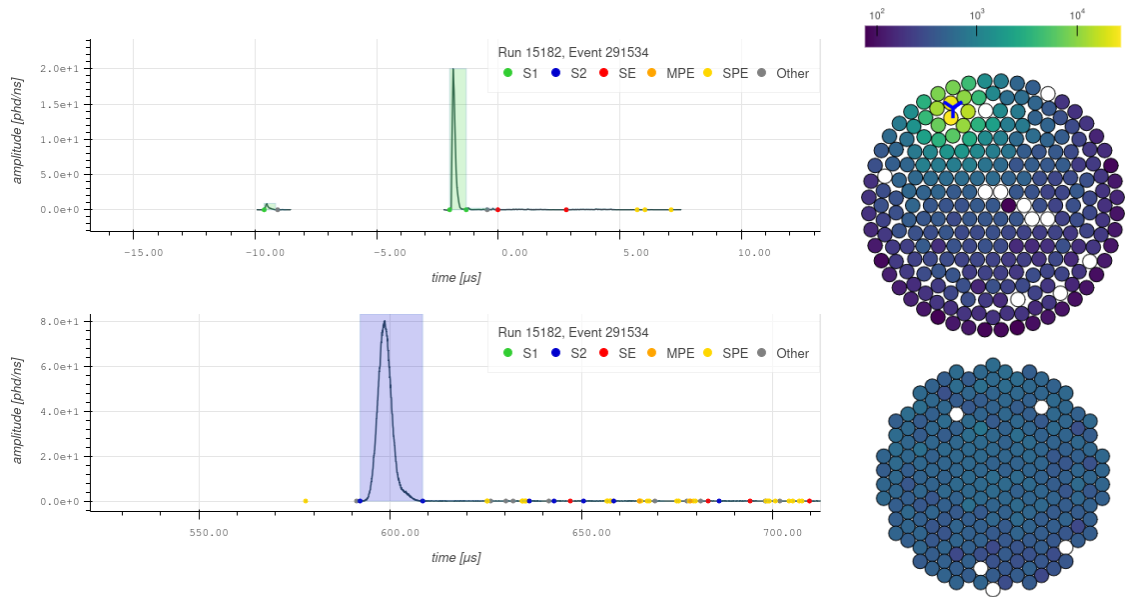


Figure 4.77: Waveforms and PMT hit maps are shown for the delayed event: run 15182, event 291534. The top left plot shows the two S1 waveforms, and the bottom left plot shows the S2 waveform. The event's PMT hit map is shown on the right for the top array (top) and the bottom array (bottom). The blue "Y" shaped marker in the top array diagram marks the S2 centroid position. The delay time of this event is about $7.5 \mu\text{s}$, and the drift time is slightly more than $600 \mu\text{s}$. This event could plausibly be an excited state ^{85}Kr decay.

Unlike the two previous delayed events, this event may be an excited state ^{85}Kr decay. The $600 \mu\text{s}$ drift time is well within the fiducial volume. The event has a single prominent

S2. The likelihood fit is left to determine the probability of this event being an excited state ^{85}Kr decay. The remaining delayed event waveforms and PMT traces are shown from Fig. A.34 to Fig. A.45 in appendix section A.1.

4.7.3 Examination of background events

The rate of events passing the selection criteria, the fiducial cut, and the S1 δ time cut are plotted by calendar date in Fig. 4.78.

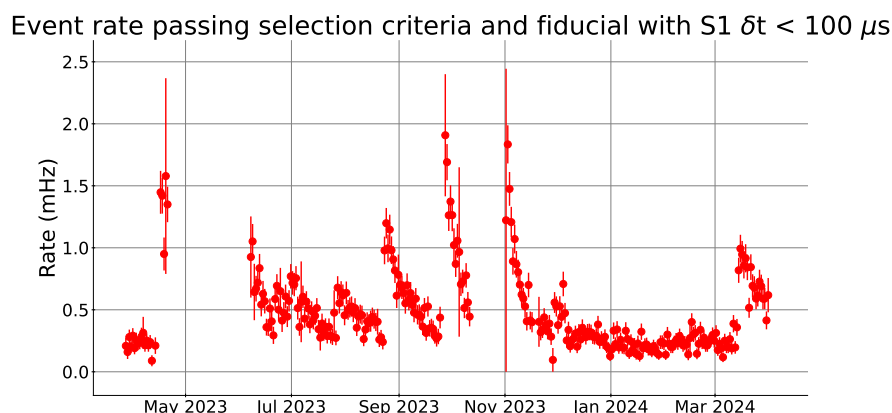


Figure 4.78: The rate of events passing initial cuts (selection criteria, fiducial, and S1 δ time) by date is shown. The rate shows multiple sharp spikes. Periods when no live time is accrued are not plotted. The two sharp rate increases that follow the extended periods of no data taking are likely due to calibrations.

The plot shows clear spikes in the event rate at certain times, followed by periods of exponential decay. Two obvious spikes are noted following the extended periods when WIMP search data was not being taken: May/June of 2023 and October of 2023. These periods are associated with detector calibrations. The obvious hypothesis is that the spike in rate is associated with an increase in accidental coincidences involving Xe activation products or lingering radioactive calibration sources. Fig. 4.79 shows the event rates when restricted to S1 δ times of less than $10\ \mu\text{s}$.

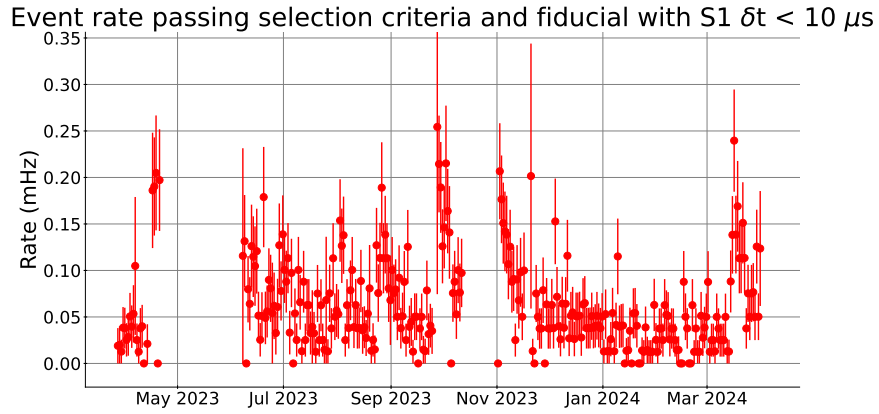


Figure 4.79: The rate of events passing initial cuts by date, with delay times less than $10 \mu\text{s}$, is shown. The shape of the plot looks nearly identical to Fig. 4.78, but with a lower rate.

The plot appears scaled down by a factor of 10 relative to Fig. 4.78, but roughly retains the same shape. Accidental coincidence pairings should be uniformly distributed in delay time. For a uniform distribution of delay times, scaling down the S1 delay time window by a factor of 10 should reduce the event rate by a factor of 10, as is observed. The eight largest spikes in event rate from Fig. 4.78 are all during periods that immediately follow calibrations.

These two plots alone suggest that activation products and lingering calibration radioactivity contributing to accidental coincidence pairs are a significant source of background. The events from Fig. 4.78 are histogrammed by their S1B and S1G in Fig. 4.80 and Fig. 4.81.

A clear peak is present around 1000 phd in both plots. The S1B plot also shows a large population of events with very small S1B. A clear spectral line should result from the combination of energy depositions producing very small S1Bs and energy depositions producing an approximately 1000 phd S1G when total energy is histogrammed. Total energies distribution of these events is shown in Fig. 4.82.

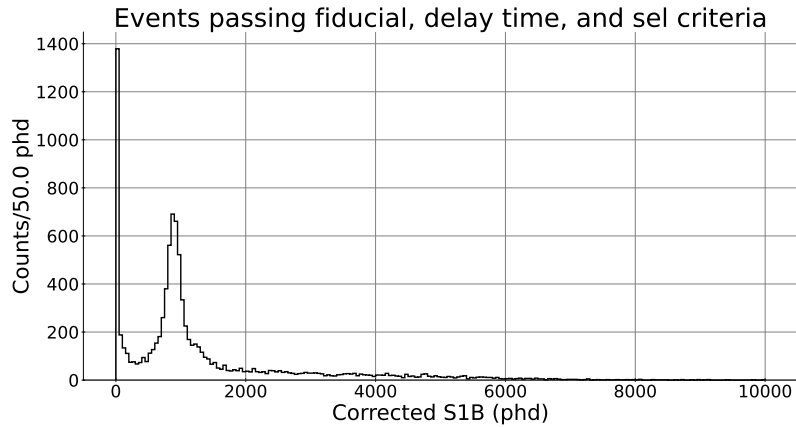


Figure 4.80: The S1B histogram of events passing the initial cuts (selection criteria, fiducial, S1 δ time) is displayed. Two very clear peaks are seen in this plot: one at very low S1 and one just below 1000 phd. The selection criteria removes all S1s smaller than 10 phd and greater than 10000 phd.

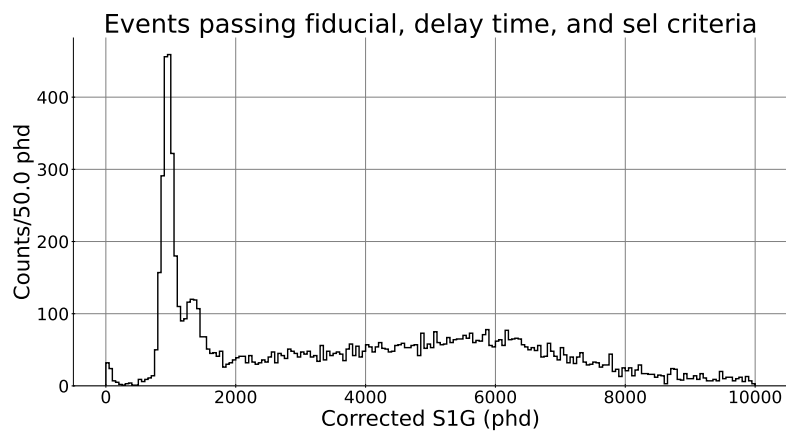


Figure 4.81: The S1G histogram of events passing the initial cuts is displayed. This plot appears to indicate a peak near 1000 phd, like the S1B plot.

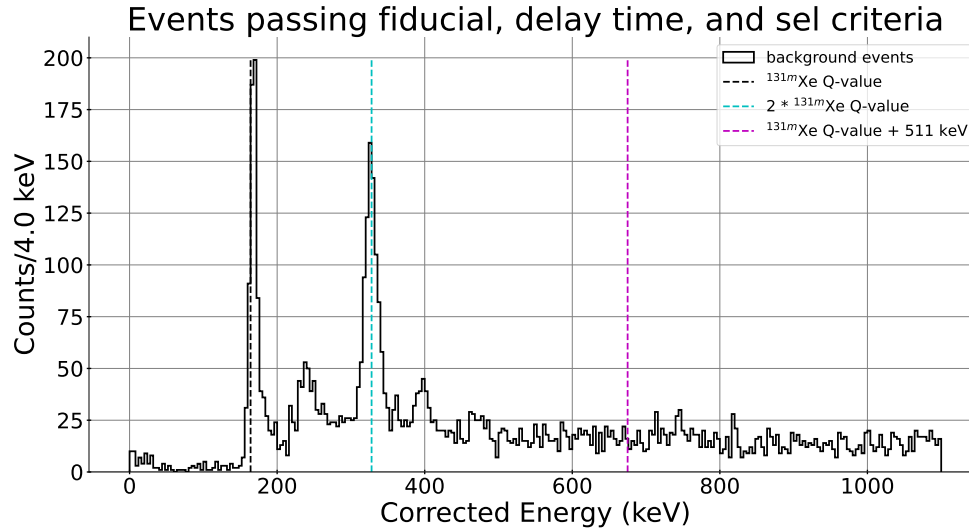


Figure 4.82: The energy histogram of events passing the initial cuts is displayed. Two energy peaks align with the 164 keV Q-value of ^{131m}Xe (marked in dashed black) and two times the Q-value of ^{131m}Xe (marked in cyan). There is no visible peak at the sum of the ^{131m}Xe Q-value and 511 keV, indicating that a ^{131m}Xe decay in coincidence with positron annihilation (for instance) is not a significant source of background.

The total energy spectrum displays a clear peak just above 164 keV. 164 keV is the energy released by a ^{131m}Xe decay, and is marked on the plot. An additional peak is observed at double the ^{131m}Xe Q-value. This plot suggests that the most common sources of background are ^{131m}Xe decays in coincidence with very small S1s and ^{131m}Xe decays in coincidence with other ^{131m}Xe decays.

^{131m}Xe S1s are not large enough to satisfy the S1G area cut. This implies that ^{131m}Xe -small S1 pairs and ^{131m}Xe - ^{131m}Xe pairs will both be rejected by the S1G cut. ^{131m}Xe must be paired with a higher energy decay to pass all cuts. The energy sum of a ^{131m}Xe decay and a γ near 514 keV (for instance, a 511 keV annihilation γ) could pass all cuts. This possible coincidence pairing energy is marked on the plot, where no significant excess is seen. Fig. 4.63 also indicates that there are no prompt or delayed events passing all cuts with an S1B area near 1000 phd. This observation confirms that no ^{131m}Xe coincidence

pairings have passed all cuts.

The high rate of small S1s in the S1B spectrum could plausibly be a part of a coincidence pair. However, no significant peaks are seen in Fig. 4.82 between the ^{85}Kr excited state energy cut boundaries. If small S1s coincidence pairs are contributing to background, they are not consistently pairing with the same mono-energetic source to pass all cuts.

4.7.4 Comparison with SR1

This technique for quantifying ^{nat}Kr was used in LZ's first science run to crosscheck the results from section 3.9.4 [65]. The 2022 study measured a ^{nat}Kr equivalent concentration of 183 ± 67 ppq (g/g). This is in agreement with the 144 ppq (g/g) of ^{nat}Kr measured by cold trap mass spectrometry.

Both studies use a relatively similar methodology and set of cuts. One noteworthy observation between the two studies is the deficit of events above $400\ \mu\text{s}$ in drift time. In the first science run, seven events passing all cuts were "prompt" (delay times of less than $5\ \mu\text{s}$) [65]. Another eight events were "delayed" (delay times greater than $5\ \mu\text{s}$), totaling 15 events passing all cuts. The drift times of events passing all cuts from LZ's first science run are displayed in Fig. 4.83.

Ignoring the events from the side band study, only two of the fifteen total events and one of the seven prompt events in the final SR1 data set have drift times less than $400\ \mu\text{s}$. This is compared with five of 27 events from the WS2024 search and two of twelve prompt events. The smallest drift time of any prompt event in either study was $265\ \mu\text{s}$. Table 4.8 summarizes the number of events in the top half of the detector in each subset of data.

Assuming that the probability of any one event occurring in the top half of the detector is 50%, the probability of four or fewer of the 19 total prompt events from SR1 and WS2024 occurring in the top half of the detector is about 1%. For four of 23 delayed events, the

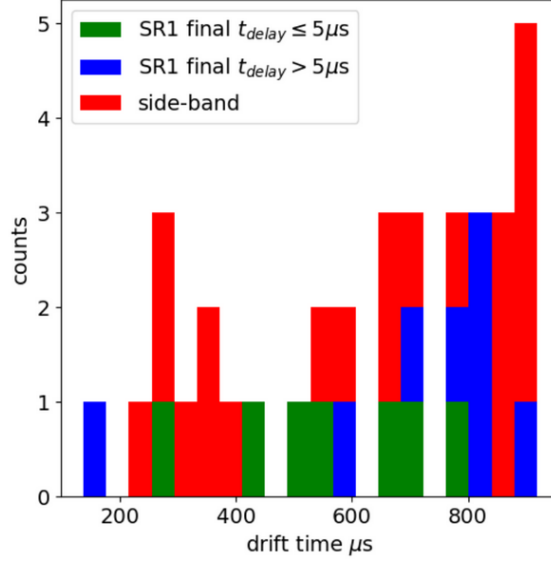


Figure 4.83: Drift times of events passing all cuts using a similar analysis from the SR1 excited state ^{85}Kr decay search are histogrammed here. Prompt events are indicated in green and delayed events are indicated in blue. "Prompt" and "delayed" are defined identically in both studies. The red side band events can be ignored for the purpose of this discussion. The detector's maximum drift time was about $100 \mu\text{s}$ less SR1 than in WS2024 (image from [65]).

(top / total)	SR1	WS2024	SR1+WS2024	$P(X \leq \text{top} N = \text{total}, p = 0.5)$
Prompt	2/7	2/12	4/19	0.0096
Delayed	1/8	3/15	4/23	0.0013
Prompt+delayed	3/15	5/27	8/42	0.00003

Table 4.8: A summary of the number of events in the top half of the detector for different subsets of data is shown. The "SR1," "WS2024," and "SR1+WS2024" columns all show $(n_{\text{top}})/(n_{\text{total}})$ for the subset of data given by the rows and the columns. The column " $P(X \leq \text{top} | N = \text{total}, p = 0.5)$ " shows the binomial probability of the number of events observed (in SR1+WS2024) or fewer occurring in the top half of the detector, given the number of events in the entire detector (in SR1+WS2024) and a 0.5 probability of an event occurring in the top half of the detector.

probability is about 0.1%. The probability of eight or fewer of the 42 total events occurring in the top half of the detector is 0.003%.

Various cuts were inspected for spatial bias. Strictly examining cuts applied to the event S1s yields interesting results. Fig. 4.84 shows the position of events passing and failing the S1 δ TBA cut after the initial cuts, the S1B cut, and S1G cut were applied.

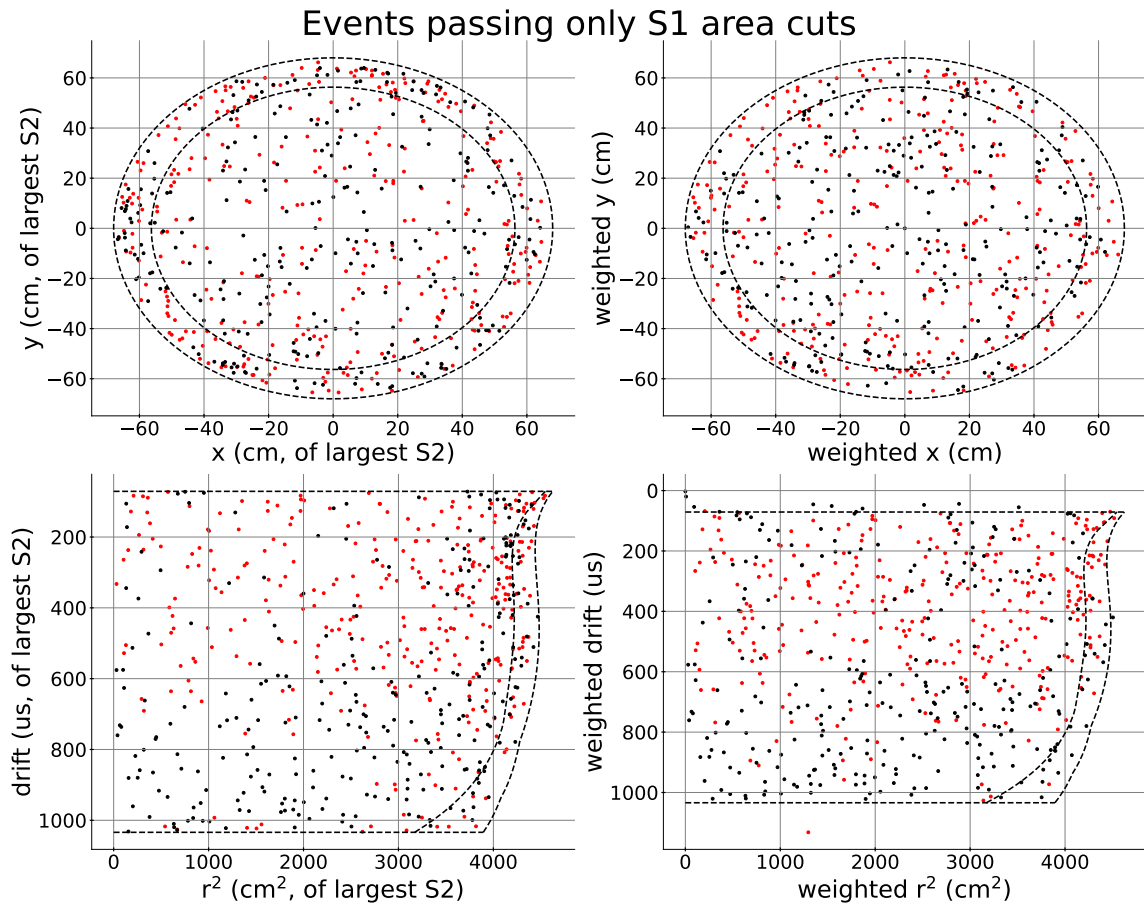


Figure 4.84: The positions of events passing the initial cuts and the two S1 area cuts are plotted here. Those that fail the S1 δ TBA are marked in red while those that pass are marked in black. The plot follows similar conventions to the previous spatial plots (see Fig. 4.70). The vast majority of the events are background. The cut is definitively better at rejecting background from the top of the detector.

The cut's propensity to remove events at the top of the detector while keeping events at the bottom of the detector is very clear. The vast majority of plotted events are backgrounds,

implying that the cut more effectively removes backgrounds from the top of the detector. To better understand why, the S1B and S1G TBAs of events in Fig. 4.84 are plotted by event drift time in Fig. 4.85.

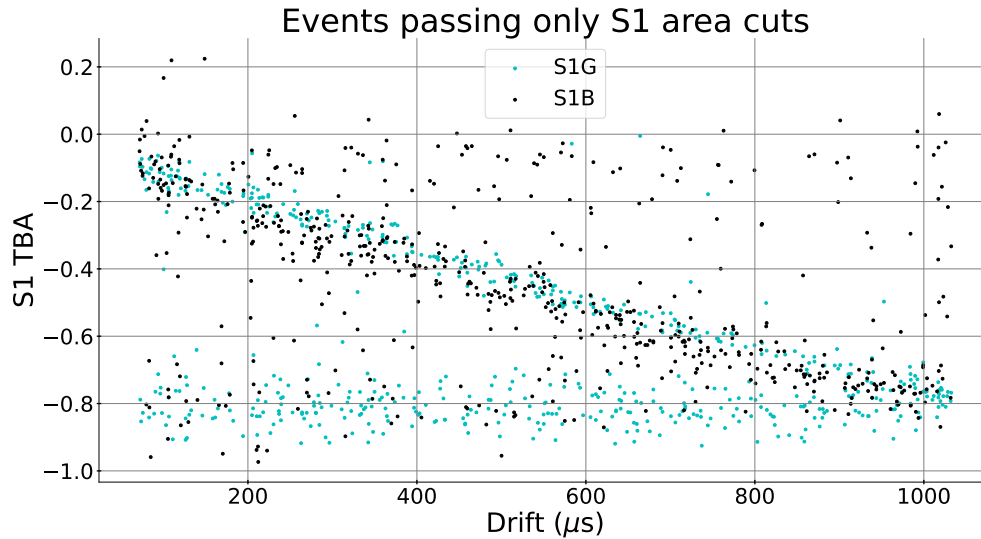


Figure 4.85: Events passing the initial cuts and the two S1 area cuts have their S1G and S1B TBAs are plotted against drift time. Cyan markers are associated with the S1G TBA and black markers are associated with the S1B. Because S1 TBA and drift are (anti)correlated, energy depositions producing an S1 and an S2 lie along the dense diagonal band in this plot. Energy depositions that produce an S1 but no S2 are not correlated with drift.

The black dots indicating the S1B and the cyan dots indicating the S1G populate the dense band along the diagonal. The energy depositions that produce the S1s along the diagonal are much more likely to contribute to the event's S2. The S1B TBAs along the diagonal are shifted slightly to the left because the drift time is measured from the S1G to the largest S2. The S1B always occurs before the S1G. Therefore, an energy deposit that produces an S1B and an S2 in coincidence with an isolated S1G always has a shorter drift time (by up to 100 μ s) than a deposit in the same location producing an S1G and an S2 in coincidence with an isolated S1B.

Energy depositions below the cathode in the RFR result in no charge collection and

have very low S1 TBAs. The high density band stretching across all drift times near -0.8 in TBA is likely due to RFR energy depositions. They are not correlated with drift because they produce no S2 and, therefore, are not associated with the event's drift time. In this case, the recorded drift time is the time difference between the non-RFR energy deposit's S2 time and the S1G time. S1Gs more densely populate the RFR band than S1Bs. Events are plotted by their S1 δ TBA and drift time in Fig. 4.86, revealing more about the bias of the cut.

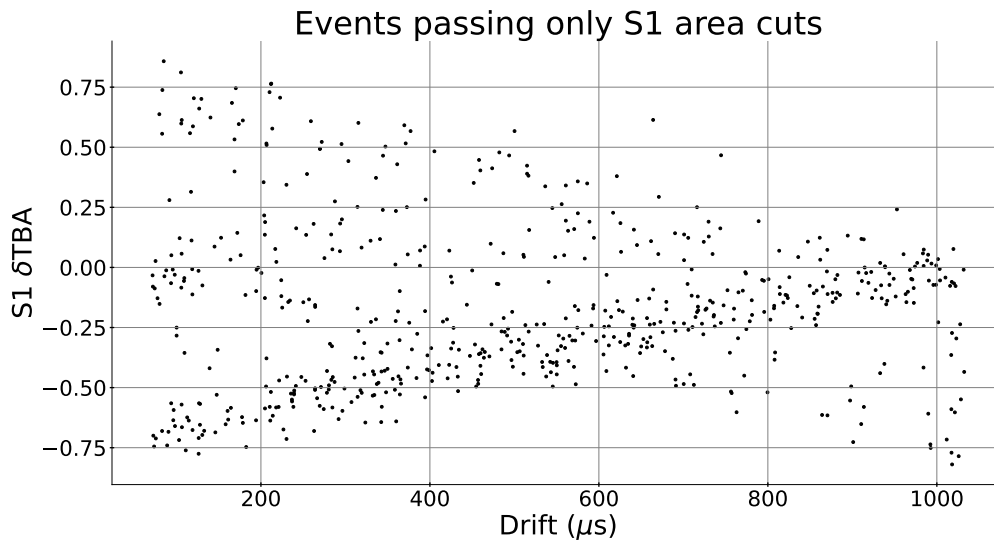


Figure 4.86: Events passing the initial cuts and the two S1 area cuts have their S1 δ TBA and drift time plotted here. A legitimate pairing of two energy depositions close in both space and time should have an S1 δ TBA near 0. Three bands seem apparent by eye. They all converge at high drift times.

By eye, three populations appear in the plot. The bottom and heaviest population is likely due to events with S1G candidates produced in the RFR (recall $\delta TBA = TBA_{S1G} - TBA_{S1B}$) in coincidence with an energy deposition producing an S1B and an S2. The band at the top of the plot is less dense and likely caused by the inverse of the scenario above. Interactions in close proximity (both spatial and temporal) that both result in an S1 and an S2 have an S1 δ TBA near zero. At high drift times (low in the detector) all three bands

converge within the cut limits of ± 0.25 .

RFR energy depositions are frequently partnered with energy depositions in the fiducial volume to form events that resemble legitimate coincidence pairs. Energy depositions lower in the fiducial volume have S1 TBAs that are more similar to RFR S1 TBAs, and therefore, more often pass the S1 δ TBA cut. The spatial effect of excluding the S1 δ TBA cut from the analysis is shown in Fig. 4.87.

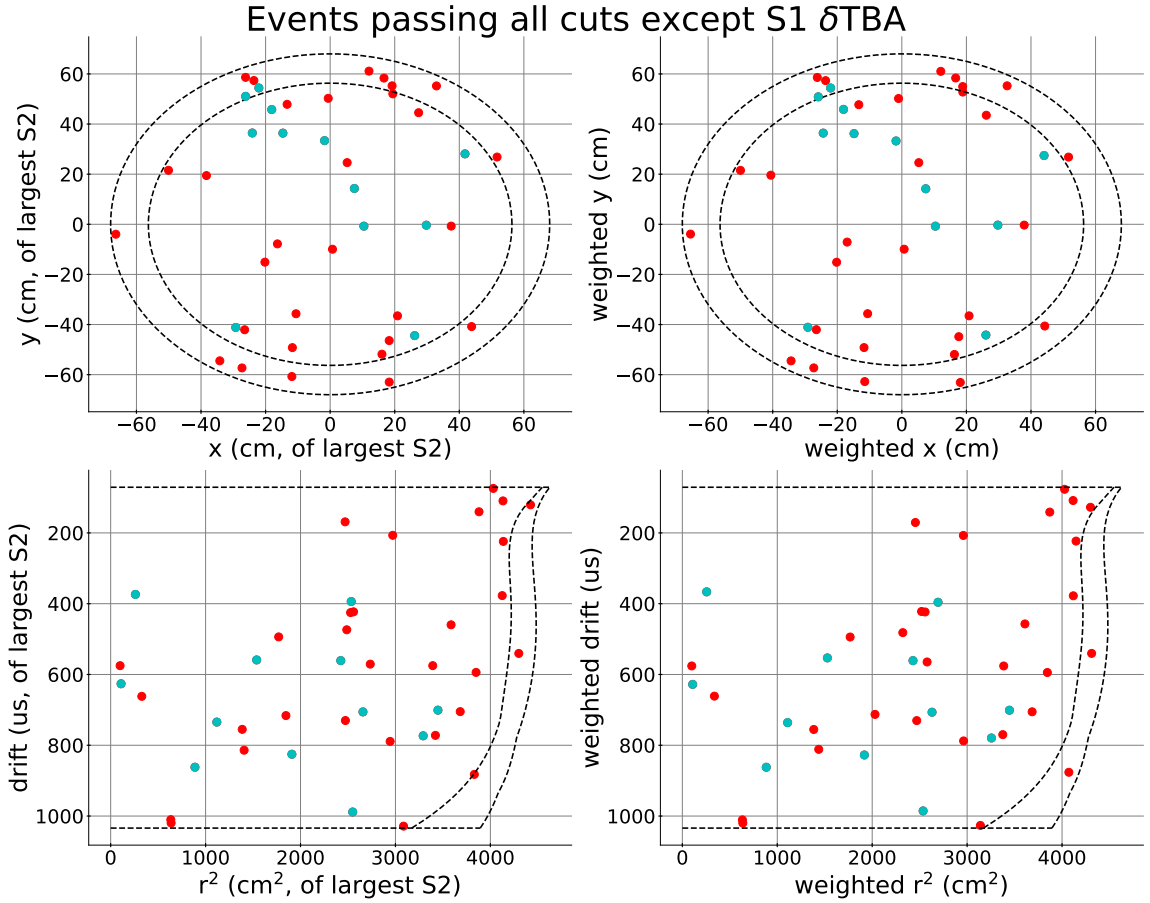


Figure 4.87: The positions of events passing all cuts except the S1 δ TBA are plotted. The plots use the same conventions as previous spatial plots. Prompt events are indicated in cyan, and delayed events are indicated in red. The deficit of delayed events in the top half of the detector no longer exists, confirming that the S1 δ TBA cut is more effective at removing low drift time (high Z position) backgrounds.

No prompt events and thirteen delayed events are added to the plot. Nine of the thirteen

are added to the top half of the detector, bringing the total number of events in the top half of the detector to thirteen out of 30. This relieves the apparent 0.1% tension between the expected and observed delayed event totals in the top half of the detector: for backgrounds, the top half probability $p \neq 0.5$.

With the S1 δ TBA cut again removed, the S1B TBA is plotted against the S1G TBA of passing events in Fig. 4.88.

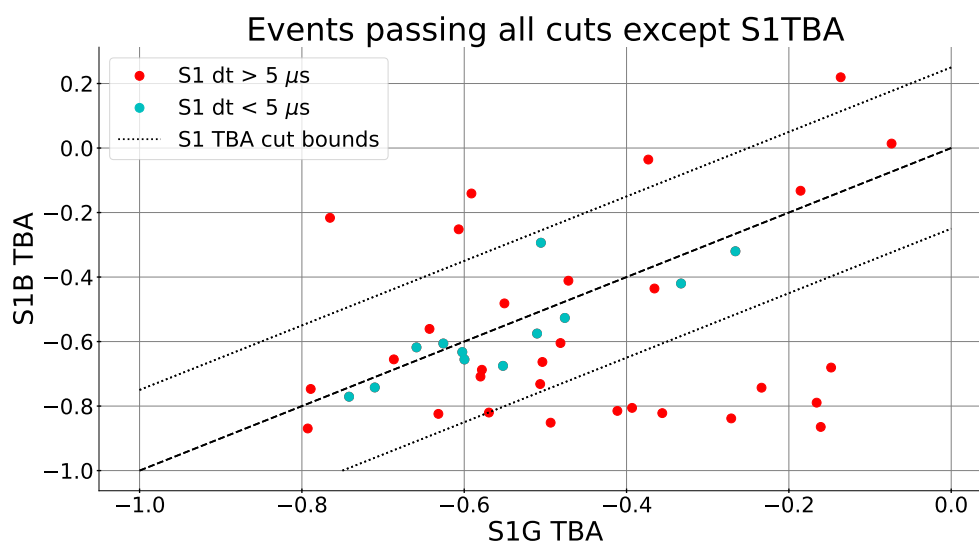


Figure 4.88: Events passing all cuts except S1 δ time are plotted by their S1B and S1G TBAs. The S1 δ TBA cut boundaries are indicated by dotted black lines. The dashed black line is S1 δ TBA = 0. Prompt events lie much closer to the line than the delayed events. A significant portion of rejected events have S1B TBAs at about -0.8. A large fraction of these are likely energy depositions in the fiducial volume producing an S1 and S2(s) coincident with RFR energy depositions.

The bounds of the δ TBA cut are outlined in the plot. The vast majority of prompt events hug the $TBA_{S1B} = TBA_{S1G}$ line. Also noted is a very clear population of events around -0.8 in S1B TBA. The cut appears to effectively remove likely RFR coincidence events while not rejecting legitimate events. The S1 δ TBA cut is less powerful at high drift times (low in the detector).

None of these observations explain why there are fewer observed prompt excited state

^{85}Kr decay candidates in the top of the detector. 50.3% of events in Fig. 4.57 passing all full simulation cuts have drift times in the top half of the detector. The spatial disparity observed in prompt events from SR1 and WS2024 combined is expected to occur about 1% of the time. While unlikely, this is plausible.

4.8 Summary of results

In 5500 ± 200 fiducial kg of Xe across 242.5 live days, the excited state ^{85}Kr decay analysis has measured the ^{nat}Kr concentration $\Phi_{nat\text{Kr}}$ to be 124^{+44}_{-37} ppq (g/g) assuming a natural abundance of $2.0 \pm 0.2 * 10^{-11}$. This is in agreement with the 182 ± 26 ppq (g/g) measured by the cold trap mass spectrometry systems in chapter 3. The analysis is found to be 0.655 ± 0.014 efficient for observing excited state decays in the fiducial volume.

Two common backgrounds are identified. First, ^{131m}Xe decays frequently pair with other energy deposits in the detector to create backgrounds. Second, accidental coincidences between energy deposits in the fiducial volume and energy deposits in the RFR are another common source of background. Both sources are heavily mitigated by the chosen cuts. The S1 δ TBA cut preferentially removes background events (delayed) near the top of the detector.

The disparity between the number of prompt ^{85}Kr candidates observed in the top and bottom halves of the detector remains unresolved. The disparity was observed in both the SR1 and WS2024 data sets. The limited sample of prompt candidates have distributions that are consistent with excited state ^{85}Kr decays across all other variables. This may simply be statistical fluctuation.

Chapter 5: Injection and Removal of Natural and Radio-labeled Methane in LZ

Tritium (^3H or T) is one of LZ's most powerful calibration sources. ^3H is the best source for calibrating detector response to low energy electron recoils. The 18.6 keV Q-value β -decay provides an exemplary source of simple, single scatter electron recoils. ^3H will populate the full energy range of the electron recoil band in the WIMP search S1-log(S2) region of interest. The better this portion of the ER band is understood, the better leakage into the low energy portion of the NR band can be understood. Because ^3H is a (short range) β emitter, it must be dissolved in the Xe. This conveniently means ^3H will spread evenly through the Xe volume to calibrate all corners of the TPC.

Many of the properties that make ^3H an attractive calibration source also make it a potentially serious background. ^3H decays will contribute to the WIMP background and can be significant in high enough quantities. The decay is *naked*, meaning no subsequent decays can be used to tag ^3H events. No energy cuts can be applied to reject individual events as background. Fiducial cuts are ineffective because of the source's spatial uniformity. In addition, the ^3H half-life is 12.3 years, and any potential problems with contamination will last for the life time of the experiment (provided no drastic intervention is taken).

Hydrogen is highly reactive. ^3H must be bound to a molecule before being injected into LZ. The candidate molecule is ideally inert (in LZ) and easily removable. When used as a calibration source, ^3H is bound to one of the H sites of a methane molecule. Tritiated

methane (CH_3T) can be removed from LZ by the noble gas purifier (also referred to as the getter).

The LUX experiment successfully injected and removed CH_3T from their 370 kg LXe TPC [68]. The observed removal time was about six hours, while the Xe purification time was around 40 hours. The event rate in the ^3H energy range eventually returned to pre-injection levels, indicating no CH_3T remained in the TPC. Unlike LUX, the LXe TPC dark matter experiment PandaX-II noted a lingering ^3H -like background after a CH_3T calibration [69]. The background was not completely mitigated by circulating Xe through a getter. In LZ, natural methane (CH_4) injected to empirically confirm its successful removal. CH_3T is injected only after verifying CH_4 is fully removed.

Removal is expected to be exponential and is fit using the simple exponential given in Eq. 5.1, where $A(t)$ is either activity or concentration at time t , A_0 is initial amplitude at $t = t_0$, t_0 is the time at the start of the methane injection, τ is the (mean) removal time, and C is a (possible) constant term. C is taken to be zero unless otherwise specified¹.

$$A(t) = A_0 * e^{-(t-t_0)/\tau} + C \quad (5.1)$$

LXe convection in the active volume can be changed by modifying TPC thermosiphon and heater settings. Generally, convection is minimized during science runs to better isolate the central volume and improve Rn tagging efficiency. When internal sources like CH_3T are injected into LZ, convection and mixing is intentionally increased to uniformly calibrate the fiducial volume. All methane injections discussed in this chapter are performed in the *mixed* or high convection state.

This chapter will begin with a discussion of the LZ's methane removal tool, the noble gas purifier, in section 5.1. Section 5.2 will discuss the procedure for injecting methane

¹A non-zero value of C does not imply that methane is not fully removed; it only implies a signal that cannot be distinguished from tritium (or methane) is detected.

into the LZ circulation system. CH_4 removal tests will be covered in section 5.3. CH_3T calibrations and their removal will be discussed in section 5.4. Section 5.5 will summarize the results.

5.1 The LZ Noble Gas Purifier (Getter)

LZ's methane removal tool is a SAES PS5-MGT50 noble gas purifier. Recall from section 2.5 that the purifier resides in the gaseous portion of the circulation system, just after the compressors, as seen in the plumbing and instrumentation diagram in Fig. 2.16. The purifier is shown in Fig. 5.1.



Figure 5.1: The LZ getter is shown operating in the Davis Cavern.

The LZ noble gas purifier is a heated zirconium getter. The getter consists of many "pills" that are heated to temperatures on the order of hundreds of degrees Celsius. The gettering pills are made of SAES St707 getter alloy and have a nominal composition of 70% Zr, 24.6% V, and 5.4% Fe [70]. Zr at the pill surface will chemically bond to nearly all non-noble impurities. At ambient temperatures, the bonded impurities will remain on the pill surface. As more bonding sites are occupied, an inert, passivated outer layer will form around the pill. Heating the getter pill material to hundreds of degrees Celsius will allow the impurities to diffuse into the bulk of the pill, opening more surface area for non-noble impurities to bond.

Methane is more difficult for the getter to remove than O₂, N₂, or other non-noble impurities [71]. Several factors are known to influence the getter's methane removal efficiency. The most significant is the diffusion time of getter surface molecules into the bulk, which is temperature dependent. Saturation in the bulk of the getter material affects removal efficiency and the flow rate across the pills may also affect the getter's removal efficiency. In LZ, the circulation system flow rate and mixing state of the TPC active volume impact methane removal time.

5.2 Injection Procedure

Calibration sources that are to be dispersed throughout the LXe volume are sent into the LZ circulation system via the *source injection panel*. The panel is connected to several locations in the gaseous portion of the main circulation path, including before and after the getter. The source injection panel has multiple sites for housing source generators (tablets coated with radioactive material, such as ²²⁸Th for ²²⁰Rn calibrations) and includes multiple ports for connecting gaseous source cylinders. These cylinders are used to hold mixtures of methane and Xe. The panel also contains a bottle for storing Xe gas. The

volume can be filled by carefully cryopumping Xe from the circulation system. This Xe is used as a carrier gas for sources in the panel. Several other pumpout ports, mass flow controllers, and pressure monitoring devices are included on the panel. Further discussion of this panel is given in [72]. A simplified diagram of the panel can be seen in Fig. 5.2.

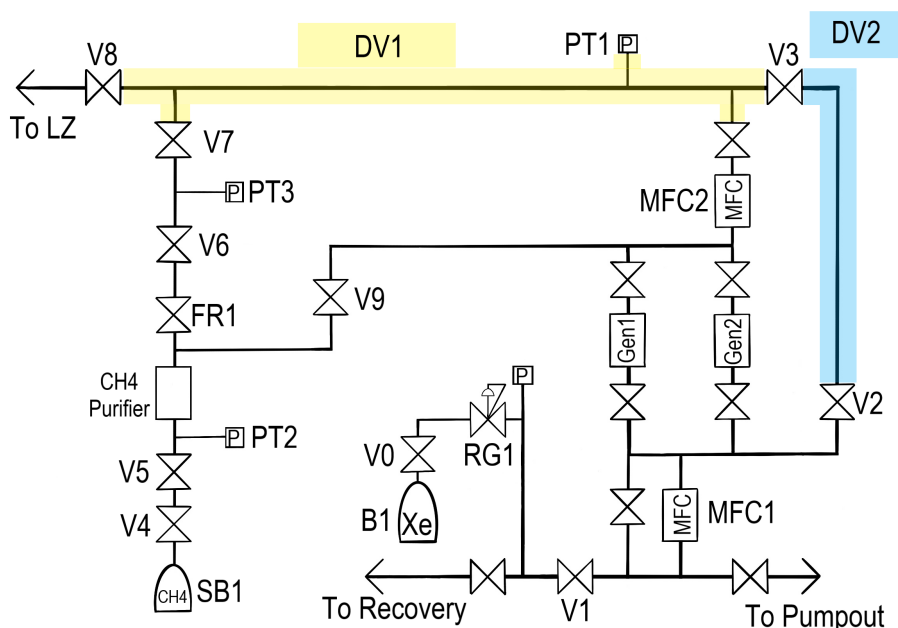


Figure 5.2: A simplified plumbing and instrumentation diagram of the LZ source injection panel is shown. A Xe-methane mixture resides in the source bottle (SB1). SB1 slowly fills the dose volume(s) DV1 and DV2, passing through the methane purifier and the flow restrictor (FR1). B1 contains a supply of Xe used to flush the dosing volumes into the circulation system, which is located behind V8. The supply Xe pressure is set with regulator RG1, and the flush rate is controlled by mass flow controller MFC1. A few other unlabeled valves and two generator source locations are also displayed, though these are not relevant to this procedure.

The methane purifier is a SAES MC1 series methane purifier, designed to remove non-noble and non-methane gas species. The purifier operates in a way that is similar to the getter, but uses a different heated material to capture impurities. The flow restrictor (FR1) is used to control the flow rate through the purifier, ensuring its effectiveness.

A rough outline of the injection procedure goes as follows. All valves in the diagram in

Fig. 5.2 are initially closed, and all volumes are at vacuum, except the Xe-methane mixture in the source bottle (SB1) and Xe in the supply bottle (B1). The methane purifier volume may be filled with a Xe-methane mixture if another injection occurred shortly before.

The *dosing* procedure occurs first. The desired dosing volume is determined to be either DV1 (15.0 cc) or DV1 + DV2 (102.3 cc), based on the intended dose size. If the larger dosing volume is to be used, V3 is opened. First, V4, V5, and V7 are opened to fill the methane purifier and flow restrictor (FR1) volume with the Xe-methane mixture. When the pressure measured by PT2 settles, V6 is opened. FR1 limits the flow rate through the methane purifier as the chosen dosing volume is filled. This procedure may take multiple hours depending on the dosing volume and bottle pressure. When the desired pressure is reached on PT3, V6 and V7 are promptly closed to complete the dosing procedure.

The *flushing* procedure begins after the panel is properly dosed. The dose volume is flushed by flowing Xe from B1 through MFC1 at 500 SCCM. The flushing time varies by injection but can last between six minutes and two hours. After flushing, the panel is (cryo)pumped to remove any residual methane. All valves are closed following the pump out. Mentioned above, the Xe-methane mixture is occasionally left in the purifier volume if another injection is scheduled in the following few days. The procedure would be executed identically, except the mixture would be in the volume bounded by V4 and V6 to start. Several other slight deviations occur during specific injections. These will be discussed more throughout the chapter.

5.3 Natural Methane Removal Tests

Before CH₃T calibrations, CH₄ is introduced into LZ to verify that the purification system is working as expected and quantify the removal. Cold trap mass spectrometry is used to measure the CH₄ concentration in LZ. Measurements are made with the Mobile

Sampling System (MSS) and the Stationary Sampling System (SSS). These systems are discussed at length in chapter 3. The main goals of the CH₄ removal tests are to determine the CH₄ removal time, determine the getter's single pass removal efficiency, verify the CH₄ concentration falls below the cold trap mass spectrometry system limit of detection, and verify that the measured CH₄ concentration (roughly) matches the expected injected CH₄ concentration. Two CH₄ removal tests have been conducted: one in October 2021 and another in August 2022.

The expected removal time can be calculated using the getter's single pass removal efficiency. The time rate of change of the CH₄ concentration $\dot{C}$ is given by Eq. 5.2, where C is the concentration, f is the (mass) flow rate through the getter, r is the getter's single pass removal efficiency, and m is the total Xe mass in the circulation system.

$$\dot{C} = \frac{-f * r}{m} * C \quad (5.2)$$

This equation has a solution of the form $C = C_0 * e^{-t/\tau_{expected}}$. $\tau_{expected}$ is given in Eq. 5.3.

$$\tau_{expected} = \frac{m}{f * r} \quad (5.3)$$

The equations above assume that the CH₄ is evenly distributed in the Xe. Various explanations could justify a disparity between observed and expected removal times but the simplest is that the Xe moving through the getter has a CH₄ concentration which differs from the average CH₄ concentration.

5.3.1 Cold trap mass spectrometry methane measurements

The RGA is the measurement device for both the MSS and the SSS. An extensive discussion of RGA operation is given in section 3.3.1. A few points relevant to measuring

CH₄ will be repeated here. The RGA detects ions of a given mass to charge ratio (AMU/q) and cannot distinguish between ions of the same mass to charge ratio. The RGA ionizes gas species passing through its ionizer's volume. The ionizer can fragment molecules, turning H₂O into H and HO for instance. The RGA may doubly ionize gas species. Each gas species will exhibit a characteristic mass to charge pattern, based on fragmentation, component isotopic ratios, and ionization probability.

CH₄ has a nominal mass of 16 AMU. A singly ionized, unfragmented CH₄ molecule will have the same mass to charge ratio as the H₂O and O₂ products: doubly ionized O₂ and the fragment O. The prevalence of H₂O and O₂ in vacuum systems renders AMU/q 16 ineffective for measuring CH₄. An RGA scan highlighting the fragmentation pattern of water is shown in Fig. 3.8. Fragmentation provides a CH₄ signal in the relatively clean AMU/q 15 channel. AMU/q 15 accounts for 39.5% of measured CH₄ [62] and is used to track CH₄.

The cold trap mass spectrometry systems can access Xe immediately upstream or downstream from the getter. Using these two ports, the MSS and the SSS are able to determine the getter's single pass removal efficiency.

5.3.2 October 2021 CH₄ removal test

The CH₄ loading procedure was first performed on October 5 and 6, 2021. 1.99 bara of a 50% Xe 50% CH₄ mixture was used to fill the 102.3 cc dosing volume on October 5, and was flushed into the LZ circulation system at 08:50 MT on October 6. The total flushing time was six minutes. 0.073 g (101.8 scc) of CH₄ were added to the system. The expected CH₄ concentration was approximately 7 ppb (parts per billion). Measurements began on October 8 and continued for the next month. Most measurements were drawn upstream of the getter but several were drawn downstream to evaluate the getter's single pass removal

efficiency.

The circulation flow rate was initially 500 SLPM but was increased to 598 SLPM just prior the first purity measurements. The flow rate remained constant until circulation stopped on the evening of October 12. Flow was gradually increased to 600 SLPM following the circulation restart. Circulation was, again, stopped for approximately one hour on the morning of October 13, after which the flow rate was raised to 600 SLPM. The flow rate was eventually reduced to 401 SLPM on October 14 around 8:00 MT. Measurements are shown in Fig. 5.3. Measurements following the circulation stoppages are included with the circulation stoppage time removed from the plot. These are not used in the removal time fit.

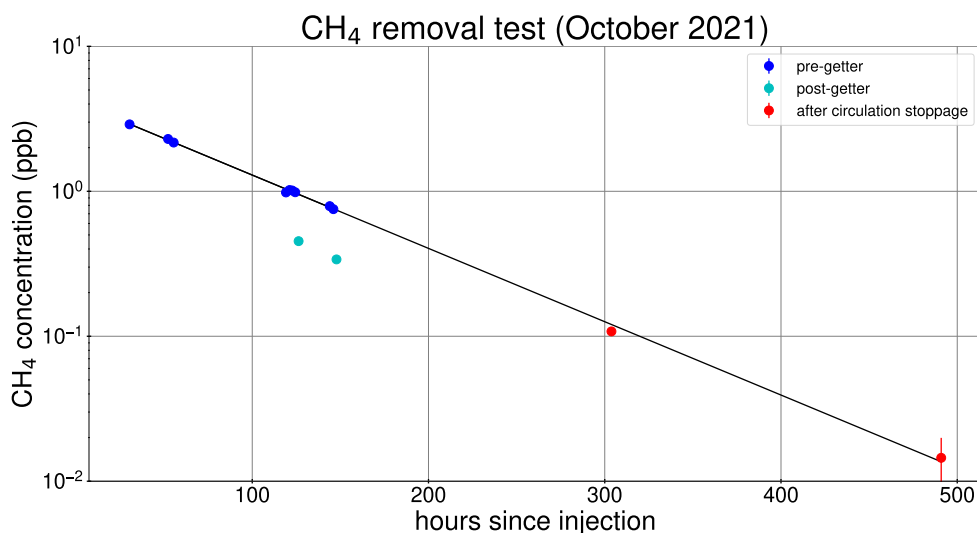


Figure 5.3: MSS Measurements of CH₄ for the October 2021 CH₄ removal test are shown. The fitted removal time is 85.8 ± 3.0 hours. Measurements are drawn before the getter (blue) and after the getter (cyan). The measured removal efficiency is 0.535 ± 0.016 . Circulation was stopped due to a power outage shortly after the final blue and cyan measurements were taken. All measurements used to fit and calculate efficiencies were drawn when the flow rate was 598 SLPM. No measurements after the initial disruption are used in any calculation. These measurements (red) are shown to compare with the projected CH₄ concentration. The time accumulated during the circulation system stoppages is removed from this plot. Later measurements (not shown) fall below the system's limit of detection.

The changes in the flow rate perturbed the circulation system's thermodynamic equilibrium. The circulation system takes days to reach equilibrium after changes. Other thermodynamic adjustments were made in the fitting period to balance the circulation system. These thermodynamic changes likely have no significant effect on the removal time measurements, although the flow rate changes themselves affect the removal time.

The measured removal time is $\tau = 85.8 \pm 3.0$ h, and the measured (fitted) concentration at the time the CH₄ is loaded into the circulation system is 4.14 ± 0.18 ppb (g/g). The measured single pass methane removal efficiency is $r = 0.535 \pm 0.016$. This was determined by finding the survival fraction $s_n = c_n(t_n)/c_{fit}(t_n)$, where $c_n(t_n)$ is the concentration of the n th post-getter measurement, at time t_n , and dividing by the fit line value at that time, $c_{fit}(t_n)$. The uncertainties for each s_n are found by propagating the uncertainties on the measurement, c_n , and the fit line, c_{fit} , at time t_n . The (in this case two) s_n are combined via weighted average, with their uncertainties propagated accordingly, to determine s , where $s = 1 - r$.

The removal time and single pass removal efficiency are notably poor. This is because the getter vessel bed temperature was around 314 °C during the test. A plot of the getter temperature before and during the removal test is shown in Fig. 5.4.

314 °C is significantly lower than the getter's nominal operating temperature of 400 °C. The getter temperature was increased before any future methane injections. Despite the lower temperature, CH₄ concentrations eventually fall below the sampling system limit of detection.

The discrepancy between the expected and measured concentrations of CH₄ is about a factor of 5/3; this is not a concern. First, there is some uncertainty on the exact fraction of CH₄ to Xe in our source bottle. There is no rigorous estimate of this uncertainty. Second, there were several (future) instances when a significant deficit between the expected injected amount of CH₃T and the measured amount of CH₃T was observed. The deficits



Figure 5.4: The getter temperature is shown before and during the October 2021 CH₄ removal test. The temperature fell below the nominal 400 °C operating temperature in late September 2021. Several minor disruptions to the circulation flow rate caused slight transients in the getter temperature prior to the test start, on the morning of October 6. The getter's steady state temperature dropped slightly when the flow rate was increased on October 8. There is a slight gap in the getter temperature data between a circulation stoppage and the flow rate reduction on October 14.

are discussed throughout section 5.4. It is unclear how this test was influenced by factors that caused the deficits. Lastly, the sampling systems were not calibrated for CH₄, and an unknown (linear) systematic is expected when measuring CH₄. Again, there is no rigorous attempt to quantify this because of the aforementioned uncertainties and because changing the linear scale factor applied to all measured CH₄ concentrations does not alter the removal time.

The expected removal time for this test is calculated using Eq. 5.3 with a flow rate $f = 212 \pm 2$ kg/h (equivalent to 598 ± 6 SLPM), an estimated Xe mass $m = 10155$ kg (negligible uncertainty) and a removal efficiency $r = 0.535 \pm 0.016$, the expected removal time is 89.9 ± 2.9 h. $\tau/\tau_{expected}$ is 0.955 ± 0.046 indicating this removal rate is consistent with the assumption that CH₄ was uniformly mixed in the Xe.

5.3.3 August 2022 CH₄ removal test

A second natural CH₄ removal test was performed on August 23 and 24, 2022. The goal of this test was to quantify the improvement in removal after increasing the getter temperature to 401 °C. The 102.3 cc dosing volume was filled with 1.453 bara of a 50% Xe 50% CH₄ mixture, which equals 0.053 g (74.3 scc) of CH₄. This was inserted in the LZ circulation system on the morning of August 24. The total flushing time was six minutes. The expected CH₄ concentration was approximately 5 ppb. The circulation system flow rate was 598 SLPM.

Unlike the previous test, CH₄ was measured with the MSS and the SSS. The SSS had not yet been calibrated for low sensitivity measurements and was calibrated after these measurements were made. The two systems have different systematic uncertainties, and the absolute normalization of measured CH₄ in each may differ. Instead of resolving the scaling factors between the systems, measurements from the two systems are fit together, with two different amplitudes, but the same removal constant. The fitted measurements are shown in Fig. 5.5.

The measured removal time is 63.9 ± 1.4 h. The SSS measured initial concentration is 4.51 ± 0.27 ppb (g/g), while the MSS measured initial concentration is 3.05 ± 0.08 ppb (g/g). The measured removal efficiency is $r = 0.794 \pm 0.009$. This is determined using the same method outlined in section 5.3.2. Later measurements are below the limit of detection and not included in the plot.

The removal time improved after the getter temperature increased. The removal efficiency increased from 59% to 79%. The fraction of expected to measured CH₄ for the MSS is similar to the previous injection: about 5/3. For the SSS, this fraction is about 7/6. Using the flow rate, the Xe mass, and the measured removal efficiency (0.794, as measured before and after the getter), the expected removal time of this test is 60.5 ± 0.8 h. Unlike

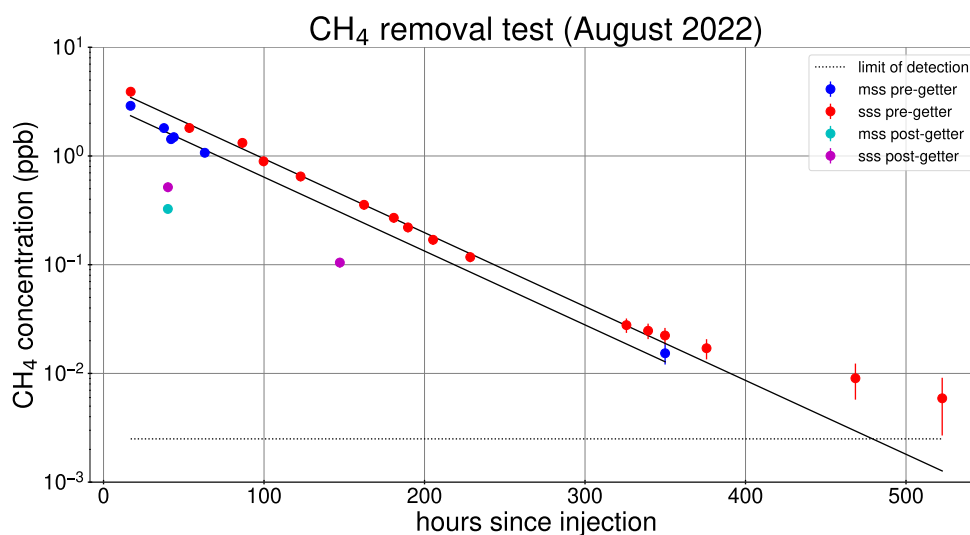


Figure 5.5: Cold trap mass spectrometry measurements taken during the August 2022 CH₄ removal test are displayed. The flow rate was 598 SLPM and the getter temperature was 401 °C. Measurements are made with both the MSS and the SSS. MSS and SSS measurements are fitted with two different amplitudes but a common floating time constant. The fitted removal time is 63.9 ± 1.4 hours, and the removal efficiency is 0.794 ± 0.009 . Later measurements (not shown) fall below the indicated limit of detection.

the October 2021 CH₄ test, the expected removal time is shorter than the observed removal time. The fraction $\tau/\tau_{expected}$ is 1.056 ± 0.027 . There is a two σ difference between the observed and expected removal times.

The two removal tests effectively show that CH₄ can be inserted into the LZ circulation system. The measured concentrations are close to the expected value. These tests demonstrate that CH₄ can be removed to concentrations that are imperceptible to the cold trap mass spectrometry systems. The measured removal time and single pass removal efficiency prove CH₃T can be safely injected in LZ and removed in a reasonable amount of time.

5.4 Tritiated Methane Calibrations

After successful CH₄ removal tests, CH₃T was deemed safe to be injected in LZ. CH₃T is injected in smaller quantities than CH₄. Cold trap mass spectrometry systems are unable to detect these small CH₃T quantities. LZ TPC measurements are used to determine injected activity and removal time. A fast analysis verifies the presence of tritium in real time. This analysis confirms ³H-like activity initially increases, and, more importantly, confirms CH₃T removal is taking place. In conjunction, a more extensive offline analysis determines the total injected activity and removal time for each CH₃T injection.

CH₃T calibration campaign timing must be carefully considered. Because ³H is a WIMP background, WIMP search data cannot be taken until ³H rates sufficiently fall. The purposes for studying CH₃T removal are quantifying the CH₃T removal time in LZ, projecting when WIMP search data taking can resume, quantifying the maximum ³H activity, and verifying that the event rate in the ³H energy range returns to pre-calibration levels. If a science run is scheduled to start when a non-negligible amount of ³H remains in LZ, the measured activity and removal time are used to determine the expected ³H background

contribution.

There are three CH₃T calibrations discussed in this chapter: one in April 2022, one in October 2022, and one in April/May of 2023. Unlike the CH₄ injections, all CH₃T injections were performed with nearly identical flow rates (around 400 SLPM) and getter temperatures (around 400 °C). The trigger used to collect ³H events is identical to WIMP search trigger. Broad cuts are implemented with the intent to capture the majority of ³H events, accepting a small fraction of non-³H events. This is permissible because the vast majority of events collected during a calibration are expected to be ³H.

Different calibration datasets were processed with different versions of the LZ event reconstruction software, *LZAP*. The analysis cuts used to identify ³H are different for each calibration. Consequently, the observed ³H efficiency and measured activity for each calibration campaign are not directly comparable. These slight differences between cuts and processing should not affect the measured removal times. The removal times of each calibration campaign are directly comparable because differences in flow rates and getter temperatures are minute.

5.4.1 April 2022 CH₃T calibration

The first CH₃T source bottle was installed on the source injection panel on April 5, 2022. The one liter bottle was prepared at University of Maryland and contained a 2.56 bara Xe-CH₃T mixture with an expected activity of about 1.33 mBq/(bar*cc) when the injections occurred.

The first CH₃T calibration campaign occurred in late April 2022, after SR1. The calibration campaign consisted of two injections. The first was a smaller *test* injection and was followed by a larger *full* injection. The circulation system flow rate was 398 SLPM throughout the campaign. Getter temperature was 403 °C at the start of the campaign and

was increased to 411 °C on April 26 at 11:31 MT. No correction is made to account for the change in getter temperature because it is small and occurs near the end of the calibration.

On April 20, 2022 at 12:43 MT the test injection was performed. The smaller dosing volume (15 ccs) was filled with 0.484 bara of the Xe-CH₃T mixture using the procedure discussed in section 5.2. This was flushed into LZ at a rate of 500 SCCM for eight minutes. The expected injected activity based on dose pressure and volume was about 9.7 mBq. The injection was monitored using TPC data to verify ³H rates decreased before additional injections were performed.

Two days later, on April 22 at 11:39 MT, the full injection was performed. The Xe-CH₃T mixture was intentionally not pumped out between V4 to V7 (as seen on Fig. 5.2) after the test injection; the full injection procedure began with this space occupied. The larger dosing volume (102.3 ccs) was filled with 1.024 bara of the Xe-CH₃T mixture. This was flushed into the circulation system for 16 minutes at a rate of 500 SCCM. The expected injection activity was 139 mBq.

The event selection includes minimal cuts to allow for a relatively high efficiency for ³H and sufficient rejection of backgrounds. All events in this calibration campaign are processed with LZAP version 5.5.1. A standard set of LZ WIMP search cuts for SR1 are defined to reject WIMP backgrounds. Of these, the fiducial volume, outer detector veto, and skin veto are used in this analysis. ³H events will experience minimal rejection from these cuts, while external backgrounds will be significantly reduced. An S1 area cut, 5 – 150 phd and a log(S2 area) cut, 3 – 4.5 (log (phd)) are implemented to reject events outside of the ³H signal energy range. The lower S1 cut boundary removes a nontrivial fraction of ³H decays, but rejects a significant number of accidental (often small) S1s. Plots of the spatial and energy distributions of events passing cuts for both injections are shown in Fig 5.6.

Events passing the cuts are grouped into one hour bins. The number of CH₃T counts per bin passing the event selection is divided by the live time per bin to calculate the event

CH₃T Calibration (April 2022)

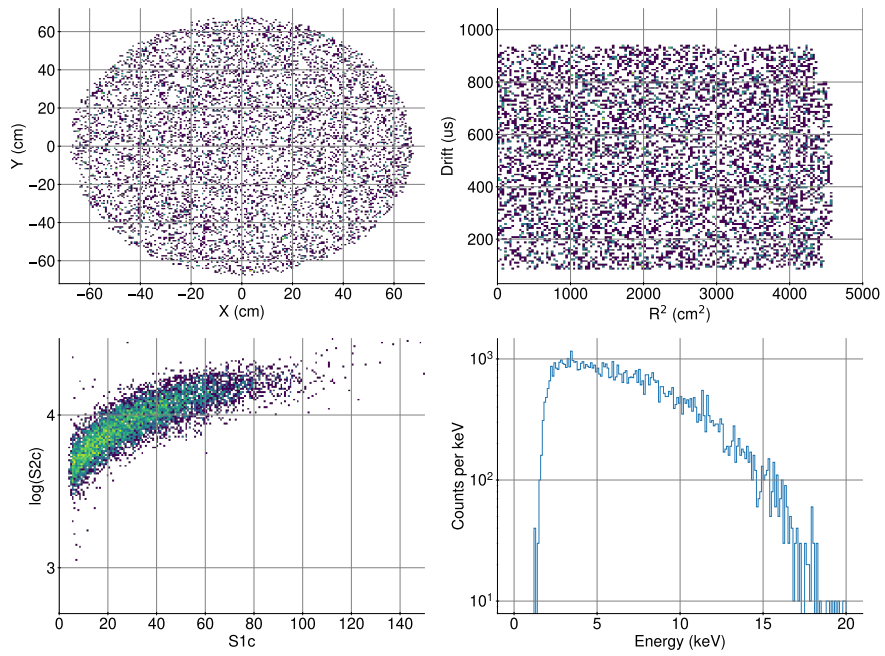


Figure 5.6: Spatial and energy plots are shown for events passing cuts during the April 2022 CH₃T calibration. The X-Y plot is at the top left, the R² drift plot is at the top right, the S1c-log(S2c) plot is at the bottom left, and the reconstructed energy spectrum is at the bottom right. The g_1 and g_2 used to produce the energy spectrum are $g_1 = 0.117$ phd/photon and $g_2 = 43.6$ phd/electron. The total number of events in this calibration is low compared to other CH₃T calibrations.

rate in a given bin. Using rates (as opposed to counts) is necessary to handle differences in live time between bins. The measurement period spans from April 20, 2022 at about 12:30 MT to April 27, 2022 at about 12:00 MT. All runs are processed with LZAP 5.5.1.

The live time must be considered to properly calculate the event rate for a given time bin. Several brief, but significant, time periods are excluded from the analysis. These include regular detector LED calibrations, underground operations known to introduce noise, and periods when the detector acquisition mode is changed. These periods can last anywhere from tens of seconds to a few hours and must be accounted for to properly calculate the event rate. Additionally, very high rate periods can reduce the live time. Improper accounting of the high rate live time losses will inflate the measured removal time.

For each event, LZAP records the *physics live time* that the detector is able to record a single scatter event between that event and the previous event. This accounts for recording time losses due to inefficiencies in the data acquisition system and losses related to event window definitions. Physics live time is summed across each bin for every event observed by the detector. A more robust live time calculation would account for additional factors like time lost due to vetoes. However, these losses are small. Only accounting for more significant losses (like excluded time periods) and systematic factors (that affect the removal time calculation) is sufficient.

The uncertainty on the rate of a given bin is calculated using the square root of the number of counts and dividing by bin live time. Bins for which the approximation is invalid (< 10 counts in a bin) are excluded from fit minimization but are still displayed in the rate plot. Few bins (mostly concentrated near the injection tails) are excluded on this basis. The measured ^3H rates from the April 2022 CH_3T calibration are shown in Fig. 5.7.

WIMP search data from April 11 through April 18 is analyzed to verify the ^3H -like background event rate is not a significant contributor to the fitted data. All data is processed with LZAP 5.5.1. The analysis includes nearly identical cuts, with the addition of the hot

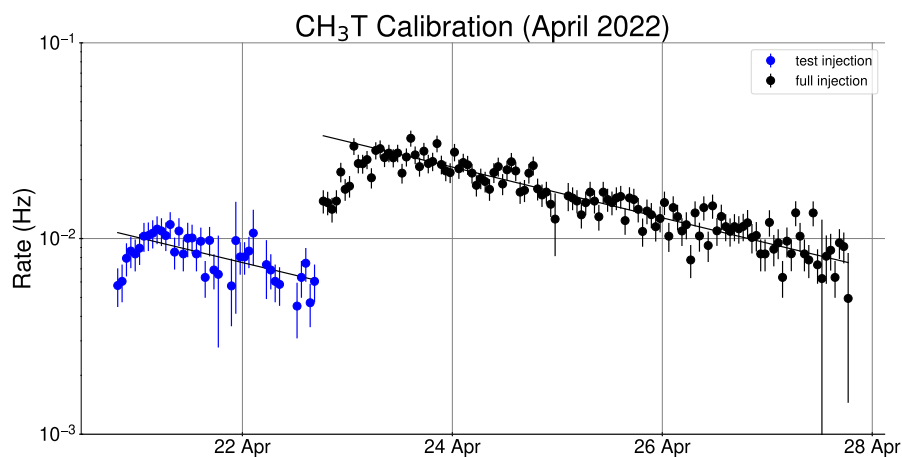


Figure 5.7: CH₃T calibration rate measurements from April 2022 are displayed. Rates reach 30 mHz. The getter temperature during the calibration was 403 °C, and the flow rate was 398 SLPM. A small "test injection" was performed with intent to verify that the rates eventually fell. Once verified, a larger "full injection" was performed. Measurements from both the test and full injections are shown. The bin size is one hour. The rise time of the rates is quite slow relative to later calibrations, taking about twelve hours to reach peak. A single fit, with different amplitudes for each injection but the same removal constant, is included. The removal time is 79.7 ± 3.2 hours. The first twelve hours of each injection are dropped from the fit, as well as several bins without sufficient counts to use the gaussian approximation for uncertainty on counting statistics. The amplitude of the full injection was expected to reach 140 mHz, but its fitted amplitude is only 33 mHz.

spot exclusion cut. There were no hot spots during the CH₃T calibration period. The event rate during the week long background period was 0.13 ± 0.02 mHz. The minimum rate during the injection period was about 5 mHz. This confirms the background makes no significant contribution to the observed rates during the calibration. Still, the background rate is included ($C = 0.13 \pm 0.02$) when fitting to a data with Eq. 5.1.

Both injections are fitted in a single chi square fit. Each amplitude and a common removal time are floated. Each injection start time (t_0) is set to the time of each respective injection. The first twelve hours following the time of each injection are excluded to account for the full ingrowth of ³H. The fitted removal time constant is 79.7 ± 3.2 hours. The total number of events passing all cuts is 7697. The fitted rates at the injection times are 10.7 ± 0.5 mHz and 33.7 ± 1.0 mHz for the test and full injections respectively. As expected, the removal time of this calibration is between the removal times of the two CH₄ removal tests.

The observed rate of the test injection is slightly greater than expected. Assuming 100% efficiency, a 9.7 mBq injection would result in an observed rate of 9.7 mHz. Losses, mostly from decays occurring outside the fiducial volume, will reduce the observed rate. For the full injection the expected rate was around 140 mHz, but only 33 mHz was observed. The shortfall will be discussed more in section 5.4.3.

These injections took noticeably longer (twelve hours) to reach their maximum activity than later injections. Later injections peak within two hours. To verify the selected twelve hour exclusion period is sufficient, fits are performed excluding the first 2 to 24 hours of each injection. Fits that include bins prior to CH₃T reaching equilibrium may prefer longer removal constants. As the pre-equilibrium bins are removed from the start of the fit, the central values of the fitted removal time should converge. The central values of each fit are plotted in Fig. 5.8 and indicate that twelve hours is a sufficient exclusion window.

The rate before and after the injection is assessed to verify that ³H is fully removed

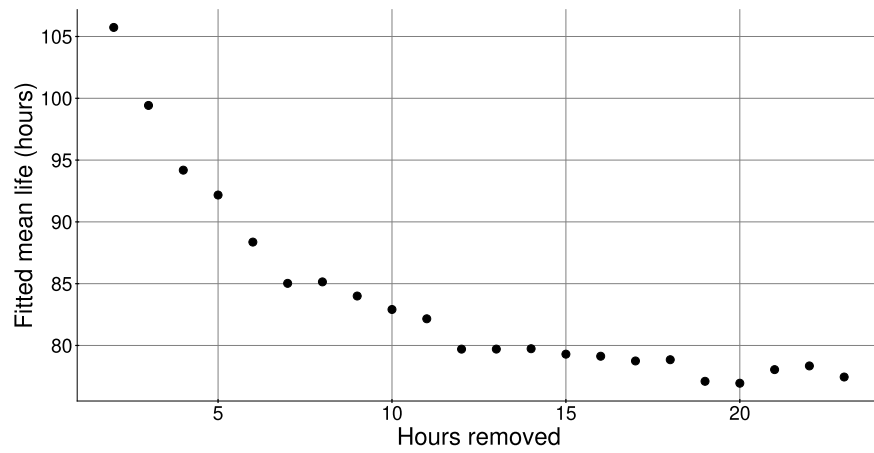


Figure 5.8: Each data point in the plot is the fitted central value of the mean removal time for a fit, with the number of hours excluded from the start of the fit on the horizontal axis. The plot is intended to assess whether excluding the first twelve hours (or bins) is sufficient to account for the slow CH_3T ingrowth and equilibration in the TPC. If the fit region includes measurements before CH_3T reaches equilibrium, a higher removal time will be measured. Fits that exclude all non-equilibrium bins should measure similar removal times. The fitted central value at twelve excluded hours is consistent with the asymptote of the fitted removal times.

and the injection did not cause the background rate to increase. Data from August 2022 is compared with data from early April 2022. The August data was not processed with LZAP version 5.5.1, so the two datasets are compared using LZAP version 5.4.7. The same cuts used for the ^3H rate calculations are applied to these datasets. The rate of events passing the selection cuts in the pre-calibration data is 0.20 ± 0.02 mHz. The event rate in the post-calibration data is 0.25 ± 0.04 mHz. The two event rates are consistent, indicating that there is no evidence of lingering CH_3T after the calibration.

Eq. 5.3 can be reinterpreted to determine the implied getter removal efficiency r_{implied} for this calibration. The equation becomes Eq. 5.4, where m and f are mass within the circulation system and (mass) flow rate respectively, and τ is now the observed removal time. This equation should hold assuming methane is well mixed within the detector and no other unexpected factors lead to misinterpretation of the removal efficiency.

$$r_{\text{implied}} = \frac{m}{f * \tau} \quad (5.4)$$

The implied removal efficiency for this calibration campaign is 0.905 ± 0.037 . This is over 10% more than the measured August 2022 CH_4 getter removal efficiency. The result implies that lower flow rates improve gettering efficiency. The effect suggests that the benefit of increasing the flow rate is slightly hampered by the loss of gettering efficiency.

5.4.2 October 2022 CH_3T calibration

The second CH_3T calibration campaign occurred in October of 2022. The first injection happened on October 12, 2022 at 13:12 MT and the final injection took place on October 20, 2022 at 13:48 MT. This calibration used the same CH_3T source bottle as the April 2022 calibration. The injections are labeled as injection A, injection B, and injection C (eight part injection). The times and measured amplitudes of the injections are shown in

Table 5.1. There were significant differences in the activity expected from the injection parameters and the observed activity during several of these injections.

Injection Part	Date	Time	Counts	Amplitude (mHz)
A	Oct 12	13:12	511	7.9 ± 0.3
B	Oct 13	11:50	18105	106 ± 1
C (part 1)	Oct 17	11:59	-	-
C (part 2)	Oct 17	19:06	9990	133 ± 2
C (part 3)	Oct 18	14:04	-	-
C (part 4)	Oct 18	18:12	15097	224 ± 2
C (part 5)	Oct 19	14:10	-	-
C (part 6)	Oct 19	18:57	16369	286 ± 3
C (part 7)	Oct 20	10:50	-	-
C (part 8)	Oct 20	13:48	68795	401 ± 3

Table 5.1: Details of the October 2022 CH₃T calibration injections are shown. This includes data from ten individual injections spanning nine days. Only the second injection of each day of the part C injections is fit. The amplitude is the fitted rate projected back to the time of the first injection on each day. The remaining activity from previous injections is not subtracted from the listed amplitude. The sum of counts in this table will not equal the total counts in the October 2022 CH₃T calibration because events between fit windows are not included in the table.

A brief unintentional getter bypass was initiated near the end of injection B on October 16 at 10:30 MT. This was caused by a misleading getter internal lifetime warning. Circulation through the getter resumed at 17:19 MT that day. Events from this time period are displayed on all plots, but the rates between the shutoff and the end of injection B are not used in the fit. Otherwise, the getter temperature was 403 °C, and the flow rate was 400 SLPM throughout the calibration.

Based on the injection parameters, the expected activity of injection A was nearly identical to the expected activity of the test injection during the April 2022 calibration period (about 9 mBq). The smaller 15.0 cc dosing volume was filled to a pressure of 0.49 bara. Injection A was flushed into LZ at a rate of 500 SCCM for six minutes. For injection B, the larger 102.3 cc dosing volume was used. The Xe-CH₃T mixture was left in the purifier

volume between injections A and B but additional Xe-CH₃T mixture was added to fill to the desired dosing pressure for injection B. Injection B was flushed into the LZ circulation system for 65 minutes at a rate of 500 SCCM. The flushing time was increased to compensate for the unexpectedly low observed rate from the April 2022 full injection. Injection B was expected to yield 133 mBq of activity (slightly less than the 137 mBq expected during the full injection in April due to ³H decay in the source bottle).

”Injection C” spanned four days with two injections each day, totaling eight injections. For simplicity, the part C injections will be grouped and referred to by the day they occurred. For example, ”injection C day 2” will refer to injection C part 3 and injection C part 4 together.

All parts of the first three days of injection C were performed using the same procedure used by injection B, with a few exceptions. These procedural changes were made to address shortfalls in observed activity. Injection C part 2 was flushed for 65 minutes, then allowed to sit in the dosing volume for an hour before being flushed for another 65 minutes. This was done to alleviate potential concerns about CH₃T getting stuck in dead end corners of the source injection panel’s dosing volume. Injection C part 4 was flushed for 120 minutes as a slight variation on the part 2 procedure to address similar concerns.

Injection C day 4 (part 7 and part 8) used a modified procedure. All volumes up to the source bottle (V5 in Fig. 5.2) were cryopumped to (rough) vacuum before the dose volume was filled for part 7. The dose volumes were filled through V9, using MFC2 to regulate flow through the methane purifier. This was intended to reduce the hour long waiting time associated with filling the large dose volume through the flow restrictor, FR1. V6 and V7 remained closed while the dosing volume was filled. The intended activity for each day 4 injection was identical to the intended activity of the previous seven injections.

The expected injection activity and the measured injection activity varied significantly between injections. The fitted rate for injection A was 7.9 mHz, roughly in agreement

with the measured activity from the test injection of the April 2022 calibration. Injection B yielded a rate of about 100 mHz from the expected injection activity of 132 mBq. Injection C day 1 was expected to yield a combined rate increase of twice injection B's rate. The two day 1 injections only increased the rate by a total of 100 mHz. The rate increase following the day 2 injections (again, with the same expected rate increase) was about 125 mHz. Day 3 showed a similar increase of about 120 mHz. The modified procedure used on day 4 increased the ^3H rate by 170 mHz. The variation between these injection activities only became apparent days after the final injection, when the data files were fully processed. The variations and shortfalls were still not understood after the October 2022 calibration. Increasing flush time did not prevent shortfalls. Further discussion of this continues in section 5.4.3.

Portions of this dataset were not processed with LZAP 5.5.1, so LZAP 5.4.9 processed data is used. All ^3H labeled data between October 12 at 13:12 and October 24 at 9:03 was analyzed. Rates are generally high enough that no extra study of the background rate is warranted, and the constant term (C) is not used when fitting to Eq. 5.1. The analysis for this calibration campaign is identical to the April 2022 CH_3T calibration, aside from slight changes to the outer detector and skin veto cuts. The spatial and energy distributions of events the passing cuts are shown in Fig. 5.9.

The ^3H rates are plotted in Fig. 5.10. The injections are grouped and fitted by injection date. Days with multiple injections have insufficient statistics to fit an exponential to the first injection of the day. Only the final injection of the day is fitted.

The injections reach equilibrium considerably faster than the April 2022 injections. Observed rates consistently peak within an hour of the injection. The bin containing the injection and the first bin following each injection are excluded from the fit. The period following the getter shutoff during injection B is also excluded. As before, all injections are fitted by floating the same removal constant but different amplitudes. All injections have

CH₃T Calibration (October 2022)

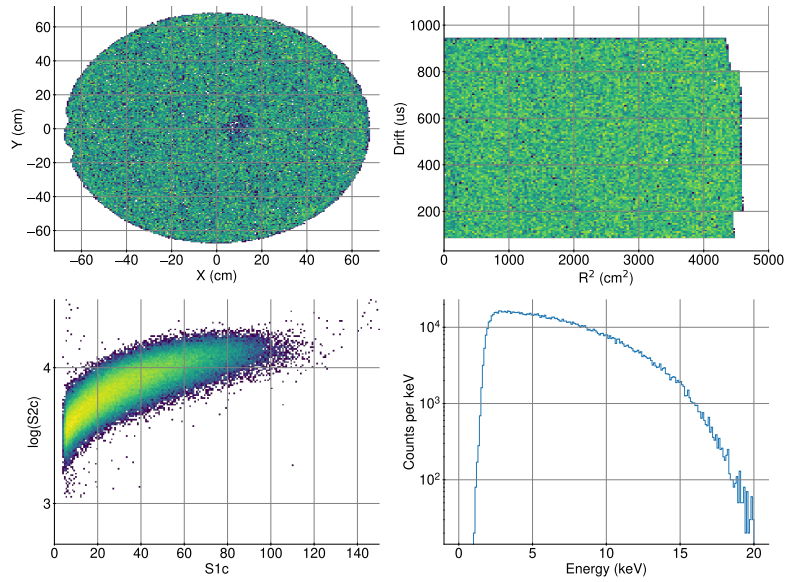


Figure 5.9: Spatial and energy plots are shown for events passing selection cuts during the October 2022 CH₃T calibration. The X-Y plot is at the top left, the R^2 drift plot is at the top right, the S1c-log(S2c) plot is at the bottom left and the reconstructed energy spectrum is at the bottom right. The g_1 and g_2 used to produce this energy spectrum are 0.113 phd/photon and 36.2 phd/electron. There were far more events in this calibration than in the April 2022 calibration plots.

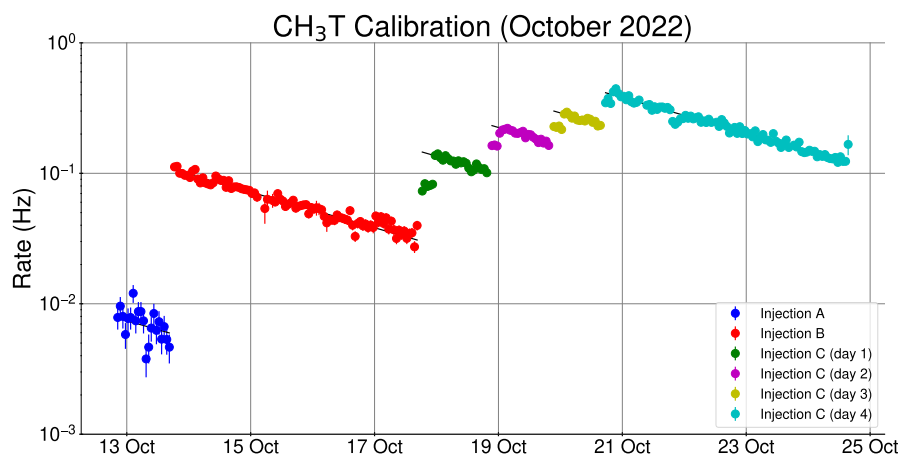


Figure 5.10: All October 2022 CH_3T rates are shown. The getter temperature was $403\text{ }^\circ\text{C}$ and the flow rate was 400 SLPM. For simplicity, the part C injections are grouped by day instead of by injection. The first injection of each day in the part C data is seen as a clustering of data points falling roughly half-way between the end of the previous day's data and the rest of the current day's data. Bins are one hour long. Rise times are clearly quicker than those in the April 2022 calibration data. Maximum activity exceeds 0.4 Hz on the fourth day of injection C. The removal time of all data fit together is 76.3 ± 0.8 hours. The first injection of each day of the part C injections are excluded from the fit. For the remaining injections, the bin when the injection occurs and the following bin are excluded to account for the delay in the rate increase. Additionally, the period after the getter shutoff during injection B is not included in the fit.

their start time (t_0) set to the time of the injection. The fitted removal time is 76.3 ± 0.8 hours.

The removal time is consistent with the April 2022 CH₃T calibration. The ³H rate exceeds 0.4 Hz in this calibration, with the total number of counts reaching 130791. Using Eq. 5.4, the implied removal efficiency $r_{implied} = 0.941 \pm 0.014$ is consistent with the previous campaign.

The second CH₄ removal test and both CH₃T tests have a getter temperature of about 400 °C. The two CH₃T calibrations have flow rates of about 400 SLPM, while the second CH₄ removal test had a flow rate of 598 SLPM. Measured removal efficiency of the second CH₄ removal test was 0.794 ± 0.008 . The implied removal efficiencies of both CH₃T calibrations are 0.905 ± 0.037 and 0.941 ± 0.014 respectively. This calibration offers further evidence that the removal efficiency depends on the flow rate.

5.4.3 April-May 2023 CH₃T calibration

The third CH₃T calibration campaign is comprised of five injections that began in April 2023 and ended in May 2023. The injections are labeled "A" through "E". Injection A is referred to as the "test injection" and occurred several weeks prior to the primary calibration. A new CH₃T source was installed in the source injection panel on April 21, 2023 for this calibration. The 1 L source bottle contained about 1.9 bara of a Xe-methane mixture with a total expected activity of about 340 Bq. The circulation system flow rate for the campaign was consistently near 390 SLPM. The getter temperature was 403 °C.

This calibration preceded the WIMP search 2024 (WS2024) data taking period. The intended calibration activity was great enough that ³H events were expected to make a non-trivial contribution to the early WIMP search background. Thus, quantifying the rate of events passing all WIMP search cuts was more important than quantifying the rate of

^3H events. Nearly all WIMP search cuts were applied to evaluate the ^3H contribution to the WIMP search event rate. Pre-calibration and post-calibration datasets were used to examine the event rate in the WIMP search ROI before and after the calibration. Table 5.2 summarizes the injections and pre/post-calibration periods, when they occurred, and their activity.

Period	Date	Time Start	Amplitude (mHz)	Counts
Pre cal	Apr 14	04:06	-	-
A (test inj)	Apr 26	11:58	13.5 ± 0.4	1501
B	May 08	14:10	15.0 ± 0.4	2074
C	May 11	11:27	462 ± 3	67193
D	May 16	10:55	205 ± 2	11141
E	May 17	09:41	430 ± 2	75953
Post cal	Jun 08	13:13	-	-

Table 5.2: Details of the May 2023 CH_3T injections and the pre-calibration and post-calibration analysis windows are shown. The pre-calibration and post-calibration periods are carefully selected to avoid lingering backgrounds from other calibrations. A few minor optical calibrations occurred in the middle of the CH_3T calibration period. Data from these periods are not included in this analysis. The counts and observed rates correspond to counts and event rates within the WIMP search ROI. The sum of counts in this table will not equal the total number of counts in the injection, as the sum does not include counts between fit windows.

Injection A was a relatively small injection using 0.016 bara of the Xe-methane mixture in the 15.0 cc dosing volume. The expected activity of 45 mBq was flushed into the circulation system at 11:58 MT on April 26 at 500 SCCM for 77 minutes. Some Xe was left in the purifier volume between injections A and B. 0.314 bara of the Xe-methane mixture was loaded into the 15.0 cc dosing volume on May 8 at 14:10 MT for injection B. This was flushed at 500 SCCM for about an hour. The injected activity was expected to be near 840 mBq. The observed rate was only 15.0 mHz.

This observed deficit cannot be related to the 102.3 cc dosing volume. Several leak tests confirmed that there was no significant leak across a valve that may have affected

the methane concentrations. Previous injections indicated that all shortfalls occurred when CH_3T was left in the purifier volume for an extended period of time. The longest methane residence time in the purifier volume was the time between injections A and B of the April and May 2023 CH_3T calibration. This also resulted in the largest observed shortfall.

The purifier space was cryopumped and refilled prior to injection C. On May 11 at 11:27 MT, a dose of 0.317 bara in the 15.0 cc dosing volume was delivered into LZ at 500 SCCM for 53 minutes. The dose pressure and expected injection activity (about 850 mBq) were nearly identical to the injection B dose, and the observed activity was 462 mHz. This was consistent with the expected ^3H detection efficiency. To repeat the methane purifier residence time effect, Xe and CH_3T were left in the purifier volume between injections C and D. A 0.316 bara dose was prepared in the 15.0 cc dosing volume on May 15. This was intended to be injected on the same day but was actually injected on May 16 at 10:55 MT using a modified flushing procedure. The observed rate increased by only 100 mHz. This relatively small rate increase is further evidence that the methane purifier reduces CH_3T . The purifier volume was cryopumped between injection D and injection E to complete the calibration. 0.156 bara of Xe-methane mixture was prepared in the 15.0 cc dosing volume and flushed into LZ at 500 SCCM for 56 minutes on May 17 at 9:41 MT. The expected injected activity was around 410 mBq, and the observed rate increase appears consistent with the expectation. The methane purifier residence time effect was later reproduced in benchtop tests at the University of Maryland.

Event rates are plotted in Fig. 5.11. All runs are processed with LZAP 5.8.0.

The analysis of this calibration differs from the analysis of the April 2022 and October 2022 CH_3T calibrations. The live time is calculated by a lightly modified version of LZ's WIMP search code. Events with S1c exceeding 80 phd are not counted in the WIMP search event rate. The cut begins to remove events at 13 keV (in electron recoil energy) and removes nearly all events above 15 keV (in electron recoil energy). While the cut results in

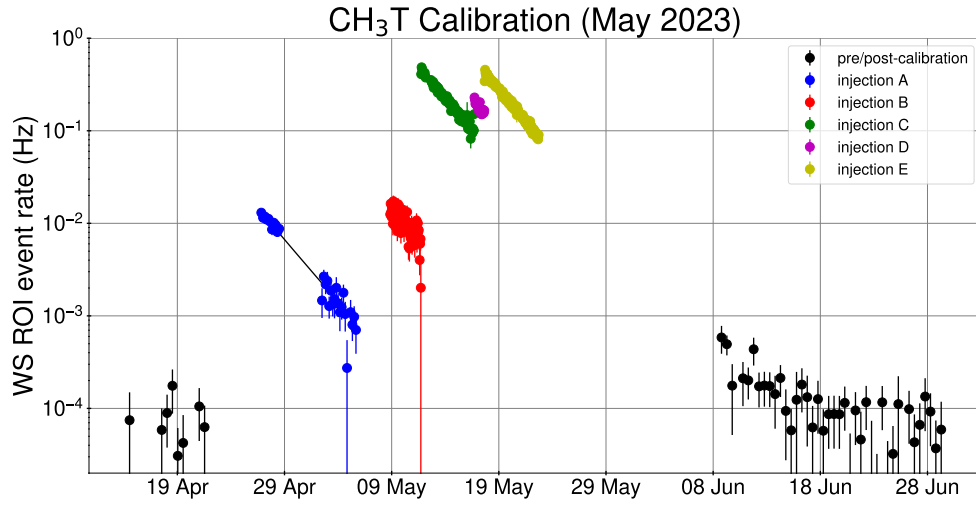


Figure 5.11: The event rates in the WIMP search region of interest (WS ROI) from all periods in the May 2023 CH₃T calibration analysis are shown. The getter temperature for this calibration was 403 °C, and the flow rate was 390 SLPM. Injections A, B, C, D, and E are explicitly labeled. The pre-calibration rates and post-calibration rates are binned in twelve hour bins, the injection A data is binned in four hour bins, and the primary calibration data is binned in one hour bins. This is done to avoid excessive zero bins in the low event rate periods while maintaining time resolution in the high event rate periods. A fit to all injections is plotted. Injections are fit with a common floating time constant but different floating amplitudes. The fitted time constant is 75.7 ± 0.5 hours. The amplitudes of individual injection fits are shown in Table 5.2.

a non-trivial efficiency reduction for ^3H events, the primary purpose of this analysis is to identify the calibration's contribution to the WIMP search rate at the start of WS2024.

Counts and live time are evaluated for each 10 minute (real time) bin. Both counts and live time are rebinned by summing from a chosen number of adjacent bins and dividing the counts by the live time to acquire a rate. The uncertainty on the rate is derived from the gaussian approximation on uncertainty for counts in each bin ($\sqrt{n}$) divided by the live time of each bin. All data points used in a fit must have at least 10 counts to ensure the approximation is valid. This is not a concern for the pre-calibration and post-calibration rates. The error bars on these rates are only for display and are not used in any fitting or calculations.

All injections are fit by floating the same removal constant with different amplitudes, anchored at the time of injection for each injection. The first and last hours of every injection are dropped from the fit. The fit results are shown in Fig. 5.11, and the final fit amplitudes are given in Table 5.2.

The combined fit removal time is 75.7 ± 0.5 h. This is consistent with the previous two calibrations. When fit independently, all injections have a removal time that is consistent with the combined fit removal time. The total number of counts in the injection B, C, D, and E fit windows is 159479. The implied removal efficiency of this calibration is 0.973 ± 0.012 , slightly greater than the previous two. This is about two σ from each of the previous two implied getter removal efficiencies. The minuscule circulation system flow rate reduction from 398 to 390 SLPM may ease the tension, since the flow rate appears to affect the removal efficiency.

From Fig. 5.11 it appears the pre-calibration event rate is consistent with the later post-calibration event rate. The event rate is compared for each window. Rates are calculated by summing counts from all bins in the window and dividing by the summed live time from all bins in the window. This avoids using the "for display only" error bars in the low rate data

mentioned above. The event rate prior to injection A is $76 \pm 18 \mu\text{Hz}$. There appears to be a tail from injection E in the post-calibration period. The rate after June 23 is compared with the event rate from the pre-calibration period. The event rate after June 23 is $66 \pm 15 \mu\text{Hz}$. These rates are averaged and included as a constant term (C) on the decaying exponential fits. The WIMP search rate returning to the pre-calibration value confirms that CH_3T is effectively removed from LZ.

Comparing the projection of the fit from injection E to the start of post-calibration data provides confirmation of the measured removal time (even when extrapolated to low rate periods) and the observed excess of events. The tail of injection E matches the start of the post-calibration data. This is shown in Fig. 5.12.

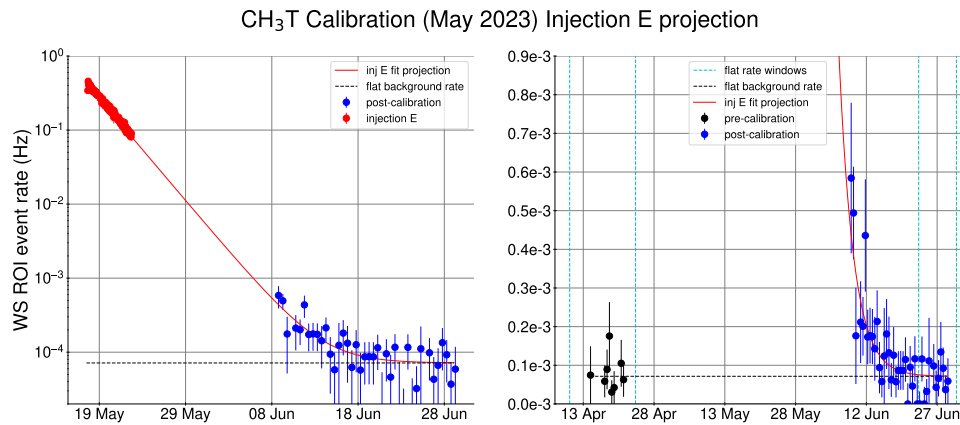


Figure 5.12: The projection of injection E to the post-calibration measurements is shown. The left plot shows injection E and the fit line projected to the end of the post-calibration period. The right plot shows a direct comparison of the background event rate in the pre-calibration window and the post-calibration window, with the injection E projection included. This again proves the getter's ability to remove CH_3T .

The methane source bottle used for this calibration campaign was accidentally contaminated with ^{14}C methane. ^{14}C is a single beta emitter with a Q-value of 156 keV and a half-life of 5700 years. The CH_3T and the $^{14}\text{CH}_4$ are chemically identical. Removal via the LZ getter is the primary depletion mechanism of both species. Thus, the presence of

$^{14}\text{CH}_4$ should not affect the measured removal time. No attempt is made to distinguish between ^3H and ^{14}C in this analysis. Independent estimates suggest the ^{14}C event rate is about 0.13 of the ^3H event rate across all energies for this calibration. This implies that nearly 98% of the excess events falling in the WS ROI are ^3H events. The S1-S2 plot and energy spectra for the WS ROI and the ER band during the primary calibration period are shown in Fig. 5.13. The spatial distribution is plotted in Fig. 5.14.

Remaining CH_3T counts in WS2024 can be calculated by integrating the activity of injection E to infinity from time t corresponding to a variable start date for WS2024. For fitted time constant τ , initial injection E activity A_0 , and injection E start time t_0 , the remaining number of counts $I(t)$ is given by Eq. 5.5.

$$I(t) = A_0 * \tau * e^{-(t-t_0)/\tau} \quad (5.5)$$

This function and its uncertainty are plotted in Fig 5.15. The plot and equation show raw counts from the calibration remaining in the WS ROI after a given date, assuming 100% detector live time (^{14}C events are included in this total). To determine the number of counts in WS2024, the equation must be convolved with the LZ WS2024 live time histograms and corrected for the (quite small) fraction of ^{14}C . The values and covariance matrix used to generate this are given in Table 5.3. Performing the convolution, the total number of ^3H and ^{14}C decays in LZ WS2024 is predicted to be 58.3 ± 3.3 .

5.5 Summary of Results

A summary of all methane campaigns is shown in Table 5.4. All CH_3T campaigns occurred with quite similar flow rates and getter temperatures, and all removal times are consistent. Future CH_3T calibrations will likely use similar parameters and should expect similar removal times of about 75-80 hours.

CH₃T Calibration (May 2023) Energy Spectrum

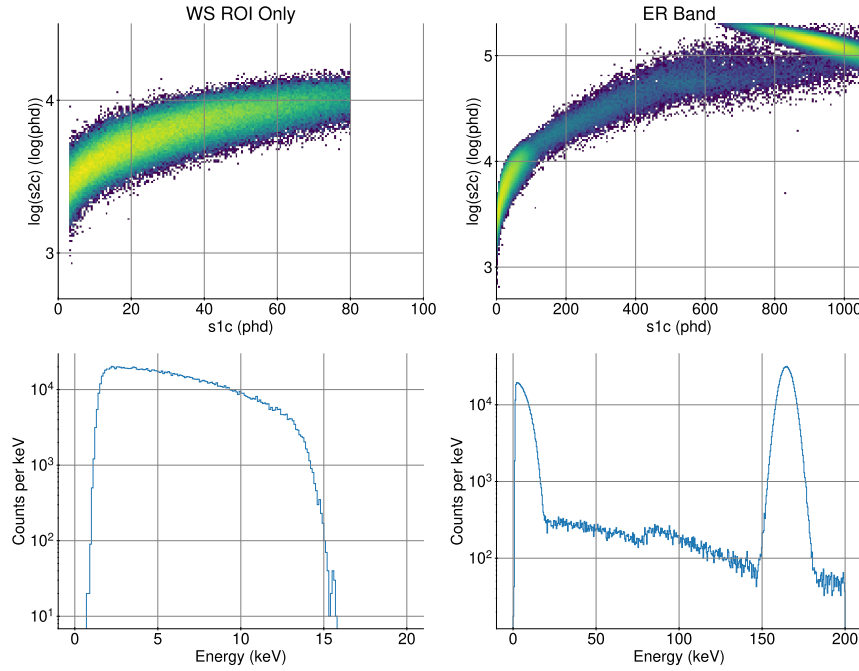


Figure 5.13: Energy spectrum (bottom) and S1-log(S2) (top) plots for the WIMP search region of interest (left) and the electron recoil band (right) to 200 keV are shown for the May 2023 CH₃T campaign. The g_1 and g_2 used to produce this energy spectrum are 0.112 phd/photon and 34.1 phd/electron. The electron recoil band is displayed here to show the presence of ^{14}C in the calibration. Only events in the WIMP search ROI are used in the rate calculations in this section. ^3H is the dominant signal below 20 keV in the bottom right plot. ^{14}C dominates between 20 and 75 keV in the bottom right plot. Without ^{14}C , the event rate would be reduced out to the ^{14}C Q-value at 156 keV. Most ^{14}C decays are too high in energy to be in the WIMP search ROI, thus the ^{14}C rate in the ROI is small compared to the ^3H rate. After subtracting out background, 98% of the WIMP search ROI events are expected to be ^3H decays. The 164 keV γ from ^{131m}Xe can be seen in the top right corner of the right S1-log(S2) plot and above 150 keV in right energy plot. The WIMP search ROI is a small fraction of the plotted electron recoil band.

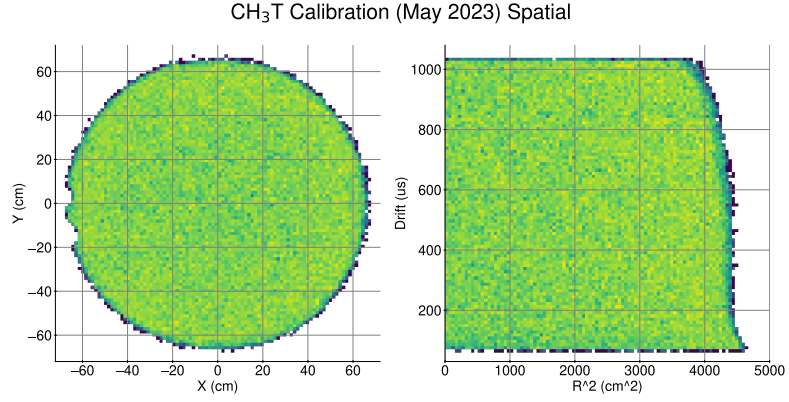


Figure 5.14: Spatial distribution of events contributing to the WIMP search rate during the May 2023 CH₃T calibration is shown. The X-Y plot is on the left and the R²-drift plot is on the right.

$\sigma_{i,j}$	$j = A_0 \text{ (Hz)}$	$j = \tau \text{ (s)}$
$i = A_0 \text{ (Hz)}$	$6.090 * 10^{-6}$	-3.269
$i = \tau \text{ (s)}$	-3.269	$3.431 * 10^6$

Table 5.3: The covariance (sub)matrix of the fit to the May 2023 CH₃T calibration is displayed. This shows the covariance elements between the amplitude of injection E (in Hz) and the removal time of the full injection (in seconds). The timestamp of the injection, the fit amplitude, and the removal time parameters are given above. This matrix is necessary to properly calculate the uncertainty on counts remaining in WS2024. The fitted removal time corresponding to this matrix is 272500 s, and the fitted amplitude is 0.430 Hz. These values reflect the event rate within the WIMP search ROI; the fraction of ¹⁴C has not been subtracted.

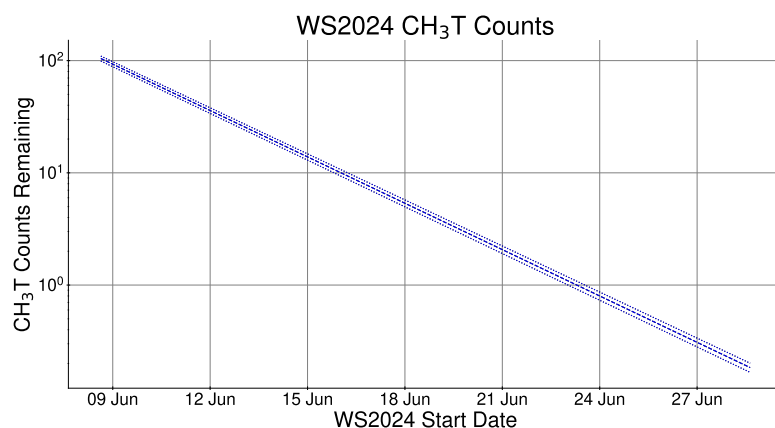


Figure 5.15: The total raw counts remaining in the WIMP search ROI by day as a result of the CH₃T calibration campaign is shown. This does not distinguish between ¹⁴C and ³H and does not account for live time losses in LZ. To properly give a number of events in WS2024 for both species, this must be convolved with the calculated live time from WS2024. By June 24, there is about one remaining event.

The getter effectively removes methane from the LZ circulation system. The CH₄ campaigns show methane can be removed to levels undetectable via cold trap mass spectrometry. Analysis before and after the April 2022 and May 2023 CH₃T calibrations proves that CH₃T is removed to levels that cannot be detected in the LZ TPC. This provides confidence that there are no lingering ³H backgrounds and CH₃T calibrations can be comfortably performed in the future.

These results provide clear evidence that gettering efficiency is affected by both the flow rate and the getter temperature. The effect of higher temperature is evident when comparing the October 2021 and August 2022 CH₄ removal times and efficiencies. Comparing the measured removal efficiency of the August 2022 CH₄ injection to the implied removal efficiency of the (lower flow rate) CH₃T calibrations shows that lower flow rates have higher removal efficiency.

The methane purifier absorbs methane left its volume for extended periods of time. The effect was unexpected but has been definitively replicated. There is still no sufficient

Campaign	$T_{\text{getter}} (^{\circ}\text{C})$	f (SLPM)	τ (h)	r	Obs/Exp τ
Oct 2021 CH ₄	314	598	85.8 ± 3.0	0.534 ± 0.016	0.955 ± 0.046
Apr 2022 CH ₃ T	403	398	79.7 ± 3.2	$0.905 \pm 0.037^*$	N/A
Aug 2022 CH ₄	401	598	63.9 ± 1.4	0.794 ± 0.008	1.056 ± 0.027
Oct 2022 CH ₃ T	403	400	76.3 ± 0.8	$0.941 \pm 0.014^*$	N/A
May 2023 CH ₃ T	403	390	75.7 ± 0.5	$0.973 \pm 0.012^*$	N/A

*indicates implied removal efficiency

Table 5.4: A summary of all fitted removal times with relevant parameters for each campaign is shown. CH₄ measurements are made using cold trap mass spectrometry. CH₃T measurements are taken with the LZ TPC. Getter vessel bed temperature (T_{getter}) and circulation system flow rate (f) are given. Removal times (τ) are given in terms of mean life, not half life, in hours. Getter removal efficiency (r) for CH₄ removal tests is determined by comparing the fitted activity of the measurements upstream of the getter with measurements taken downstream from the getter. The implied getter removal efficiency for the CH₃T campaigns is calculated with Eq. 5.4, assuming methane is uniformly mixed in the Xe. Observed/expected removal time (Obs/Exp τ) is the fraction of the measured fitted removal time and the expected removal time ($\tau/\tau_{\text{expected}}$). The expected removal time is based on the getter efficiency and the flow rate and is calculated with Eq. 5.3. A value of 1 indicates observed and expected give identical results.

explanation for the slow rise time seen during the April 2022 CH₃T calibration.

Chapter 6: Conclusions

The search for WIMP dark matter continues. LZ has set a world leading limit on WIMP interaction cross section across the expected WIMP mass range with a minimum limit of $2.1 \times 10^{-48} \text{ cm}^2$ at $36 \text{ GeV}/c^2$ [73]. This would not be possible without meticulous efforts to minimize, monitor, and quantify backgrounds that could otherwise restrict the sensitivity of LZ. The LZ WIMP search 2024 science run WIMP-nucleon spin independent cross-section limit curve is shown in Fig. 6.1.

Chapter 3 describes the cold trap mass spectrometry measurement techniques, implementation, and results. The cold trap mass spectrometry technique measured $182 \pm 26 \text{ ppq}$ (g/g) of Kr during the WIMP search 2024 science run. One of the most valuable aspects of the technique that has not been explicitly acknowledged is the volume of data it produces. Minimal operator effort was required to measure impurities by the end of the WIMP search 2024 science run. Multiple hundreds of measurements have documented the impurity concentrations in LZ Xe. Improvements made prior to and during WS2024 have allowed the systems to operate at a higher duty cycle. The measurements are useful for assigning an entry in a backgrounds table, but they also provide insight that would not otherwise be obtained. LZ was seemingly lucky that Kr concentrations matched the storage pack expectation. Had the concentrations differed by a factor of four (like LUX Kr or LZ Ar for instance), it would have been difficult to quantify Kr with conviction. Looking forward to a next generation experiment, coupling cold trap mass spectrometry with a method for drawing liquid phase Xe would be incredibly powerful.

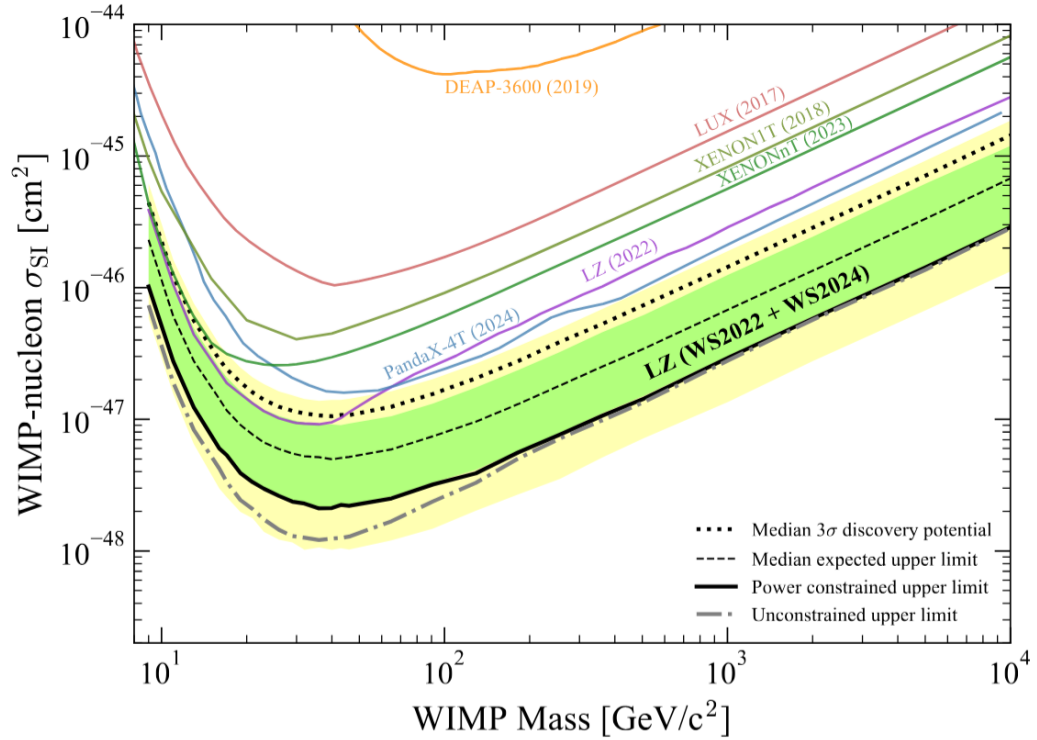


Figure 6.1: Limits on the WIMP nucleon cross-section from several experiments are shown. The solid black line is the 90% C.L. (power constrained) upper limit from the LZ WIMP search 2024 science run. The limit is world leading across all plotted WIMP mass ranges exceeding 10 GeV/c² (image from [73]).

Chapter 4 describes a complimentary technique for quantifying Kr using a ^{85}Kr decay branch that proceeds through ^{85m}Rb . This rare decay branch was used to calculate a ^{nat}Kr equivalent concentration of 124^{+44}_{-37} ppq (g/g) assuming a natural abundance of 2.0×10^{-11} ($^{85}\text{Kr}/^{nat}\text{Kr}$). There is no significant background for the search so the dominant uncertainty on the technique is from low signal statistics. This technique's precision scales with the number of Kr atoms in the active volume, not the Kr concentration. A next generation liquid Xe dark matter experiment would ideally have lower Kr concentration, but larger Xe mass. While the technique loses sensitivity when Kr concentrations are reduced, the technique recovers sensitivity from the Xe mass increases. This technique may be a viable method for measuring Kr in a next generation experiment. Improving the agreement be-

tween simulations and data may permit cut boundaries to be selected more precisely for better background rejection. The absence of prompt signal candidates high in the detector should be monitored and further explored.

As final note on Kr, the half-life of the problematic isotope, ^{85}Kr , is 10.76 years. The observed recent reduction in Kr ingress suggests the constraint on ingress from a leak is lower than the limit set by cold gas ingress measurements: $\leq 49 \pm 7$ ppq/y. If there was absolutely no air leak, all ^{85}Kr in LZ (including ^{85}Kr in TPC plastics) would deplete with a 10.76 year half-life. LZ has operated for a non-trivial fraction of the half-life. It is possible that the natural ^{85}Kr abundance of 2.0×10^{-11} ($^{85}\text{Kr}/^{nat}\text{Kr}$) is not the abundance in LZ because ^{85}Kr is decaying and not being replenished. It is difficult to quantify the abundance without knowing the leak rate. The excited state measurement technique quantifies the problematic ^{85}Kr isotope and converts to a ^{nat}Kr equivalent using the assumed ^{85}Kr abundance, while the cold trap mass spectrometry technique quantifies ^{nat}Kr directly. If the measured ^{nat}Kr from cold trap mass spectrometry and the ^{nat}Kr equivalent from the excited state measurement are observed to diverge as LZ ages, this would imply natural ^{85}Kr abundance is not the ^{85}Kr abundance in LZ. This should be considered in the experiment's background model. If the natural and LZ abundances differ, there is clear value in carefully handling and reusing ^{85}Kr -depleted LZ Xe for a next generation LXe dark matter experiment.

Using CH_3T as a calibration source in LZ is very powerful. The value of calibrating with CH_3T hinges on the ability to remove it from the Xe. Methane removal was quantified in chapter 5. The measured methane removal time of the CH_3T calibration prior to the WIMP search 2024 science run was $\tau = 75.7 \pm 0.5\text{h}$. CH_4 was reduced to concentrations below the sensitivity of the cold trap mass spectrometry systems. CH_3T was reduced to concentrations that could not be detected by the LZ TPC. These results indicate that CH_3T is a safe calibration source for LZ and there is no reason CH_3T cannot be used in a next

generation LXe dark matter experiment.

Appendix A: Appendix

A.1 Appendix A

Fig. A.1 to Fig. A.24 are fits to energy, corrected S1, and corrected S2 for various γ decays from section 4.4. These are used to compare data and simulations for the ^{85}Kr excited state decay measurement.

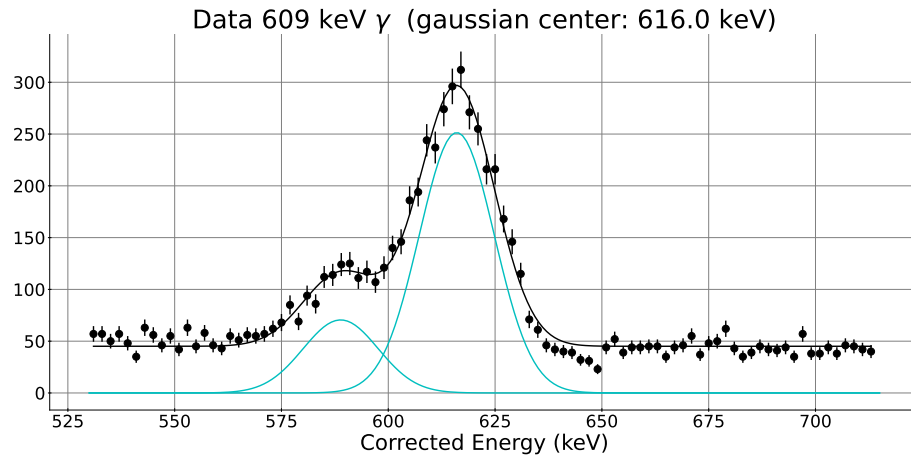


Figure A.1: A fit to the corrected energy spectrum of WIMP search data in the energy range near the 609 keV ^{214}Bi γ . A second Gaussian is added to the fit to account for the small peak near 585 keV. The primary Gaussian centroid is 616.0 keV and the width is 8.8 keV. The cyan lines show the individual contribution of the two Gaussians, and the black line shows the sum of the two components and a constant.

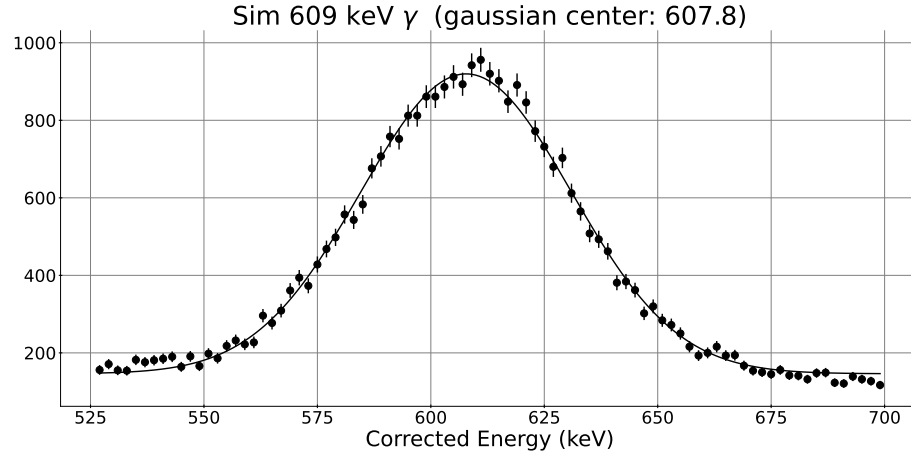


Figure A.2: A fit to the corrected energy spectrum of Rn decay chain simulations in the energy range near the 609 keV ^{214}Bi γ . A constant is included in the fit. The fitted Gaussian centroid is 607.8 keV and the width is 23.2 keV. The black line shows the sum of the Gaussian and the constant.

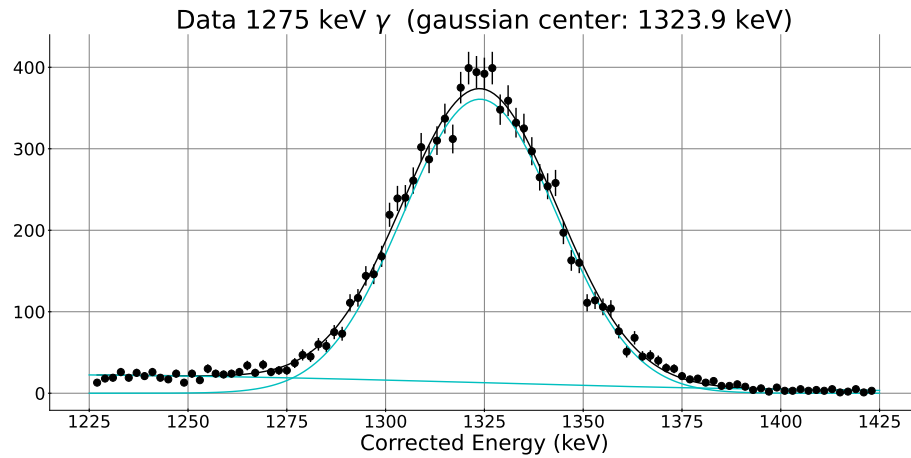


Figure A.3: A fit to the corrected energy spectrum of ^{22}Na calibration data in the energy range near the 1275 keV γ . The Gaussian centroid is 1323.9 keV and the width is 19.5 keV. The cyan lines show the individual Gaussian and sigmoid contributions to the fit, and the black line shows the sum of the two components.

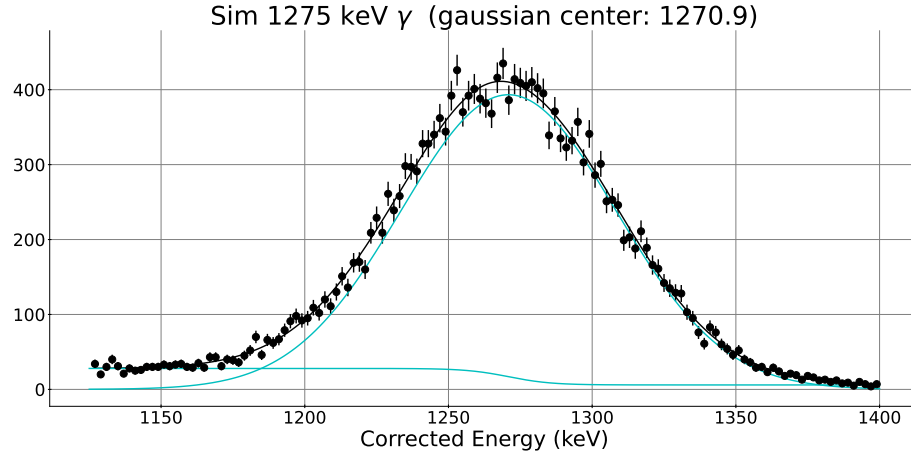


Figure A.4: A fit to the corrected energy spectrum of ^{22}Na simulations in the energy range near the 1275 keV γ . The Gaussian centroid is 1270.9 keV and the width is 37.4 keV. The cyan lines show the individual Gaussian and sigmoid contributions to the fit, and the black line shows the sum of the two components.

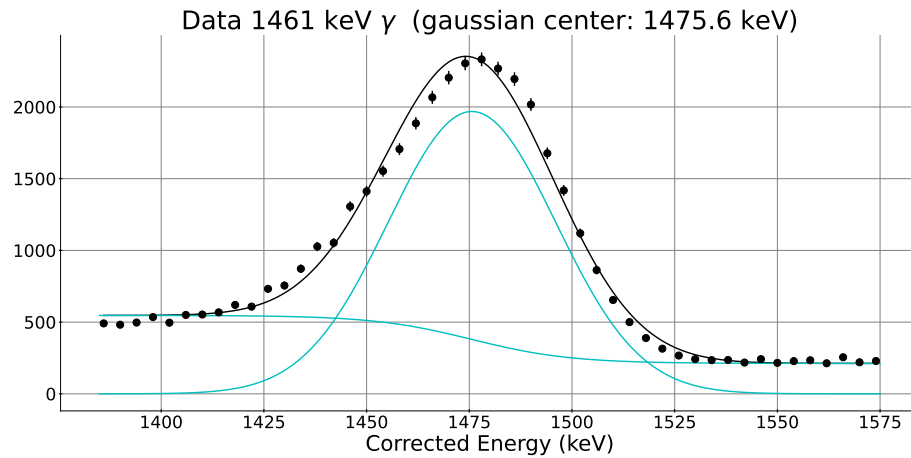


Figure A.5: A fit to the corrected energy spectrum of WIMP search data in the energy range near the 1461 keV ^{40}K γ . The Gaussian centroid is 1475.6 keV and the width is 8.8 keV. The cyan lines show the individual Gaussian and sigmoid contributions, and the black line shows the sum of the two components.

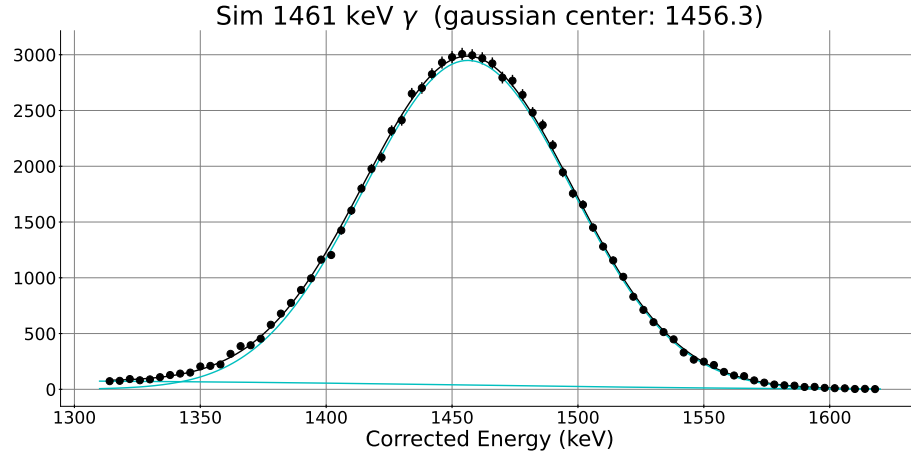


Figure A.6: A fit to the corrected energy spectrum of ^{40}K simulations in the energy range near the 1461 keV γ . The Gaussian centroid is 1456.3 keV and the width is 41.5 keV. The cyan lines show the individual Gaussian and sigmoid contributions, and the black line shows the sum of the two components.

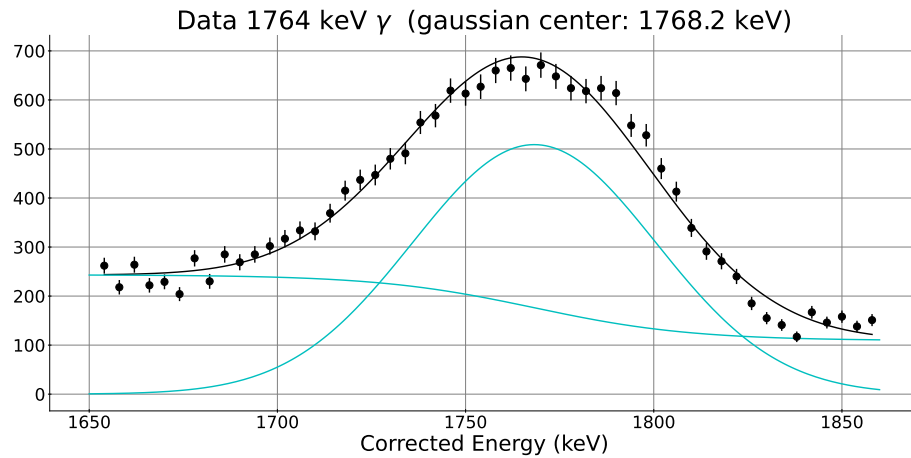


Figure A.7: A fit to the corrected energy spectrum of WIMP search data in the energy range near the 1764 keV ^{214}Bi γ . The Gaussian centroid is 1768.2 keV and the width is 32.4 keV. The cyan lines show the individual Gaussian and sigmoid contributions, and the black line shows the sum of the two components.

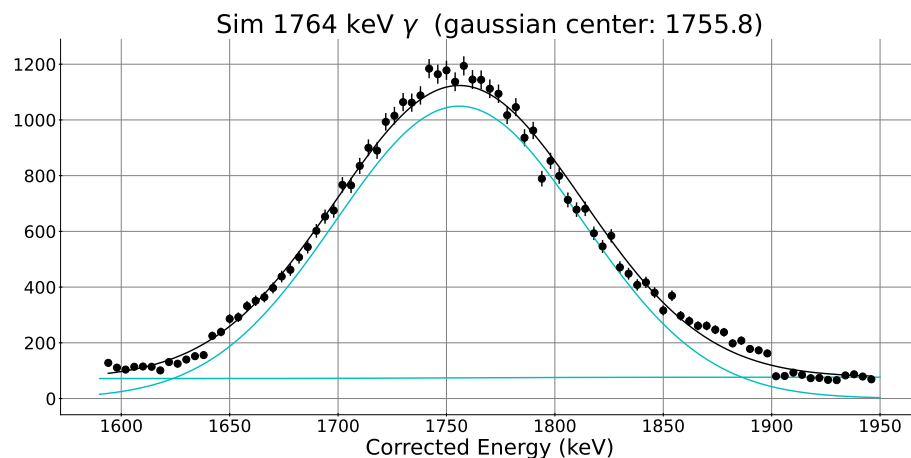


Figure A.8: A fit to the corrected energy spectrum of Rn decay chain simulations in the energy range near the 1764 keV ^{214}Bi γ . The Gaussian centroid is 1755.8 keV and the width is 57.0 keV. The cyan lines show the individual Gaussian and sigmoid contributions, and the black line shows the sum of the two components.

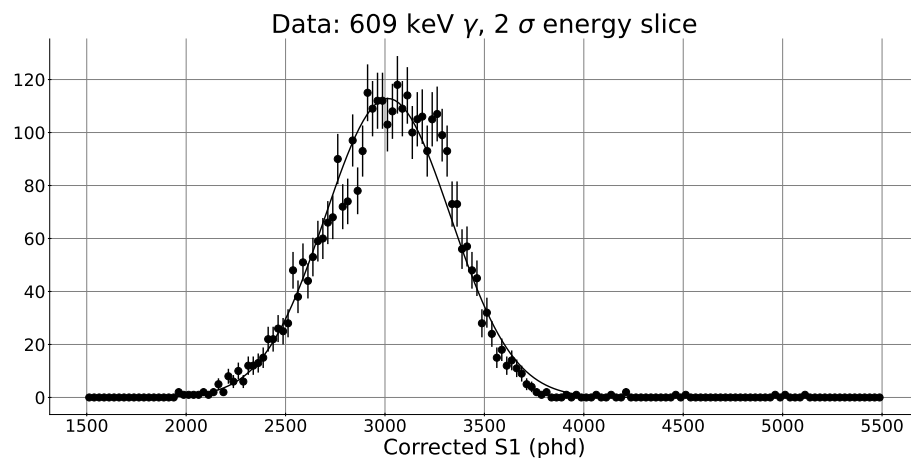


Figure A.9: A fit to the corrected S1 area of the 2σ energy slice of data associated with the 609 keV γ . The fitted centroid and width are 3015 and 315 phd.

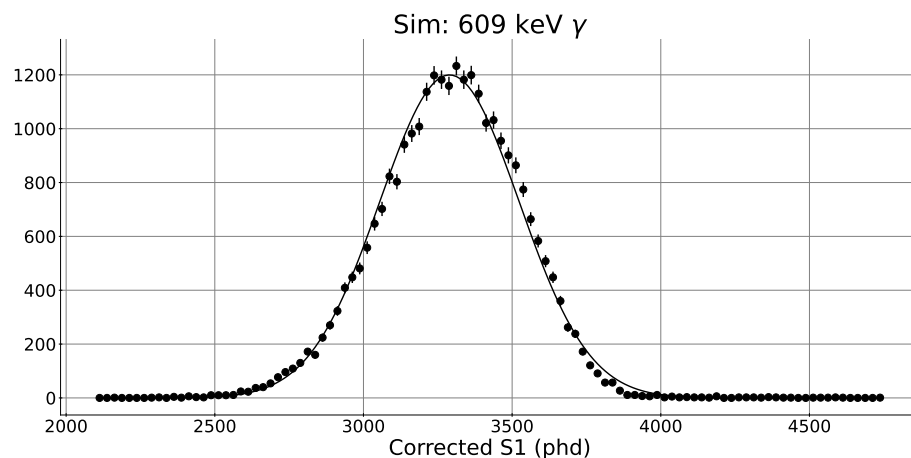


Figure A.10: A fit to the corrected S1 area of the 2σ energy slice of simulations associated with the 609 keV γ . The fitted centroid and width are 3289 and 235 phd.

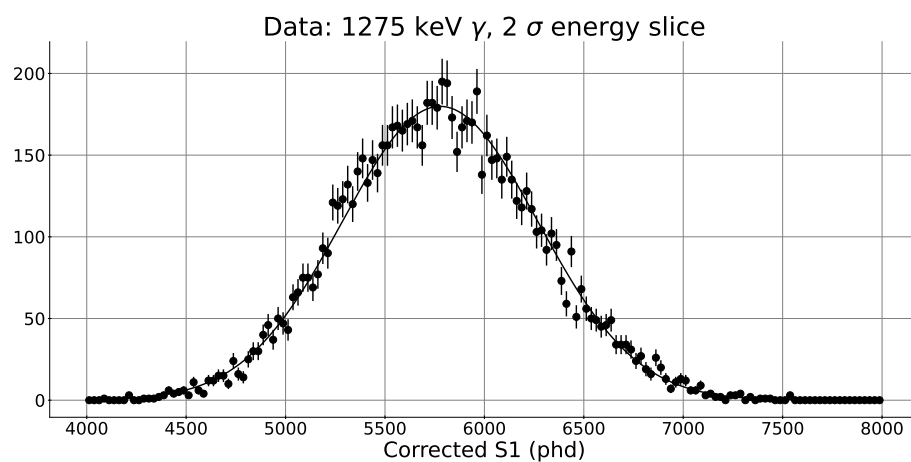


Figure A.11: A fit to the corrected S1 area of 2σ energy slice of data associated with the 1275 keV γ . The fitted centroid and width are 5777 and 493 phd.

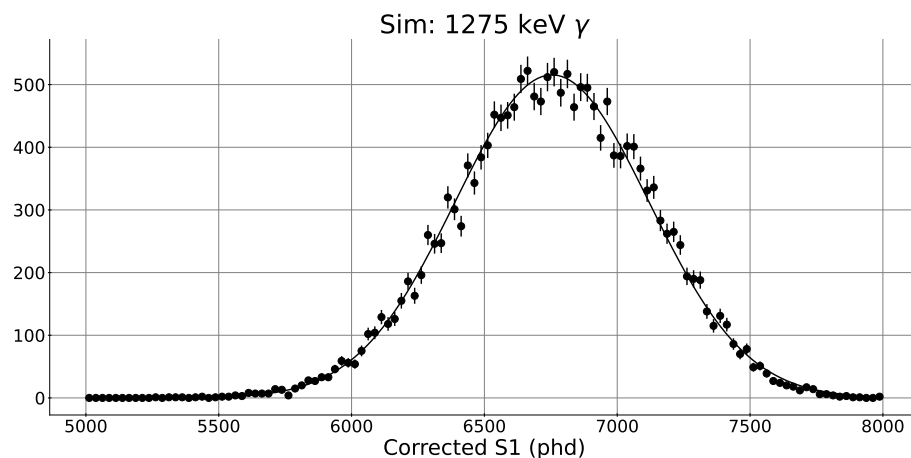


Figure A.12: A fit to the corrected S1 area of the 2σ energy slice of simulations associated with the 1275 keV γ . The fitted centroid and width are 6755 and 365 phd.

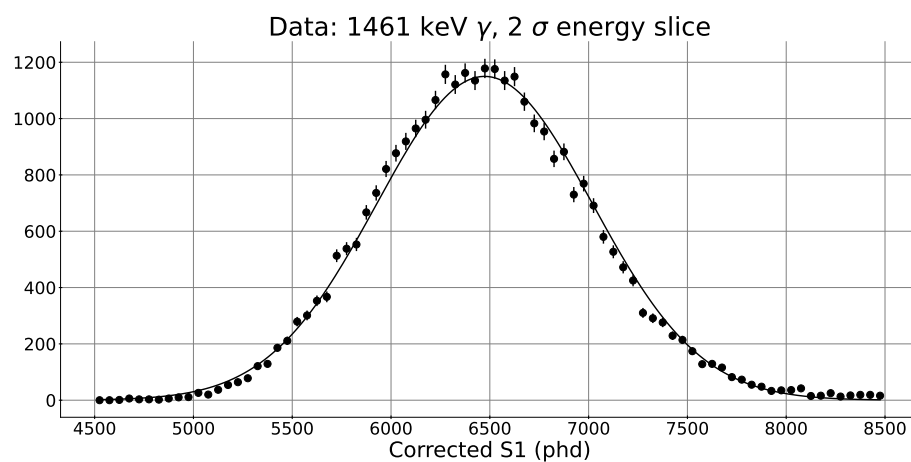


Figure A.13: A fit to the corrected S1 area of 2σ energy slice of data associated with the 1461 keV γ . The fitted centroid and width are 6473 and 546 phd.

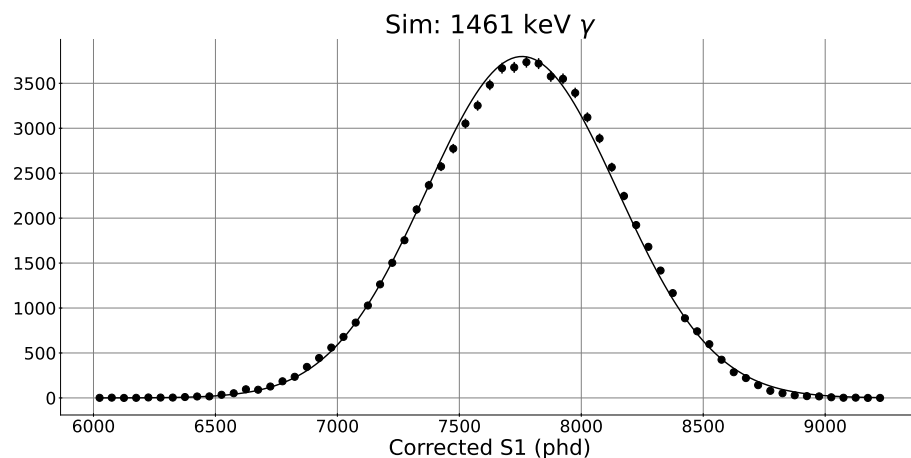


Figure A.14: A fit to the corrected S1 area of the 2σ energy slice of simulations associated with the 1461 keV γ . The fitted centroid and width are 7757 and 392 phd.

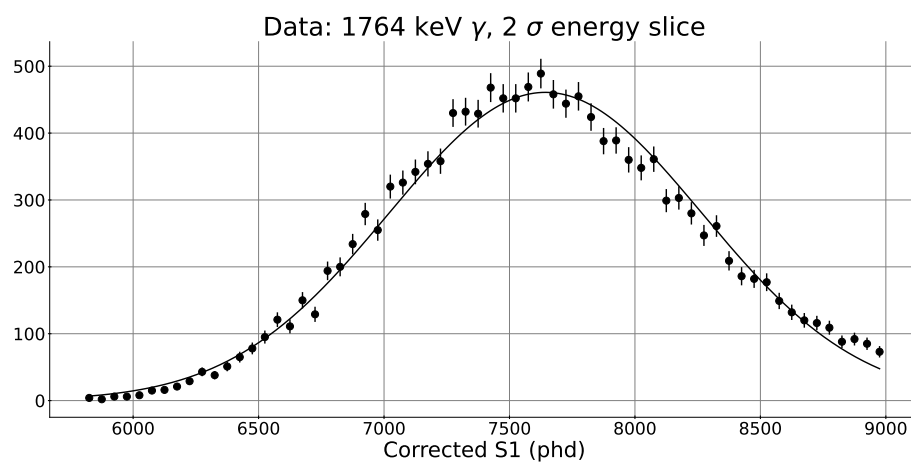


Figure A.15: A fit to the corrected S1 area of 2σ energy slice of data associated with the 1764 keV γ . The fitted centroid and width are 7766 and 828 phd.

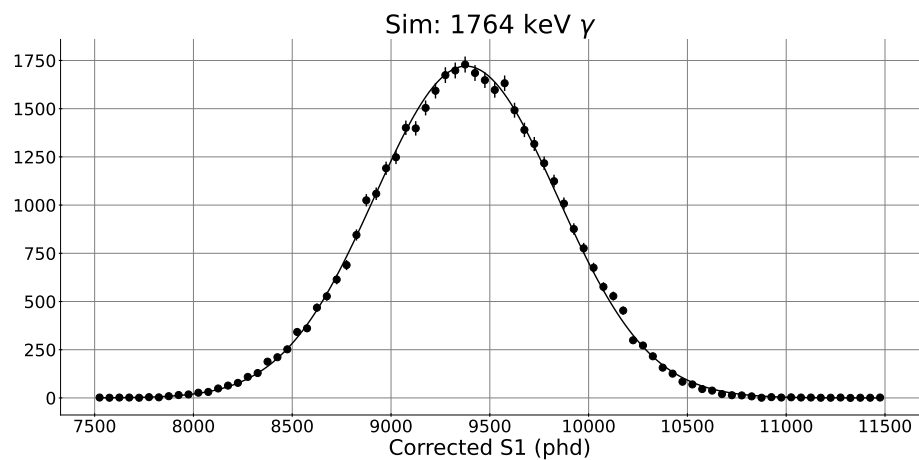


Figure A.16: A fit to the corrected S1 area of the 2σ energy slice of simulations associated with the 1764 keV γ . The fitted centroid and width are 9380 and 464 phd.

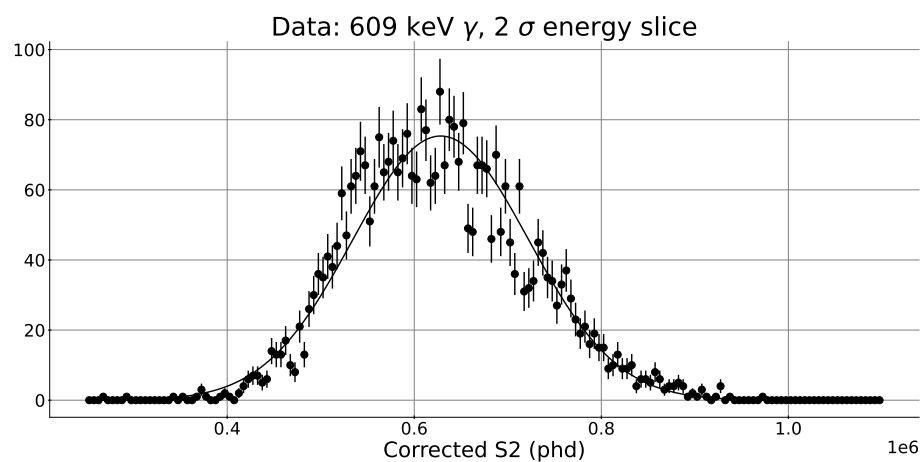


Figure A.17: A fit to the corrected S2 area of the 2σ energy slice of data associated with the 609 keV γ . The fitted centroid and width are 628000 and 94000 phd.

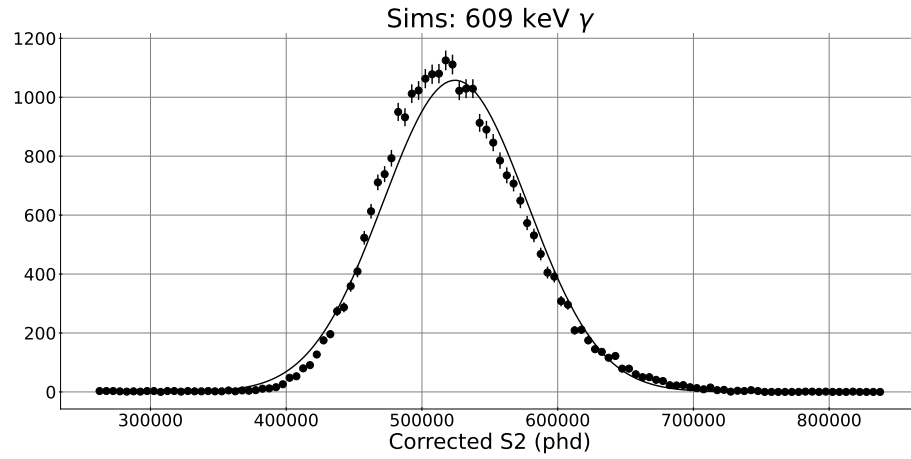


Figure A.18: A fit to the corrected S2 area of the 2σ energy slice of simulations associated with the 609 keV γ . The fitted centroid and width are 524000 and 53000 phd.

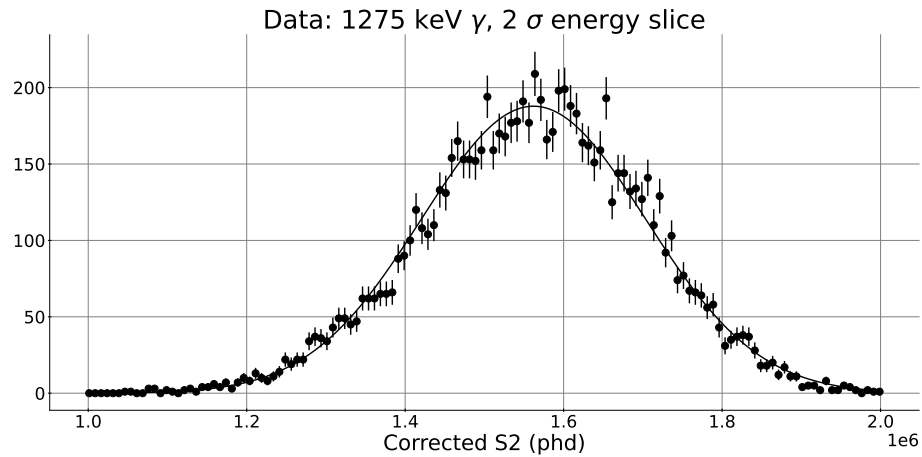


Figure A.19: A fit to the corrected S2 area of the 2σ energy slice of data associated with the 1275 keV γ . The fitted centroid and width are 1560000 and 140000 phd.

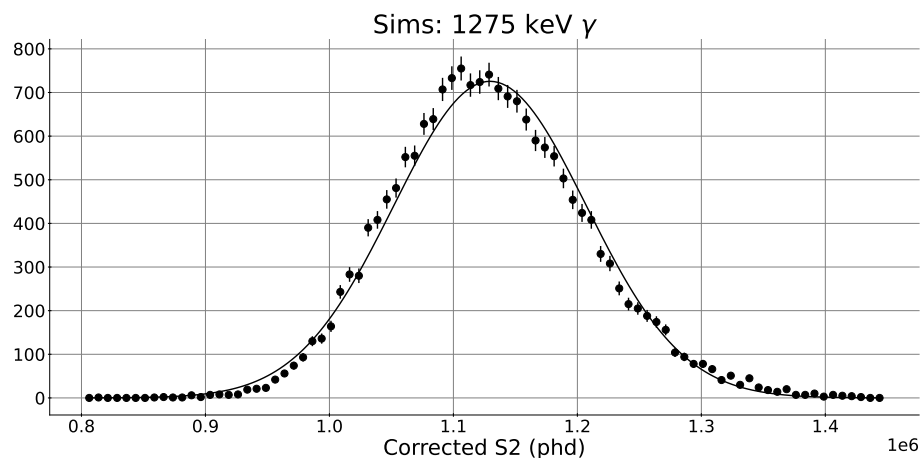


Figure A.20: A fit to the corrected S2 area of the 2σ energy slice of simulations associated with the 1275 keV γ . The fitted centroid and width are 1130000 and 78000 phd.

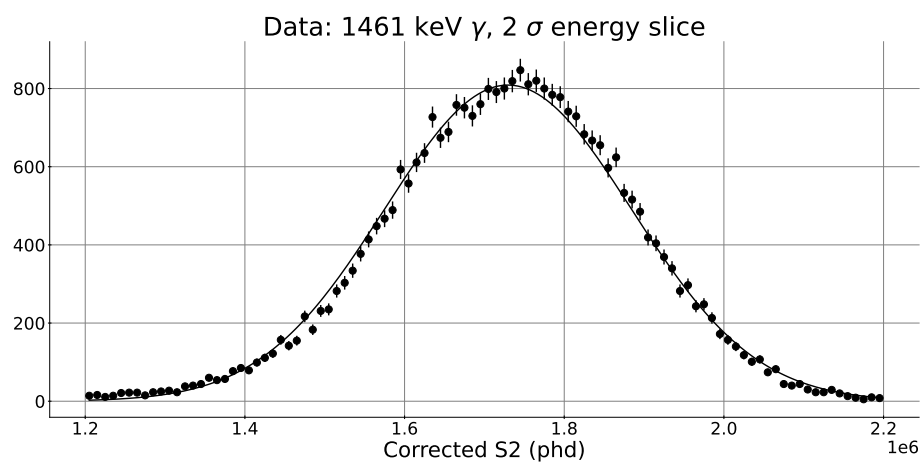


Figure A.21: A fit to the corrected S2 area of the 2σ energy slice of data associated with the 1461 keV γ . The fitted centroid and width are 1720000 and 150000 phd.

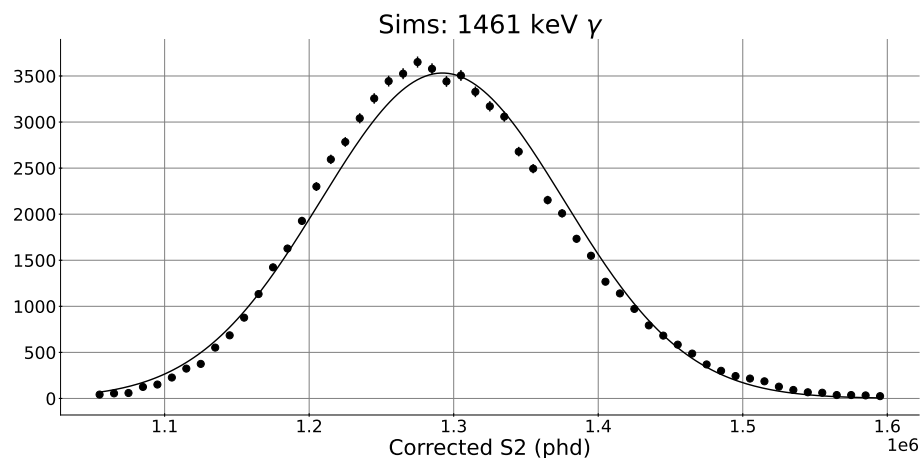


Figure A.22: A fit to the corrected S2 area of the 2σ energy slice of simulations associated with the 1461 keV γ . The fitted centroid and width are 1290000 and 84000 phd.

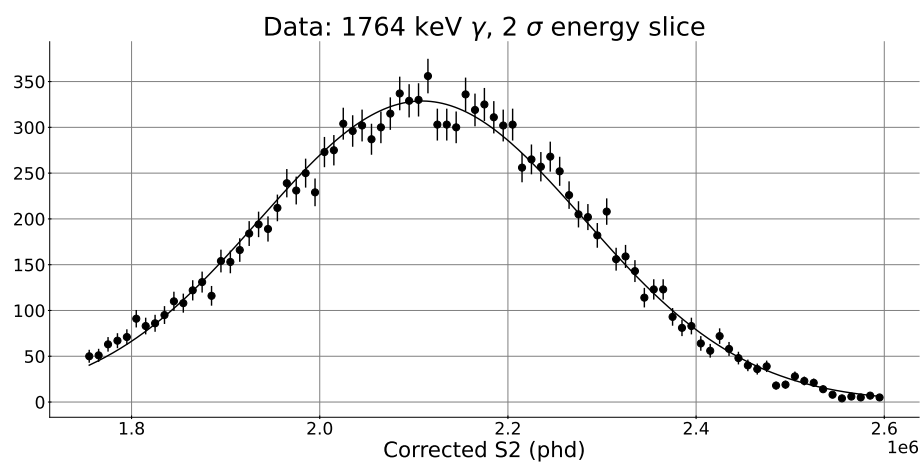


Figure A.23: A fit to the corrected S2 area of the 2σ energy slice of data associated with the 1764 keV γ . The fitted centroid and width are 2110000 and 170000 phd.

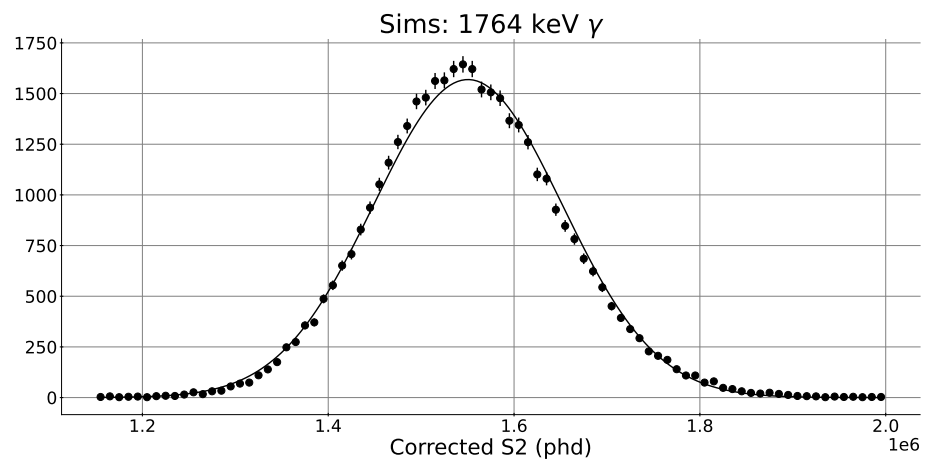


Figure A.24: A fit to the corrected S2 area of the 2σ energy slice of simulations associated with the 609 keV γ . The fitted centroid and width are 1550000 and 100000 phd.

Fig. A.25 to Fig. A.33 are wave forms and PMT hit maps for prompt events ($S1 \delta$ time $< 5 \mu s$) passing all ^{85}Kr excited state decay cuts. These candidate events are originally discussed in section 4.7.2.

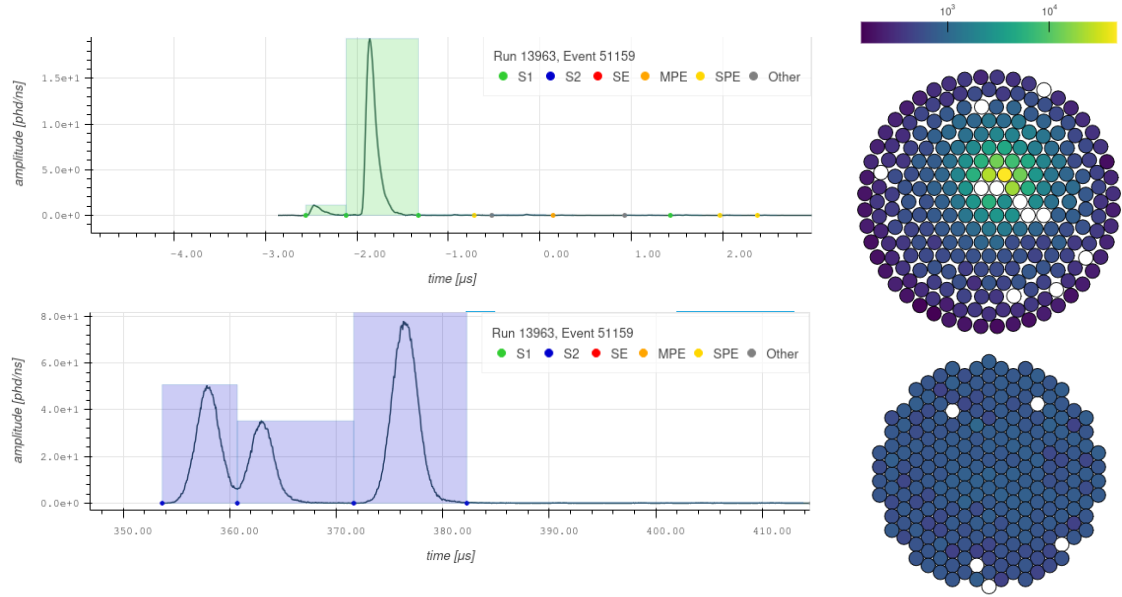


Figure A.25: Waveforms and PMT hit maps are shown for the prompt candidate: run 13963, event 51159. The top left plot shows the two S1 waveforms highlighted in green. The bottom left plot shows the S2 waveforms highlighted in blue. The event's PMT hit map is shown on the right for the top array (top) and the bottom array (bottom). The delay time of this event is less than one μs , and the drift time is about 370 μs .

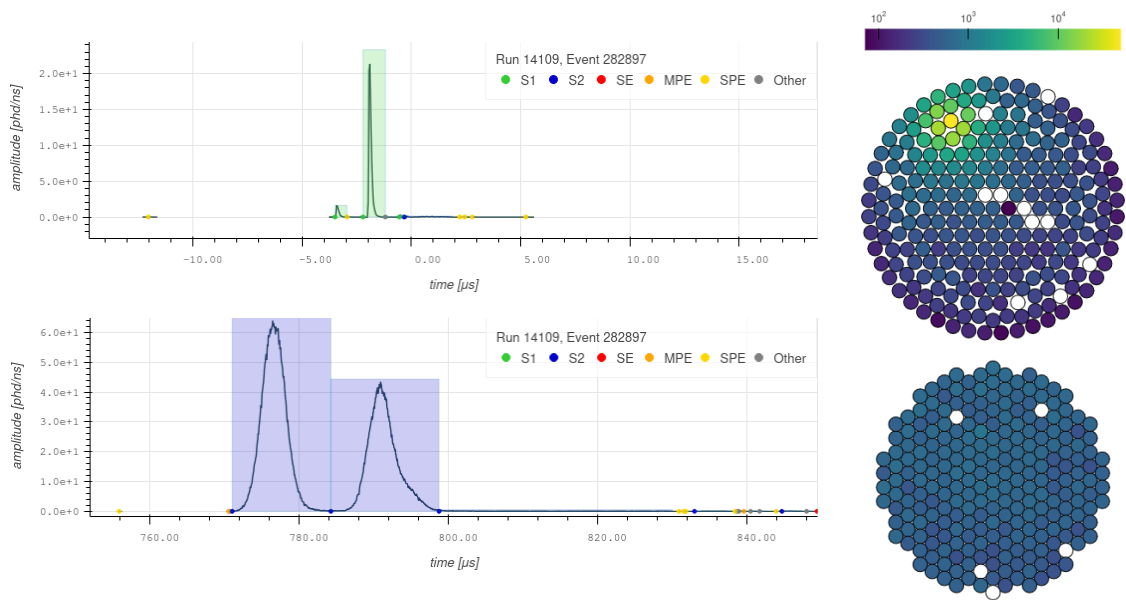


Figure A.26: Waveforms and PMT hit maps are shown for the prompt candidate: run 14109, event 282897. The top left plot shows the two S1 waveforms highlighted in green. The bottom left plot shows the S2 waveforms highlighted in blue. The event's PMT hit map is shown on the right for the top array (top) and the bottom array (bottom). The blue "Y" shaped markers in the top array diagram mark the S2 centroid positions. The delay time of this event is about $1.5 \mu\text{s}$, and the drift time is about $770 \mu\text{s}$.

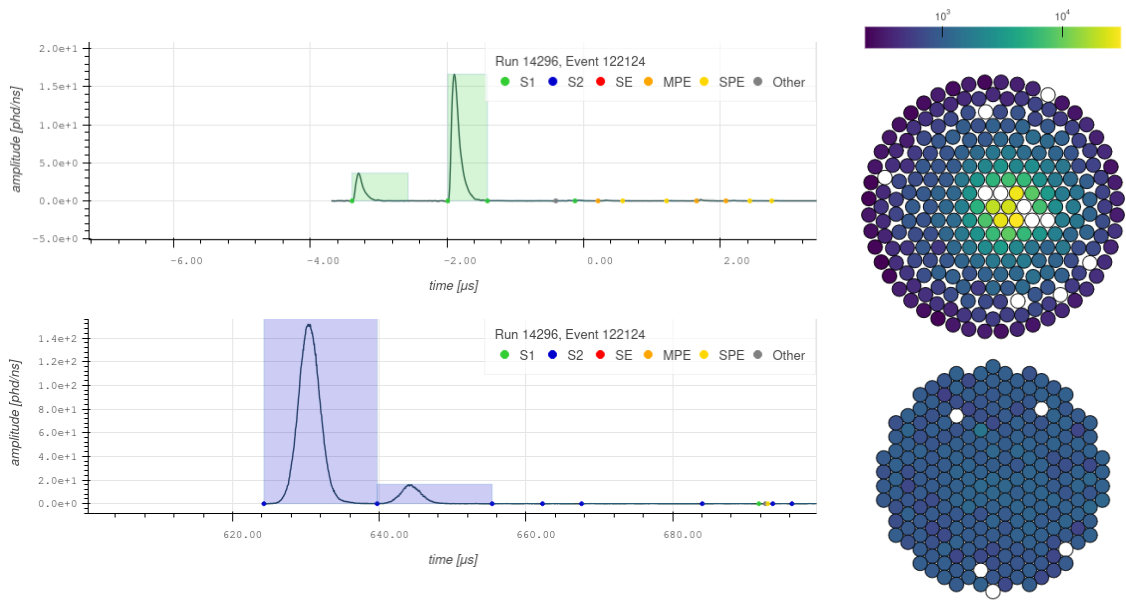


Figure A.27: Waveforms and PMT hit maps are shown for the prompt candidate: run 14296, event 122124. The top left plot shows the two S1 waveforms highlighted in green. The bottom left plot shows the S2 waveforms highlighted in blue. The event's PMT hit map is shown on the right for the top array (top) and the bottom array (bottom). The delay time of this event is about $1.5 \mu\text{s}$ and the drift time is about $620 \mu\text{s}$.

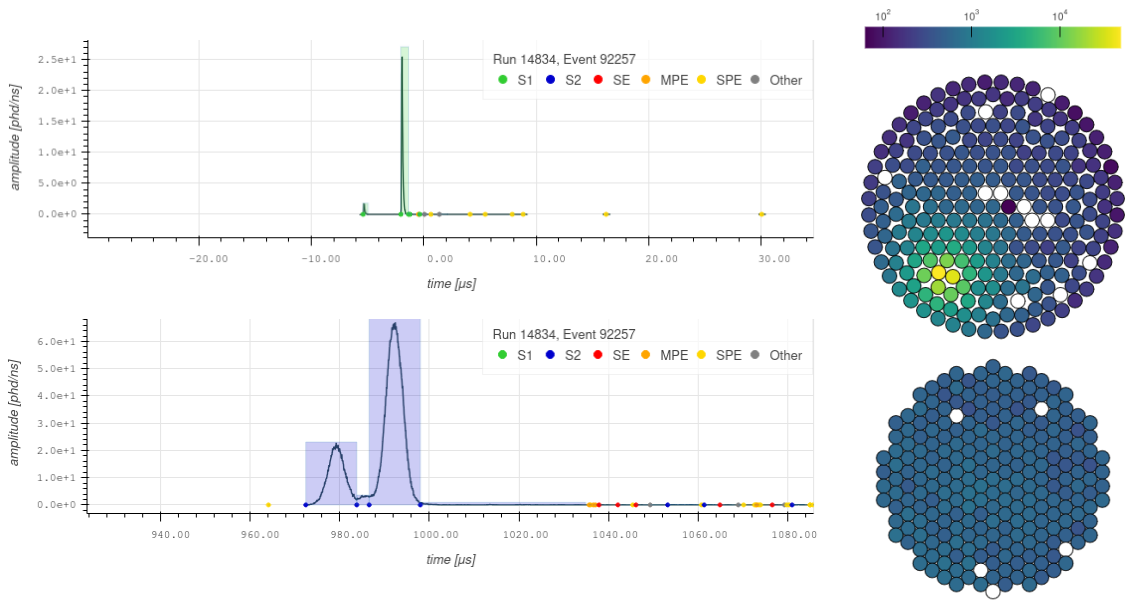


Figure A.28: Waveforms and PMT hit maps are shown for the prompt candidate: run 14834, event 92257. The top left plot shows the two S1 waveforms highlighted in green. The bottom left plot shows the S2 waveforms highlighted in blue. The event's PMT hit map is shown on the right for the top array (top) and the bottom array (bottom). The delay time of this event is about $4 \mu\text{s}$, and the drift time is about $970 \mu\text{s}$.

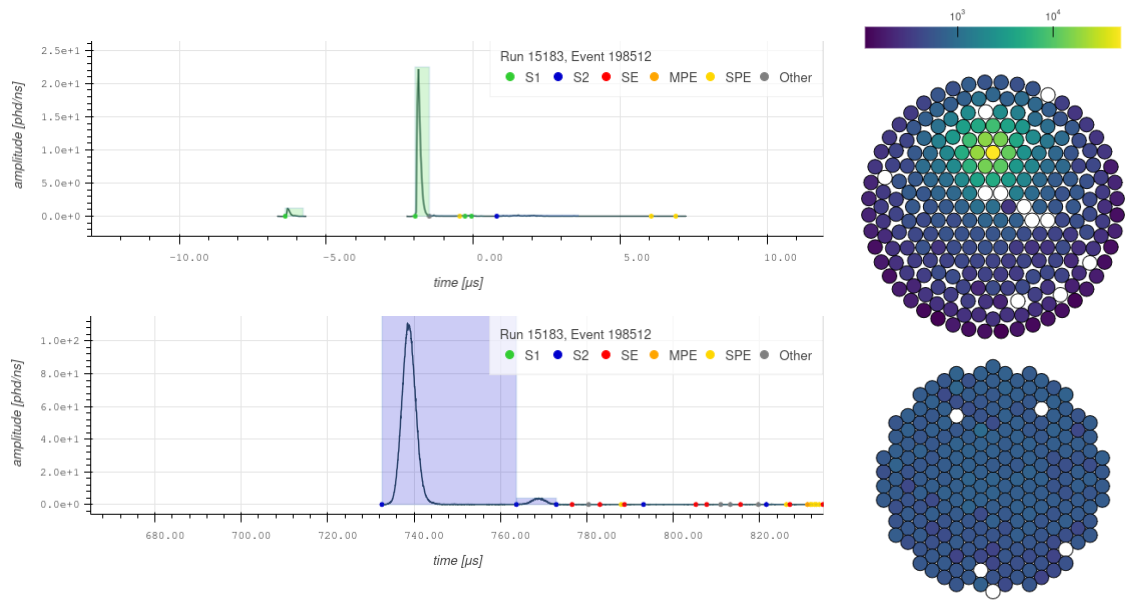


Figure A.29: Waveforms and PMT hit maps are shown for the prompt candidate: run 15183, event 198512. The top left plot shows the two S1 waveforms highlighted in green. The bottom left plot shows the S2 waveforms highlighted in blue. The event's PMT hit map is shown on the right for the top array (top) and the bottom array (bottom). The delay time of this event is about $5 \mu\text{s}$, and the drift time is about $730 \mu\text{s}$.

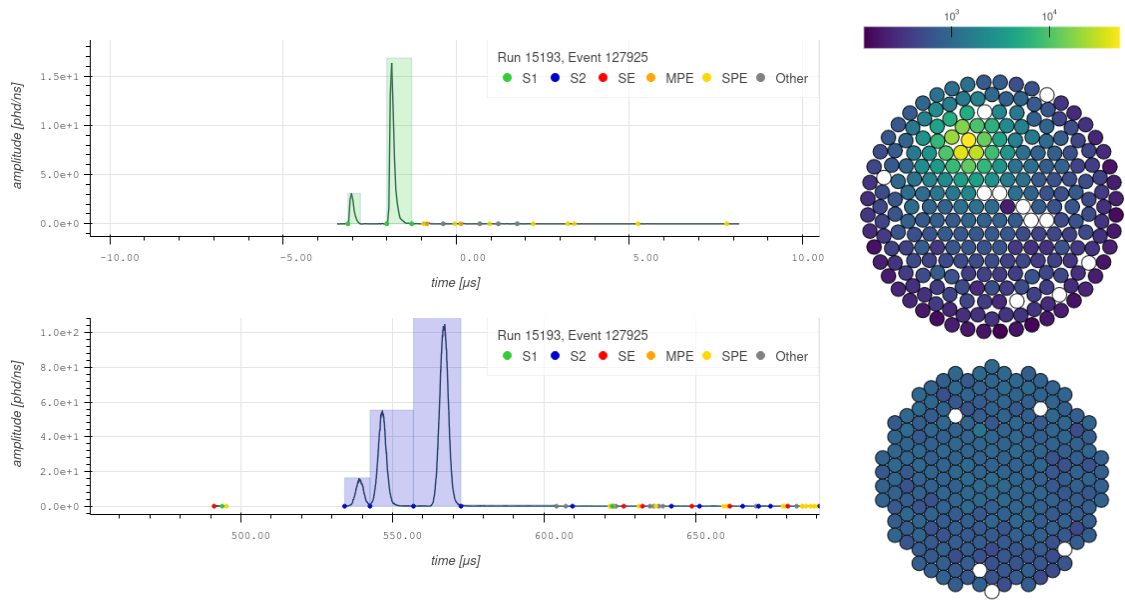


Figure A.30: Waveforms and PMT hit maps are shown for the prompt candidate: run 15193, event 127925. The top left plot shows the two S1 waveforms highlighted in green. The bottom left plot shows the S2 waveforms highlighted in blue. The event's PMT hit map is shown on the right for the top array (top) and the bottom array (bottom). The delay time of this event is about $1 \mu\text{s}$, and the drift time is about $560 \mu\text{s}$.

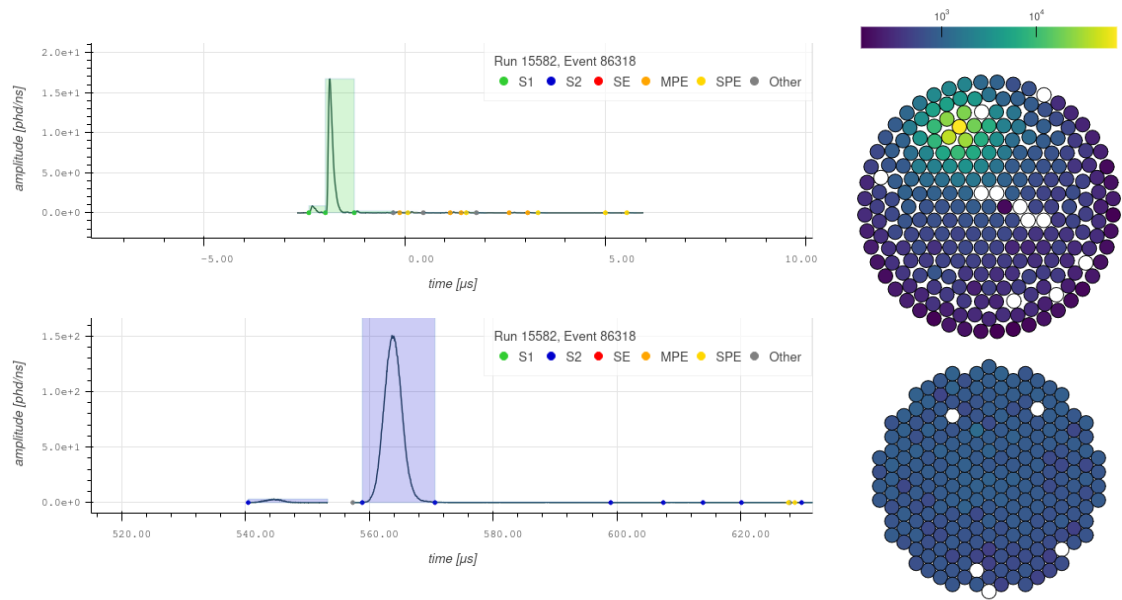


Figure A.31: Waveforms and PMT hit maps are shown for the prompt candidate: run 15582, event 86318. The top left plot shows the two S1 waveforms highlighted in green. The bottom left plot shows the S2 waveforms highlighted in blue. The event's PMT hit map is shown on the right for the top array (top) and the bottom array (bottom). The delay time of this event is about $0.5 \mu\text{s}$, and the drift time is about $560 \mu\text{s}$.

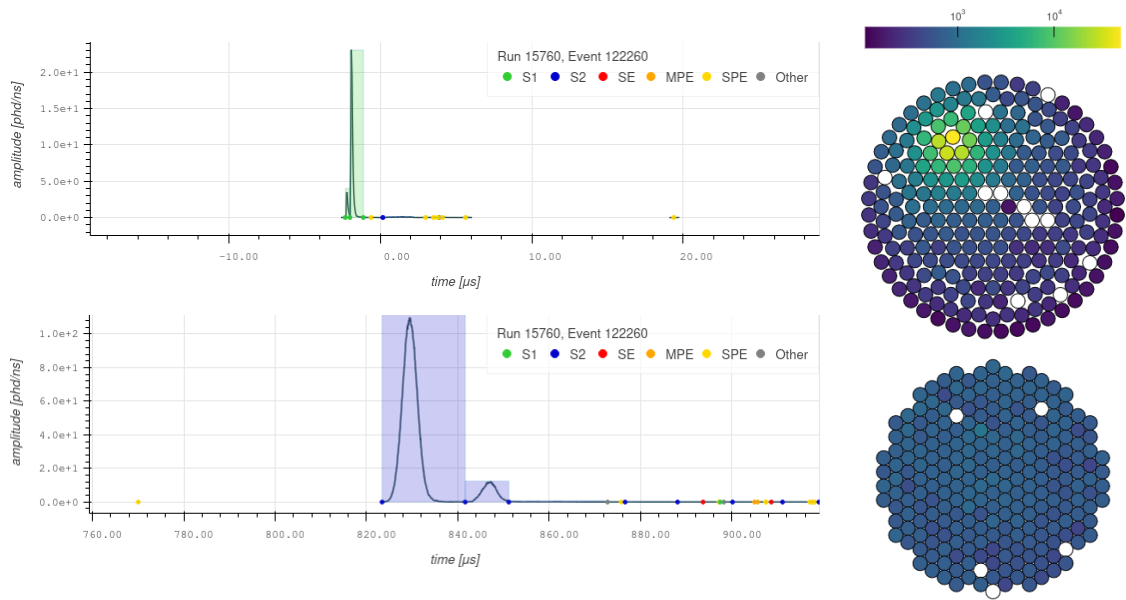


Figure A.32: Waveforms and PMT hit maps are shown for the prompt candidate: run 15760, event 122260. The top left plot shows the two S1 waveforms highlighted in green. The bottom left plot shows the S2 waveforms highlighted in blue. The event's PMT hit map is shown on the right for the top array (top) and the bottom array (bottom). The delay time of this event is about $0.3 \mu\text{s}$, and the drift time is about $820 \mu\text{s}$.

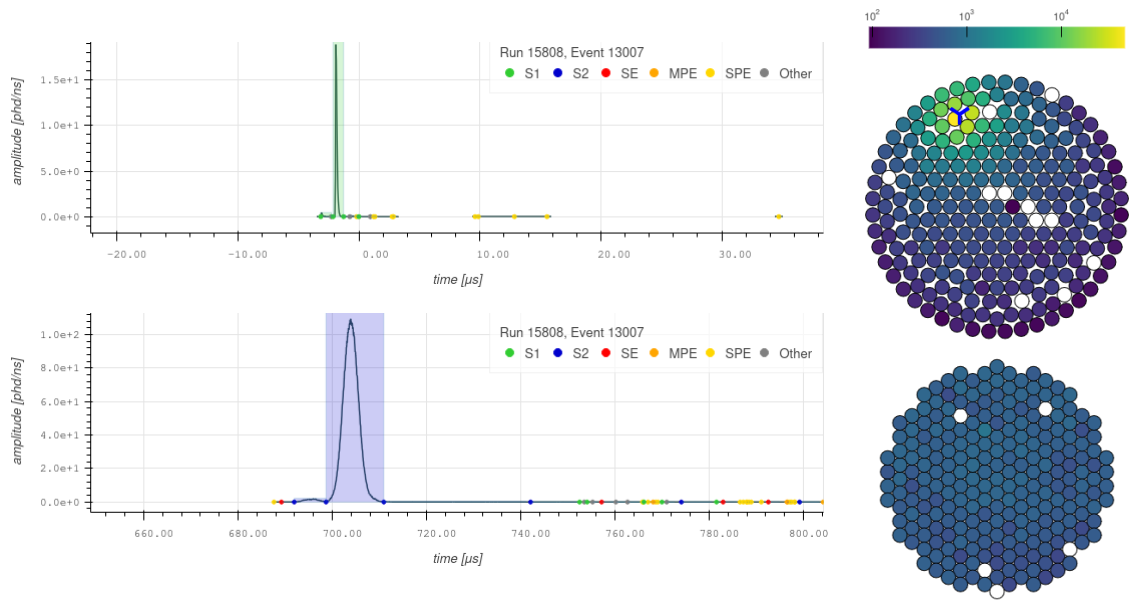


Figure A.33: Waveforms and PMT hit maps are shown for the prompt candidate: run 14109, event 282897. The top left plot shows the two S1 waveforms highlighted in green. The bottom left plot shows the S2 waveforms highlighted in blue. The event's PMT hit map is shown on the right for the top array (top) and the bottom array (bottom). The delay time of this event is about $1.5 \mu\text{s}$, and the drift time is about $700 \mu\text{s}$.

Fig. A.34 to Fig. A.45 are wave forms and PMT hit maps for delayed events ($S1 \delta$ time $> 5 \mu s$) passing all ^{85}Kr excited state decay cuts. These events are originally discussed in section 4.7.2.

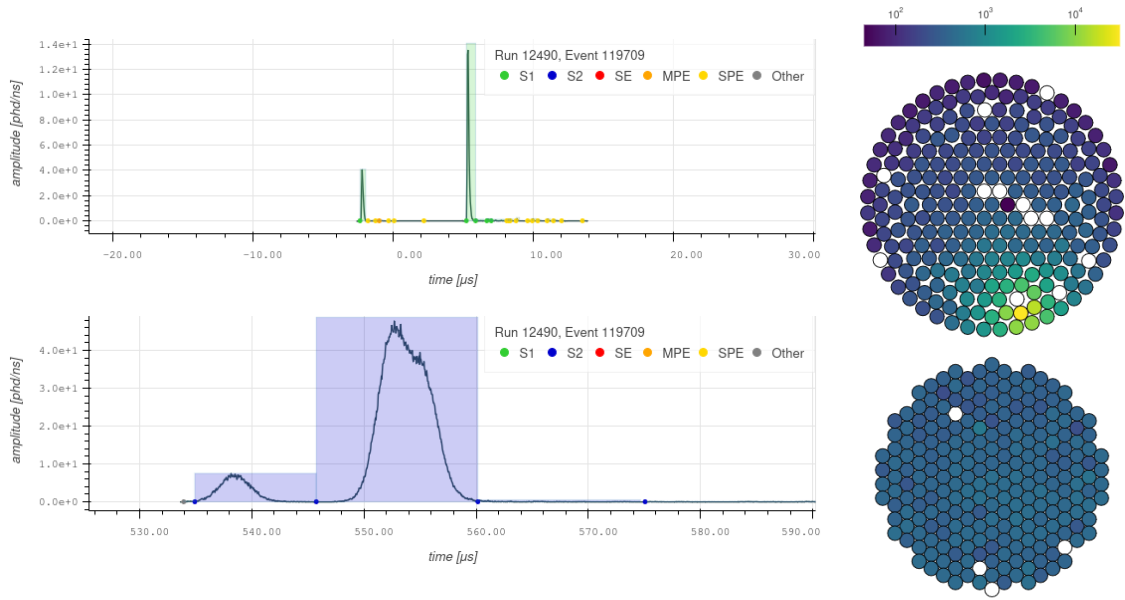


Figure A.34: Waveforms and PMT hit maps are shown for the delayed event: run 12490, event 119709. The top left plot shows the two S1 waveforms highlighted in green. The bottom left plot shows the S2 waveforms highlighted in blue. The event's PMT hit map is shown on the right for the top array (top) and the bottom array (bottom). The delay time of this event is about $8 \mu s$, and the drift time is about $550 \mu s$.

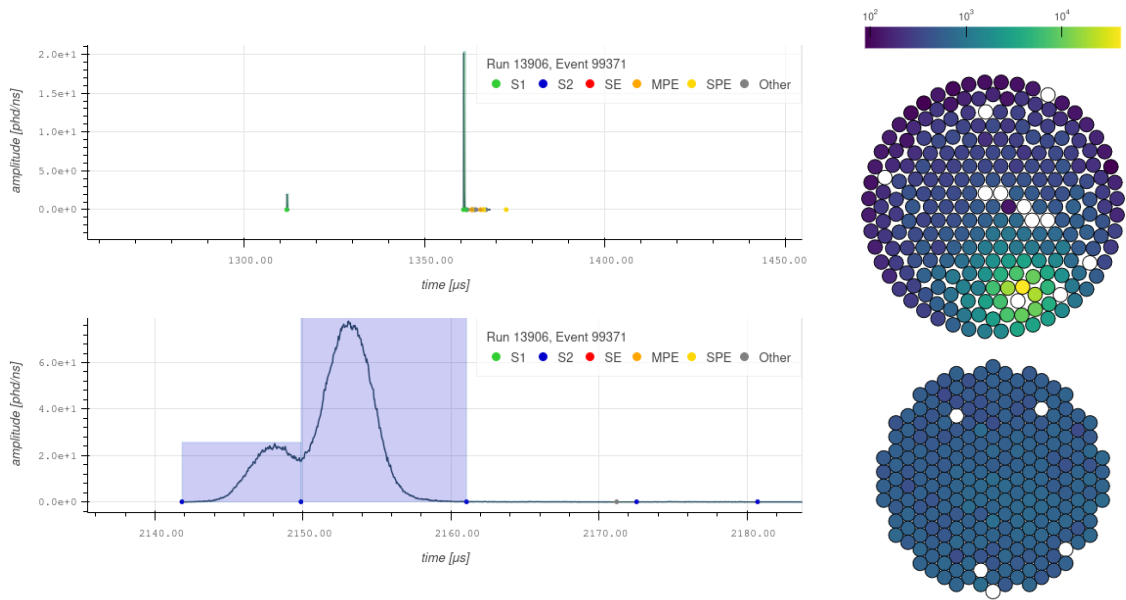


Figure A.35: Waveforms and PMT hit maps are shown for the delayed event: run 13906, event 99371. The top left plot shows the two S1 waveforms highlighted in green. The bottom left plot shows the S2 waveforms highlighted in blue. The event's PMT hit map is shown on the right for the top array (top) and the bottom array (bottom). The delay time of this event is about $50 \mu\text{s}$, and the drift time is about $800 \mu\text{s}$.

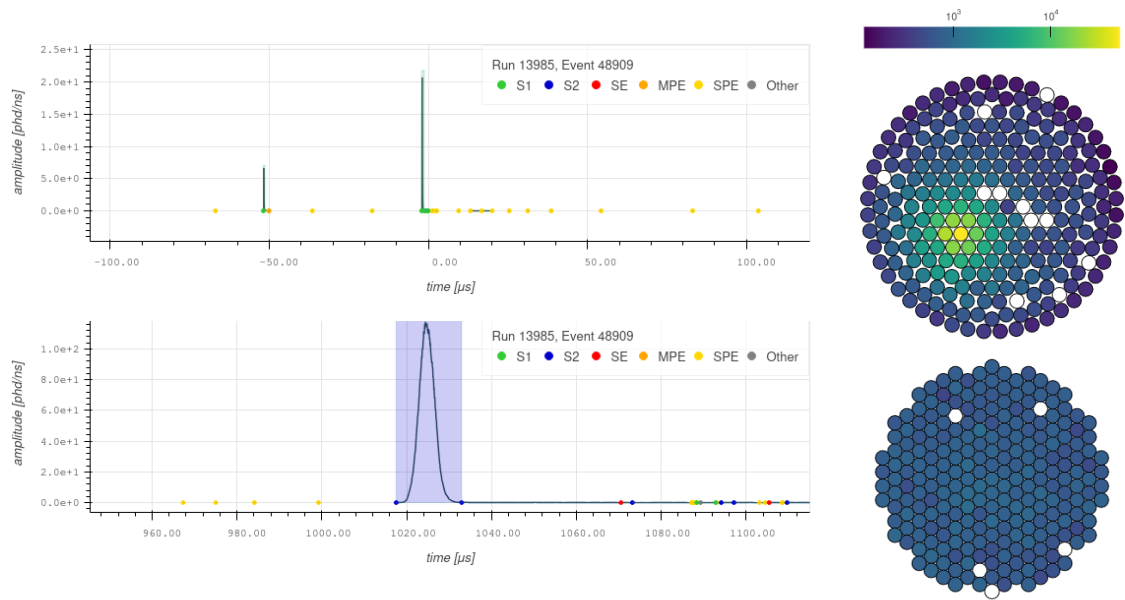


Figure A.36: Waveforms and PMT hit maps are shown for the delayed event: run 13985, event 48909. The top left plot shows the two S1 waveforms highlighted in green. The bottom left plot shows the S2 waveform highlighted in blue. The event's PMT hit map is shown on the right for the top array (top) and the bottom array (bottom). The delay time of this event is about $500 \mu\text{s}$, and the drift time is about $1020 \mu\text{s}$.

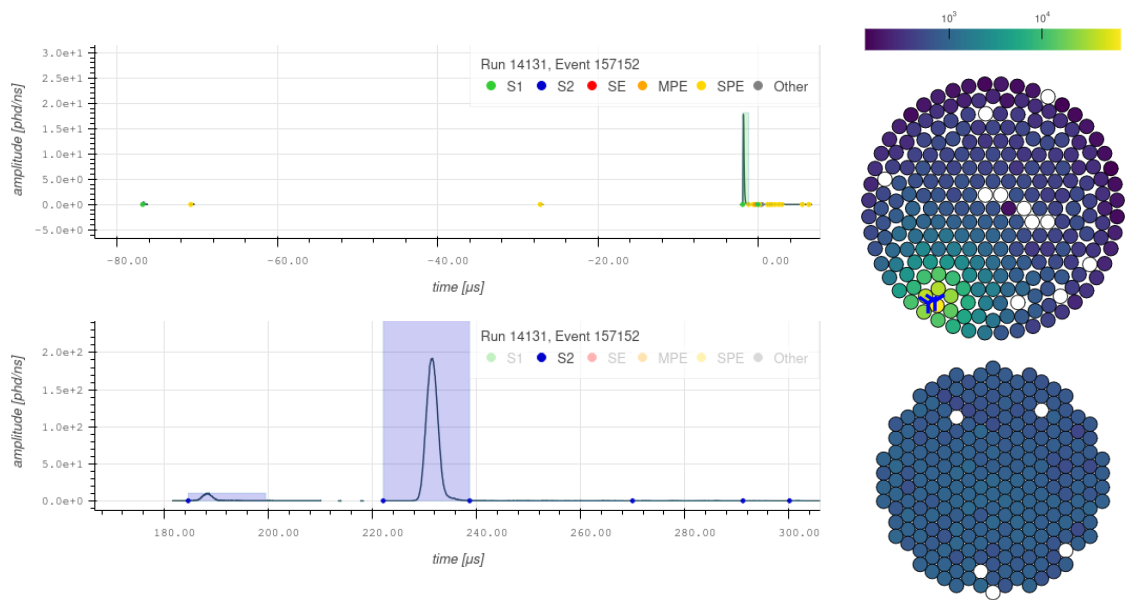


Figure A.37: Waveforms and PMT hit maps are shown for the delayed event: run 14131, event 157152. The top left plot shows the two S1 waveforms highlighted in green. The bottom left plot shows the S2 waveforms highlighted in blue. The event's PMT hit map is shown on the right for the top array (top) and the bottom array (bottom). The blue "Y" shaped markers in the top array diagram mark the S2 centroid positions. The delay time of this event is about $75 \mu\text{s}$, and the drift time is about $220 \mu\text{s}$.

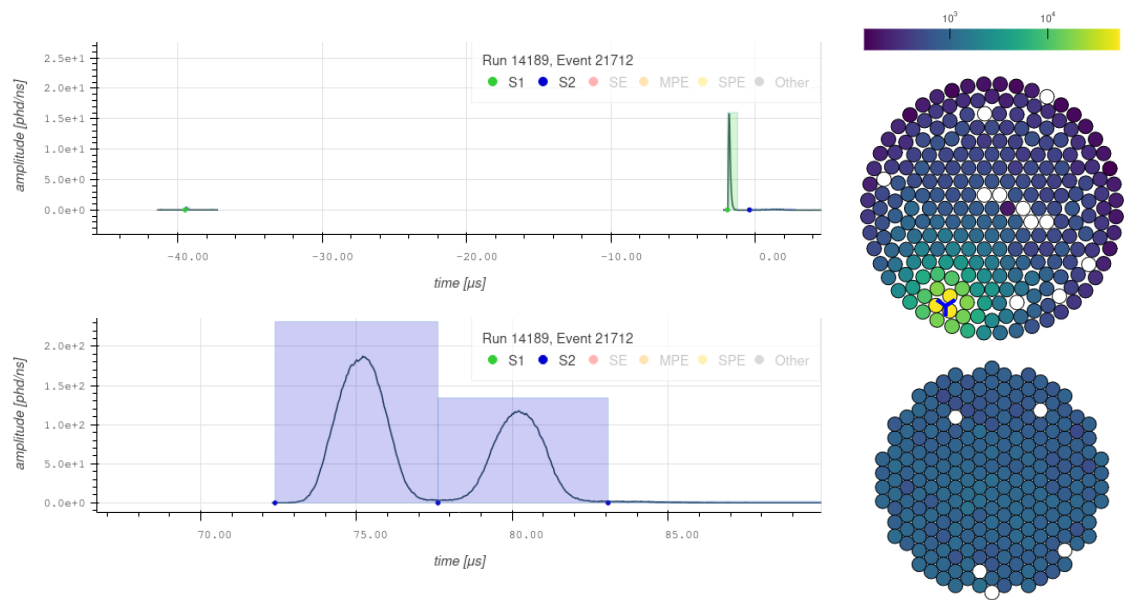


Figure A.38: Waveforms and PMT hit maps are shown for the delayed event: run 14189, event 21712. The top left plot shows the two S1 waveforms highlighted in green. The bottom left plot shows the S2 waveforms highlighted in blue. The event's PMT hit map is shown on the right for the top array (top) and the bottom array (bottom). The blue "Y" shaped markers in the top array diagram mark the S2 centroid positions. The delay time of this event is about $40 \mu\text{s}$, and the drift time is about $75 \mu\text{s}$.

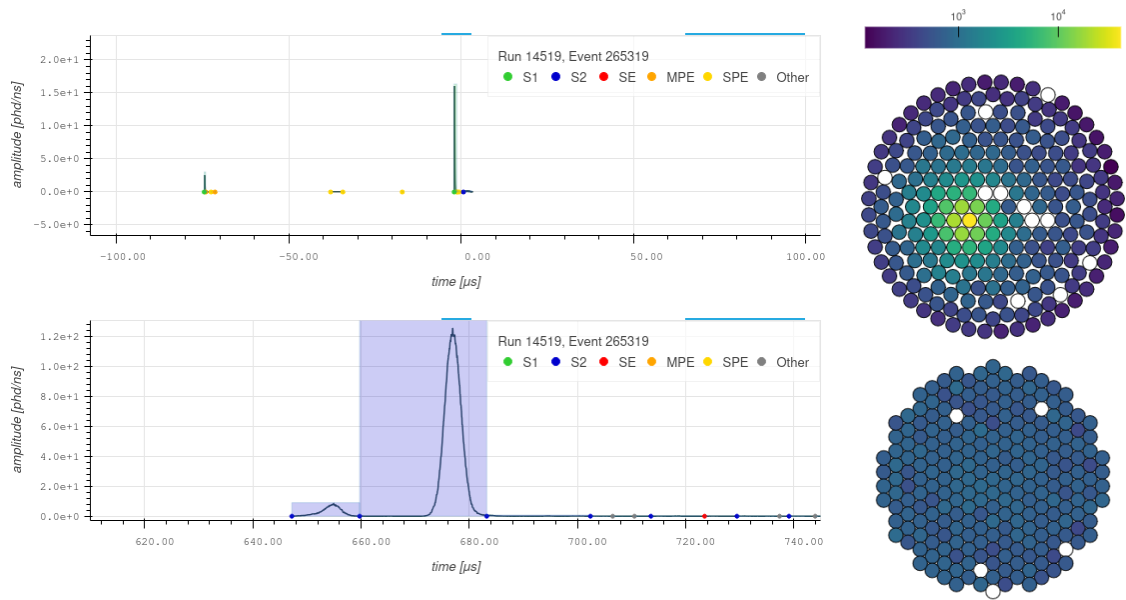


Figure A.39: Waveforms and PMT hit maps are shown for the delayed event: run 14519, event 265319. The top left plot shows the two S1 waveforms highlighted in green. The bottom left plot shows the S2 waveforms highlighted in blue. The event's PMT hit map is shown on the right for the top array (top) and the bottom array (bottom). The delay time of this event is about $75 \mu\text{s}$, and the drift time is about $650 \mu\text{s}$.

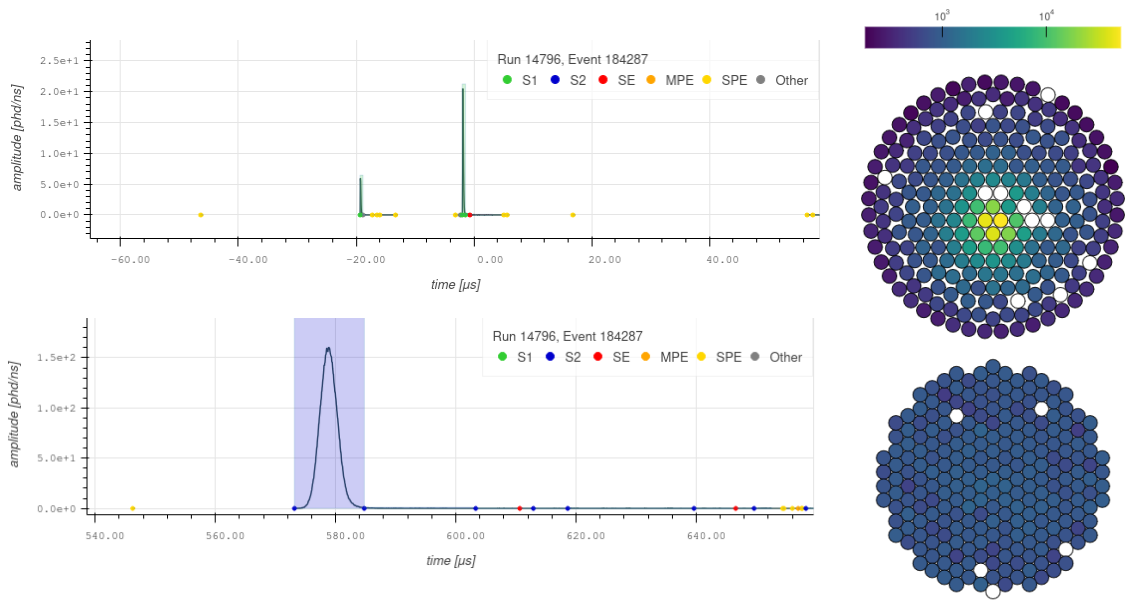


Figure A.40: Waveforms and PMT hit maps are shown for the delayed event: run 14796, event 184287. The top left plot shows the two S1 waveforms highlighted in green. The bottom left plot shows the S2 waveform highlighted in blue. The event's PMT hit map is shown on the right for the top array (top) and the bottom array (bottom). The delay time of this event is about $20 \mu\text{s}$, and the drift time is about $580 \mu\text{s}$.

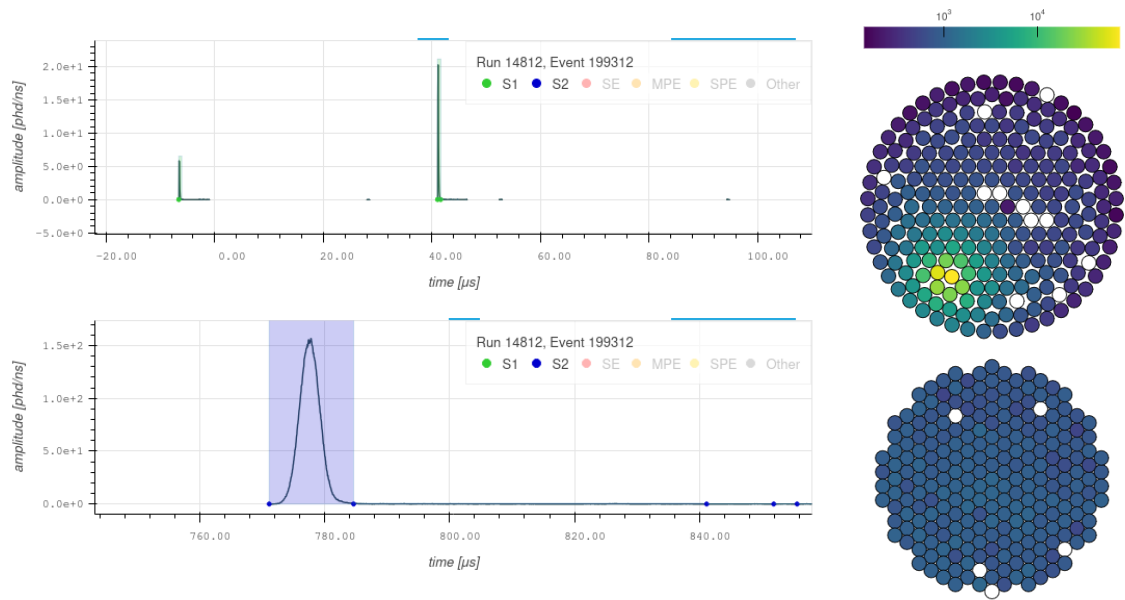


Figure A.41: Waveforms and PMT hit maps are shown for the delayed event: run 14812, event 199312. The top left plot shows the two S1 waveforms highlighted in green. The bottom left plot shows the S2 waveform highlighted in blue. The event's PMT hit map is shown on the right for the top array (top) and the bottom array (bottom). The delay time of this event is about $50 \mu\text{s}$, and the drift time is about $730 \mu\text{s}$.

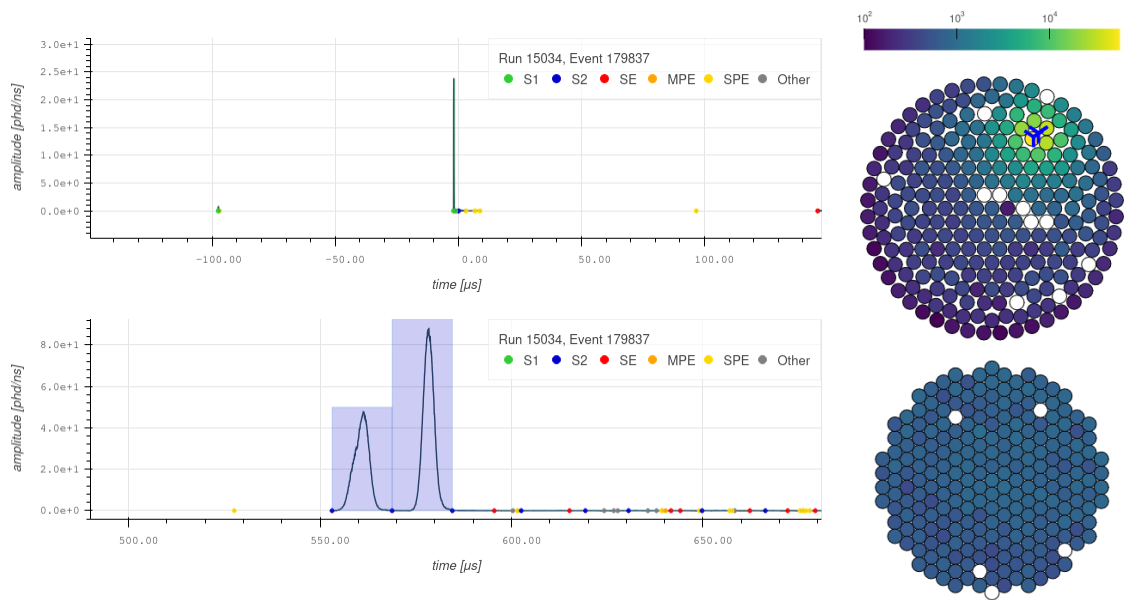


Figure A.42: Waveforms and PMT hit maps are shown for the delayed event: run 15034, event 179837. The top left plot shows the two S1 waveforms highlighted in green. The bottom left plot shows the S2 waveforms highlighted in blue. The event's PMT hit map is shown on the right for the top array (top) and the bottom array (bottom). The blue "Y" shaped markers in the top array diagram mark the S2 centroid positions. The delay time of this event is about 95 μs , and the drift time is about 570 μs .

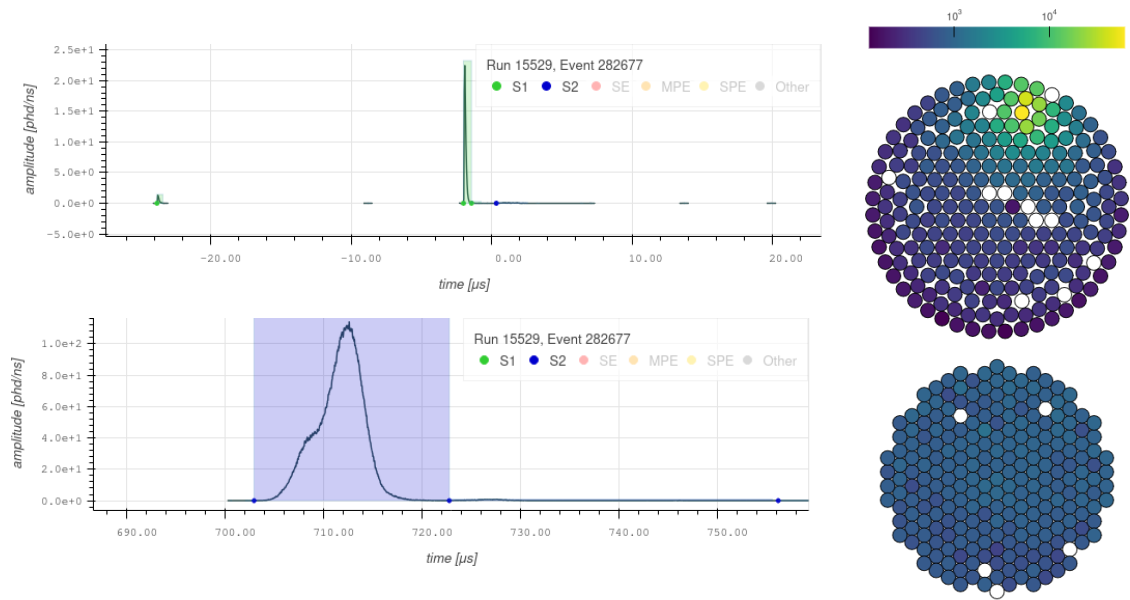


Figure A.43: Waveforms and PMT hit maps are shown for the delayed event: run 15529, event 282677. The top left plot shows the two S1 waveforms highlighted in green. The bottom left plot shows the S2 waveform highlighted in blue. The event's PMT hit map is shown on the right for the top array (top) and the bottom array (bottom). The delay time of this event is about $20 \mu\text{s}$, and the drift time is about $700 \mu\text{s}$.

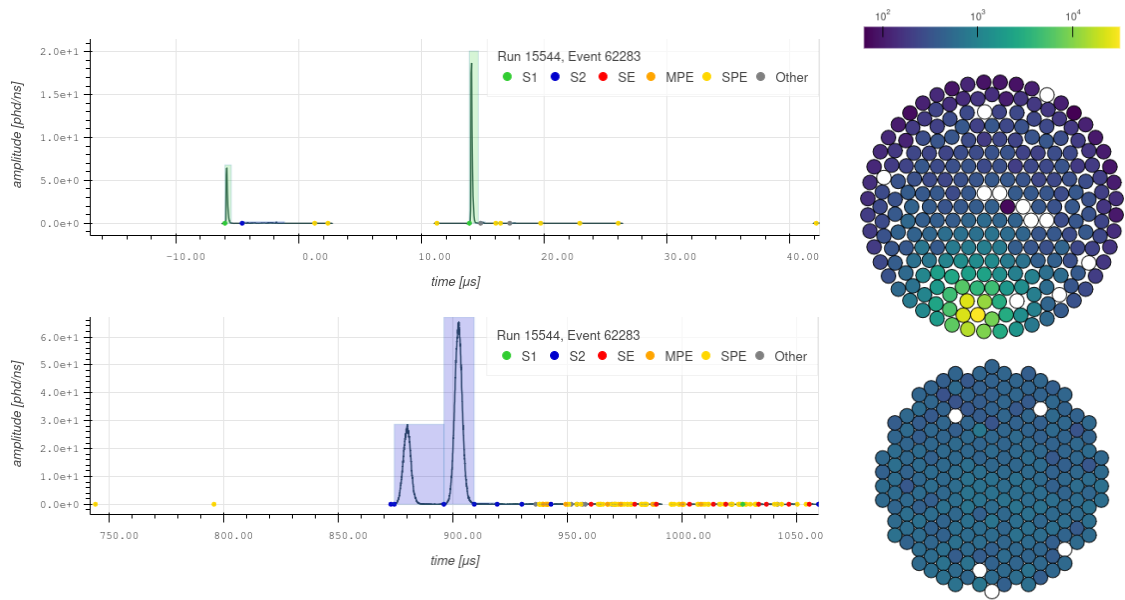


Figure A.44: Waveforms and PMT hit maps are shown for the delayed event: run 15544, event 62283. The top left plot shows the two S1 waveforms highlighted in green. The bottom left plot shows the S2 waveforms highlighted in blue. The event's PMT hit map is shown on the right for the top array (top) and the bottom array (bottom). The delay time of this event is about 20 μ s, and the drift time is about 890 μ s.

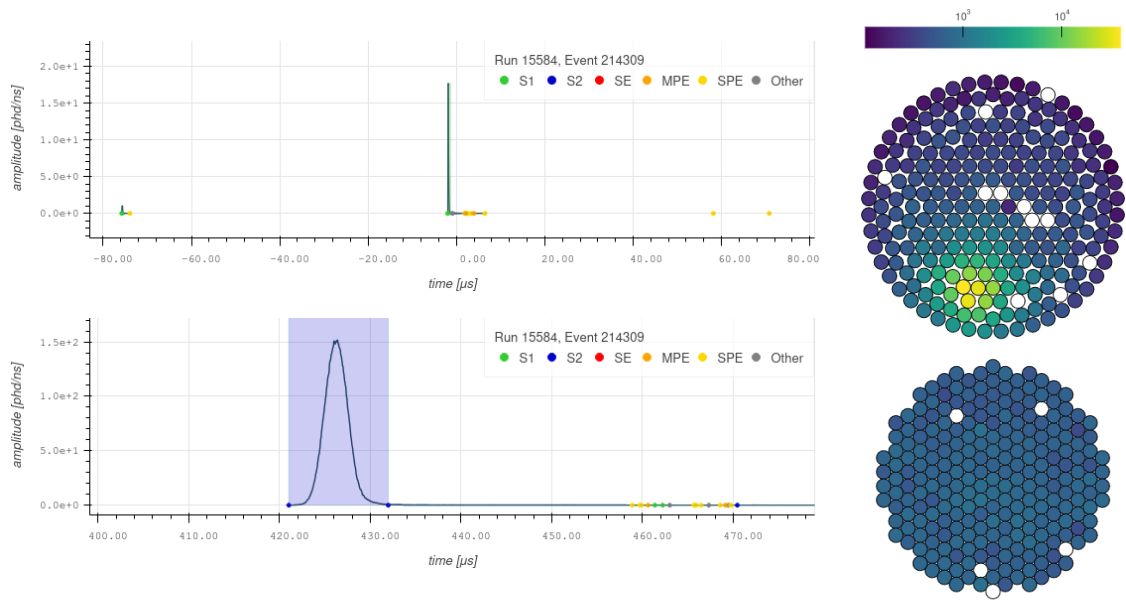


Figure A.45: Waveforms and PMT hit maps are shown for the delayed event: run 15584, event 214309. The top left plot shows the two S1 waveforms highlighted in green. The bottom left plot shows the S2 waveform highlighted in blue. The event's PMT hit map is shown on the right for the top array (top) and the bottom array (bottom). The delay time of this event is about $75 \mu\text{s}$, and the drift time is about $420 \mu\text{s}$.

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