

Electric Fields and their Implications in the LUX-ZEPLIN Time Projection Chamber



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*To my beautiful grandparents
Anima Chanda and Hari Narayan Chanda
- Diddi and Dadda, I love you*

If I have seen further it is by standing on the shoulders of giants

— I. Newton

Acknowledgements

I have returned to this page many times, convinced that writing these acknowledgements would be simple, only to realise that it is anything but. Not because I do not know what to say, but because there are too many people to thank. That, in itself, feels like a quiet measure of how fortunate I have been. Over the last four years, I have had the privilege of meeting and working with people I might never otherwise have known, each leaving their own imprint on my life and on this journey. It is their kindness, patience, unique personalities, and generosity that have shaped these years, and the memories made along the way are ones I will always treasure.

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* * *

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Abstract

Dark matter, though traced by its gravitational and cosmological imprints, continues to evade direct detection. The LUX–ZEPLIN (LZ) experiment, a dual-phase xenon time projection chamber, stands at the forefront of this pursuit. This thesis interrogates the microscopic and macroscopic roles of electric fields in LZ and their consequences for charge transport, event reconstruction, and low-energy sensitivity through enhanced signal–background discrimination and targeted background mitigation. Measurements of drift velocity and longitudinal diffusion in liquid xenon yield a self-consistent transport model that anchors field reconstruction and exhibits quantitative concordance with the Cohen–Lekner formulation of electron transport. A data-driven and simulation-informed programme then maps time-evolving and azimuthally asymmetric fields and introduces a novel surface-charge modelling framework that reveals charge redistribution on PTFE walls. These methods refine field mapping and, in turn, the description of charge drift, reducing biases and uncertainties in position reconstruction while clarifying diffusion-induced broadening. They also inform a low-energy ionisation-only analysis that demonstrates operation below the scintillation threshold. The advances reported here strengthen LZ’s forthcoming WIMP searches as sensitivities approach the neutrino fog, building on world-leading performance for $m_\chi \gtrsim 9 \text{ GeV}/c^2$, and they support a wide suite of physics analyses, including $0\nu\beta\beta$, by tightening charge-transport and field systematics. Taken together, these studies furnish field-motivated design guidance for the next-generation XLZD detector and underscore the role of electric fields as a central, quantitative lever among the determinants of performance, calibration, and physics reach.

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Foreword

Dark matter remains one of the most enduring mysteries in modern physics, inferred through its gravitational and cosmological imprints—from the formation of the cosmic web and the dynamics of galaxies and clusters to the relic signatures in the cosmic microwave background (CMB) and the constraints of big-bang nucleosynthesis (BBN). Among the leading experiments seeking to unveil its nature is the LUX–ZEPLIN (LZ) detector, a dual-phase xenon time projection chamber situated deep underground to shield against background radiation. Dual-phase TPCs such as LZ lie at the heart of direct-detection efforts, translating minute energy deposits into measurable light and charge signals. Within these instruments, the electric field defines everything: it governs how ionisation electrons drift, how recombination unfolds, and how faithfully we can reconstruct the position and energy of each event. In LZ, these same fields reveal a deeper story—one that connects microscopic charge transport to macroscopic detector performance.

The studies presented in this thesis examine that relationship in detail: mapping electric-field distortions, quantifying their impact on event reconstruction, and probing the limits of low-energy sensitivity through an ionisation-only analysis. Together, these investigations form a narrative that begins with understanding electron behaviour in liquid xenon, extends to optimising the present LZ detector, and culminates in design insights for the next-generation XLZD instrument, where electric-field control will again define what physics can be reached.

CHAPTERS 1 & 2 establish the scientific context of this work. The first motivates dark matter through astrophysical and cosmological evidence, outlines key candidate particles, and frames their expected interactions with ordinary matter. The second introduces direct detection with dual-phase xenon TPCs, culminating in the LUX–ZEPLIN experiment as a flagship instrument delivering unprecedented sensitivity to WIMP scattering. Within this broader framework, the author contributed through active involvement in LZ’s accidentals group, where a suite of ionisation-based selection cuts was designed and tuned for both WS 2022 and WS 2024 to improve control of one of the experiment’s least well-constrained background classes—problematic by nature rather than by rate. This toolkit achieved approximately 95% rejection of accidental backgrounds (e.g. isolated ionisation signals) after preliminary data-quality preselection while maintaining near-unity signal acceptance across both WIMP searches. The details of this contribution are not presented in this thesis.

CHAPTER 3 focuses on charge transport in liquid xenon, presenting measurements of drift velocity and the longitudinal diffusion coefficient in LZ and, from the same dataset, deriving a self-consistent set of charge-transport parameters—drift velocity, longitudinal and transverse diffusion coefficients, and the effective electron momentum-transfer cross-section—in a regime of operation relevant to many dark-matter experiments and beyond. These results are consistent with Cohen–Lekner expectations and the opening of multiple momentum-transfer channels with field. The calibrated parameters serve as inputs to the electric-field modelling in the next chapter, fixing the drift-time-to- z mapping and quantifying how field non-uniformities bias reconstructed position and energy. The framework is now used in LZ’s ionisation and detector-response simulations and updates the charge-transport literature relevant to future detector designs. This chapter presents work undertaken by the author in full, except for the waveform-analysis-derived diffusion-coefficient study (the “IRF” study, E. Jacquet), which serves as an independent cross-check.

CHAPTER 4 characterises and models the electric fields in LZ, linking microscopic charge transport to large-scale detector behaviour. Using an ionisation-based framework anchored to calibration data, the chapter reconstructs the time-evolving fields, quantifies azimuthal non-uniformities, and propagates their effects to fiducialisation and energy or position bias. A patch-based surface-charge model with eigenmode analysis is developed to expose and control degeneracies between neighbouring patches, revealing a stable, cathode-proximal redistribution pattern rather than monotonic accumulation. The study also explains the apparent migration of the $^{131\text{m}}\text{Xe}$ -derived ionisation wall during WS 2024 as large-scale charge redistribution on the inner PTFE. The practical gains include improved field mapping for WIMP searches, tighter priors for radial bias, and clarified coupling between TPC fields and the surrounding xenon skin response—insights useful both for background rejection and for future, larger detectors.

Key results: (i) first explicit characterisation and demonstration of charge redistribution on PTFE surfaces; (ii) validation of field impact within the TPC and on the xenon-skin response; (iii) quantification of field-induced biases in position reconstruction. A paper reporting on this work is currently in preparation.

Acknowledgements and authorship. Wall-profile tracking is credited to the Wall Group (led by A. Musalhi). Comparisons to official $^{83\text{m}}\text{Kr}$ -derived fields were provided by B. Schafer and to $^{131\text{m}}\text{Xe}$ -derived fields by M. Murdy. Credit is due to M. Hernandez for data-driven tuning of the skin response. Where figures or data from these contributors are used, this is indicated explicitly. All remaining field-characterisation work is the author’s, including development of LZEF (inherited from R. Watson), the full charge-profile matching code, and subsequent analyses.

CHAPTER 5 develops background-rejection methods for the principal pathologies in an ionisation-only search and applies them to a proof-of-concept analysis using a subset of WS 2022 data, demonstrating LZ’s capability to operate without reliance on scintillation. The study establishes baseline ionisation-only limits and indicates a clear path to sub- keV thresholds and sensitivity to lighter dark-matter candidates in the sub- GeV/c^2 regime. Work toward the full analysis is ongoing; using methodology consistent with that developed here, it is expected to deliver competitive limits that further expand LZ’s physics reach.

Acknowledgements and authorship. The ionisation-only team is acknowledged for developing key livetime-based analysis cuts and for producing the clean calibration datasets used for tuning and validation. A. Wang and T. Pershing developed the statistical framework; the author made minor amendments to this code to obtain the final results. The primary contributions of the author in this chapter are the design and tuning of the background-rejection cuts presented herein.

CHAPTER 6 synthesises the findings of this thesis to inform the preliminary design of the XLZD time projection chamber, field cage, and surrounding skin veto—developed within the newly formed XLZD collaboration. The chapter integrates insights from the author’s studies of electric fields, electron transport, and backgrounds to refine fundamental design requirements and update earlier literature assumptions. Field-related motivations are quantified to guide grid geometry, high-voltage operation, and extraction efficiency, while mechanical and background-rejection considerations are incorporated into the overall cryostat and veto layout.

SPECIAL NOTE ON APPENDIX A. The appendix revisits the xenon electroluminescence yield at cryogenic conditions and provides an updated gain model now adopted as the LZ simulation baseline. Its implementation resolves the long-standing tension in light-collection modelling without recourse to unphysical optical parameters, enabling more realistic tuning of material reflectivities and reducing a key systematic in charge-based reconstruction. This parametrisation is taken as the baseline for the conclusions in this chapter.

A short study of preliminary results from the HYDROX experiment at SLAC is also presented. The author contributed to the experiment through construction of the circulation panel—undertaken with the full SLAC team—and, principally, through the design of the gas TPC. Although this work is not reported in detail in the thesis, a brief exploratory analysis conducted by the author on the impact of hydrogen-doped GXe on single-electron yields is included, based on diagnostic data from one of HYDROX’s earliest runs and on preliminary GARFIELD++ simulations by Y. Qie, extended in part by the author.

Together, these studies provide a physics-driven foundation for XLZD’s next-generation detector design, ensuring that the experiment’s ultimate reach is limited only by nature itself.

List of Abbreviations

$0\nu\beta\beta$	Neutrinoless double beta decay
1-D, 2-D	One- or two-dimensional, referring to spatial dimensions
$2\nu\beta\beta$	Two-neutrino double beta decay
AC	Accidental coincidences
ADC	Analog-to-Digital Converter
AFT	Area Fraction Time
AIC	Akaike Information Criterion
BACCARAT	Basically A Component-Centric Analog Response to AnyThing
CDF	Cumulative Distribution Function
$CE\nu NS$	Coherent Elastic Neutrino–Nucleus Scattering
CL	Confidence Level
CMB	Cosmic Microwave Background
CSD	Calibration Source Deployment
DAQ	Data Acquisition
DD	Deuterium–Deuterium, a neutron calibration source
DER	Detector Electronics Response
EL	Electroluminescence
ER	Electronic Recoil; also used to denote the Extraction Region where clear from context
FFR	Forward Field Region
FSR	Field Shaping Ring
FV	Fiducial Volume
GdLS	Gadolinium-doped Liquid Scintillator
GXe	Gaseous Xenon
HV	High Voltage
ICV	Inner Cryostat Vessel
iRRS	in-line Radon Reduction System
IRF	Impulse Response Function
LCE	Light Collection Efficiency
LUX	Large Underground Xenon experiment

LXe	Liquid Xenon
LZ	LUX-ZEPLIN
LZEF	LZ Electric Fields software
Λ CDM	Lambda Cold Dark Matter cosmological model
MS	Multiple Scatter
NEST	Noble Element Simulation Technique
NR	Nuclear Recoil
OCV	Outer Cryostat Vessel
OD	Outer Detector
PBH	Primordial Black Hole
PDF	Probability Density Function
phd	Photons detected
PLR	Profile Likelihood Ratio
PMT	Photomultiplier Tube
PSD	Pulse Shape Discrimination
PTFE	Polytetrafluoroethylene
RFR	Reverse Field Region
RMS	Root Mean Square
ROI	Region of Interest
S1c	Corrected primary scintillation signal area
S2c	Corrected secondary scintillation signal area
SEM	Standard Error of the Mean
SNR	Signal-to-Noise Ratio
SS	Single Scatter
SURF	Sanford Underground Research Facility
TBA	Top-Bottom Asymmetry
TOF	Time of Flight
TPC	Time Projection Chamber
VUV	Vacuum Ultraviolet
WIMP	Weakly Interacting Massive Particle
WS	WIMP Search
XLZD	XENON-LUX-ZEPLIN-Darwin, a proposed future LXe observatory
ZEPLIN	ZonEd Proportional scintillation in Liquid Noble gases

“How can I be substantial if I do not cast a shadow? I must have a dark side also, if I am to be whole.”

— C. G. Jung, *Modern Man in Search of a Soul*

Part I

The Landscape of Dark Matter Searches

1

Dark Matter

OBSERVATIONS ACROSS ASTROPHYSICS AND COSMOLOGY reveal a non-luminous matter component that dominates the mass budget of the Universe. Its presence is traced in many ways, including flat galactic rotation curves, the binding of clusters, gravitational lensing, and the temperature–polarisation anisotropies of the cosmic microwave background; taken together these imply that dark matter comprises $\sim 85\%$ of the cosmic matter density. In this sense, dark matter denotes a predominantly non-luminous component required by dynamics, lensing, and early-Universe probes (CMB and BBN), for which no confirmed particle explanation currently exists. This chapter assembles the observational case and the ensuing physical requirements for dark matter, surveys the principal dark-matter candidates within and beyond the Λ CDM framework, and outlines the experimental search strategies that motivate the analyses in this thesis.

1.1 Evidence for Dark Matter

The case for dark matter rests upon a convergence of independent observations across vastly different scales—from galactic dynamics to the cosmic microwave background (CMB). Together they reveal a persistent discrepancy between the gravitational potential inferred from luminous matter and that required to explain observed motions, lensing, and anisotropies. The inferred dark component must be stable, non-baryonic, and effectively collisionless on cosmological timescales.

Except where otherwise noted, the discussion in this section draws primarily on several comprehensive review articles [1–3], which summarise the observational evidence, theoretical candidates, and experimental approaches to dark matter. Individual works are therefore not cited exhaustively; the purpose here is to motivate the search for dark matter rather than to provide a comprehensive survey of the evidence.

1.1.1 Galactic Rotation Curves

The first compelling evidence arose from measurements of galactic rotation curves. Under Newtonian gravity, the circular velocity of an object orbiting a mass distribution $M(r)$ should obey

$$v_c(r) = \sqrt{\frac{GM(r)}{r}}. \quad (1.1)$$

Beyond the luminous stellar disk, where $M(r)$ is dominated by visible matter, one expects $v_c \propto r^{-1/2}$. Observations beginning with Babcock, and later Rubin and Ford, demonstrated instead that the velocity profiles of spiral galaxies remain approximately constant to the largest measured radii. Such “flat” rotation curves imply a mass density $\rho(r) \propto r^{-2}$ extending far beyond the optical disk.

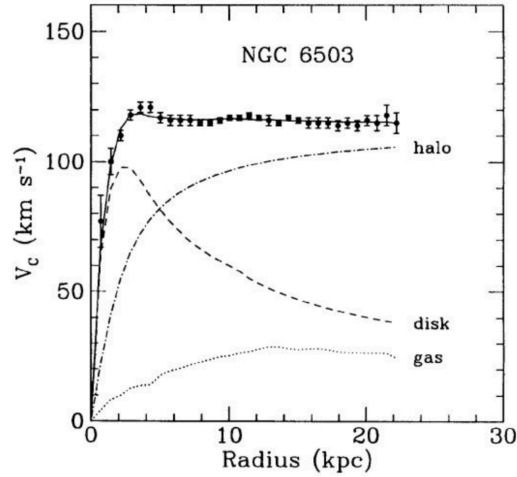


Figure 1.1: Observed rotation curve of the spiral galaxy NGC 6503. The measured circular velocity $v_c(r)$ (points) remains approximately flat beyond the stellar disk, while the contributions from gas and stars decline. The inferred dark-matter halo component dominates the gravitational potential at large radii. Taken from [4].

This behaviour is reproduced in diverse systems—dwarf spheroidals, low-surface-brightness galaxies, and massive spirals alike—indicating that each galaxy is embedded within an extended dark halo whose mass exceeds that of its luminous component by an order of magnitude. Empirical profiles such as the Navarro–Frenk–White (NFW) form,

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

provide an adequate description of halo structure across a wide mass range and arise naturally in cosmological N -body simulations of cold dark matter.

1.1.2 Clusters of Galaxies

At larger scales, the mass discrepancy persists in galaxy clusters. Zwicky’s 1933 study of the Coma cluster, applying the virial theorem to galaxy velocity dispersions,

$$2\langle T \rangle + \langle U \rangle = 0, \quad (1.3)$$

yielded a total mass nearly two orders of magnitude greater than that inferred from starlight. Subsequent X-ray and gravitational-lensing observations have confirmed that the majority of the mass in clusters resides not in galaxies but in an extended, gravitationally bound dark component. Cluster mergers such as the Bullet Cluster (1E0657-56) offer direct, geometric evidence for dark matter: the spatial separation between the baryonic plasma, traced by X-ray emission, and the gravitational potential, mapped through weak lensing, demonstrates that the dominant mass component is effectively collisionless. The same conclusion holds across other colliding systems, providing a dynamical test of dark-matter self-interaction and setting stringent bounds on its cross-section per unit mass.

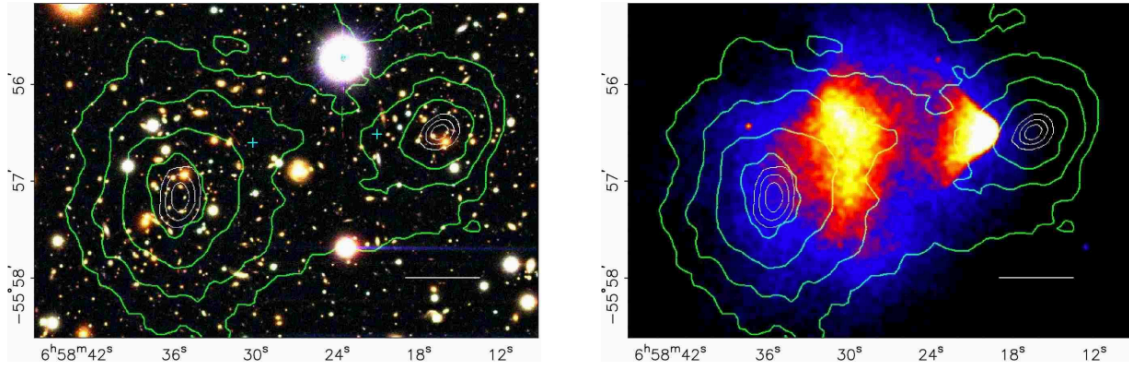


Figure 1.2: Weak gravitational lensing (green contours) overlaid on optical (left) and X-ray (right) images of the merging galaxy cluster 1E0657–558 (the Bullet Cluster). The lensing mass peaks (white contours) trace the collisionless dark-matter halos rather than the hot intracluster gas seen in X-rays, providing direct evidence that most of the gravitating mass is non-baryonic. Taken from [5].

1.1.3 Gravitational Lensing

Gravitational lensing furnishes a purely geometric probe of mass, independent of dynamical assumptions. Deflection of light by intervening matter distorts and magnifies background sources according to the projected gravitational potential Φ , producing convergence κ and shear γ fields measurable in deep surveys. Strong-lensing arcs around massive clusters require total surface densities an order of magnitude higher than can be accounted for by baryons alone, while weak-lensing surveys have mapped the large-scale dark-matter distribution over hundreds of square degrees. The resulting “cosmic shear” power spectra trace the growth of structure and agree closely with predictions of the Λ CDM model when normalised by the CMB.

1.1.4 Cosmic Microwave Background and Large-Scale Structure

The most precise measurement of the dark-matter abundance comes from the anisotropies of the CMB. Acoustic oscillations in the primordial photon–baryon plasma imprint a characteristic pattern of peaks in the temperature power spectrum, whose relative heights depend sensitively on the matter–radiation ratio and the baryon fraction (parametrised by Ω_b). Fits to the latest *Planck* data yield implies that non-baryonic cold dark matter (with density parameter Ω_c) comprises $\sim 26\%$ of the present-day energy density of the Universe. Complementary evidence from baryon acoustic oscillations and large-scale structure surveys supports the same cosmological parameters, reinforcing the Λ CDM paradigm - a model in which cold dark matter and a cosmological constant Λ dominate cosmic dynamics. Simulations incorporating a cold, collisionless matter component reproduce the observed hierarchy of cosmic structure—from filamentary large-scale clustering to virialised haloes—whereas baryons alone cannot account for the depth and coherence of the potential wells in which galaxies form.

1.1.5 Summary and Requirements

The consistency of these observations across independent physical regimes establishes dark matter as an essential constituent of the Universe. Its inferred properties may be summarised as follows:

- **Massive and non-relativistic:** must be cold at matter–radiation equality to permit hierarchical structure formation.

- **Stable:** lifetime $\tau \gg t_{\text{Universe}}$ to persist until today.
- **Non-baryonic:** the cosmic baryon fraction measured by the CMB (and supported by large-scale structure) is far below the total matter density, so the dominant dark component cannot be ordinary baryons.
- **Neutral or milli-charged:** electromagnetic interactions must be negligible.
- **Predominantly gravitational:** no substantial coupling to Standard-Model fields beyond gravity.

These criteria delineate the landscape of viable dark-matter candidates explored in the following section.

1.2 Dark Matter Candidates

A wide range of candidates have been proposed to explain the non-baryonic component of the Universe. The requirement that they be stable on cosmological timescales, neutral, and cold (non-relativistic during structure formation) severely constrains the viable parameter space. The brief survey that follows samples leading ideas - from ultra-light bosonic fields to weak-scale thermal relics - touching on compact astrophysical possibilities, aiming to situate the reader within a diverse theoretical landscape rather than to be exhaustive. A closing subsection outlines alternative paradigms and competing frameworks to keep that landscape in honest tension.

1.2.1 Axions

The axion was originally introduced not to solve the dark-matter problem but to resolve the strong-CP problem in quantum chromodynamics (QCD) through the Peccei–Quinn (PQ) mechanism. In this framework a new global $U(1)_{\text{PQ}}$ symmetry is spontaneously broken at scale f_a , promoting the CP–violating QCD angle to a dynamical field whose pseudo–Nambu–Goldstone boson is the axion a . Non-perturbative QCD effects generate a small axion mass inversely proportional to f_a ,

$$m_a \simeq 5.7 \mu\text{eV} \left(\frac{10^{12} \text{ GeV}}{f_a} \right),$$

up to $\mathcal{O}(1)$ uncertainties from chiral inputs. The axion couples very weakly to Standard-Model particles; the axion–photon coupling can be written as

$$g_{a\gamma\gamma} = \frac{\alpha}{2\pi f_a} C_{a\gamma},$$

where α is the fine-structure constant and $C_{a\gamma} \sim \mathcal{O}(1)$ encodes model dependence.

In the early Universe, axions are efficiently produced by the *misalignment mechanism*: when the Hubble rate H drops below m_a the homogeneous field begins coherent oscillations about its minimum and redshifts as non-relativistic matter, providing cold dark matter for plausible initial conditions in the μeV – meV mass range (equivalently $f_a \sim 10^9$ – 10^{12} GeV).

Experiments exploit $g_{a\gamma\gamma}$ to convert ambient axions into photons in strong magnetic fields. Resonant cavity haloscopes (ADMX, HAYSTAC, ORGAN) target m_a in the few–40 μeV range; dielectric haloscopes (MADMAX) and

lumped-element LC circuits (ABRACADABRA, DMRadio) extend coverage to higher and lower masses, respectively. Helioscopes (e.g. CAST) and stellar-cooling arguments provide complementary constraints on couplings [6]. Axion-like particles (ALPs) relax the QCD mass–coupling relation and are sought with the same techniques across a broader parameter space.

1.2.2 Neutrinos

Neutrinos provide the only confirmed example of stable, weakly interacting particles beyond the photon. Their established properties clarify what a viable dark-matter candidate must satisfy, and why neutrinos themselves do not. Standard-Model neutrinos decouple from the primordial plasma while still relativistic (at $T \sim \text{MeV}$); the relic cosmic neutrino background today has a temperature of about 1.95 K and a correspondingly tiny energy density [7]. Cosmological analyses constrain the summed neutrino mass to $\sum m_\nu \lesssim 0.12 \text{ eV}$, implying a contribution to the matter density that is negligible compared with $\Omega_{\text{DM}} h^2$. Complementing these bounds, the kinematic tritium β -decay experiment KATRIN sets the strongest direct laboratory limit on the effective electron-neutrino mass, $m_\beta < 0.8 \text{ eV}$ (90% C.L.) [8].

Neutrinos remain relativistic until well after matter–radiation equality, so their large thermal velocities erase small-scale perturbations by free-streaming out of primordial overdensities. The resulting suppression of power on sub-Mpc scales is incompatible with the hierarchical assembly of galaxies that characterises cold-dark-matter cosmologies [7, 9]. They therefore constitute a classic example of *hot* dark matter and cannot account for the dominant cold component inferred from cosmological and astrophysical observations.

Extensions of the neutrino sector introduce heavier, *sterile* states that interact only via mixing with the active flavours. For masses of order keV, such sterile neutrinos are produced while relativistic in the early Universe and later become non-relativistic, behaving as *warm* dark matter—suppressing sub-galactic structure while remaining consistent with large-scale structure data [9]. Their radiative decay, $\nu_s \rightarrow \nu \gamma$, would yield a monochromatic X-ray line at $E_\gamma \simeq m_{\nu_s}/2$, motivating dedicated searches for spectral excesses in astrophysical observations [10]. Although current limits disfavour much of the simplest parameter space, sterile-neutrino models remain one of the few minimal extensions capable of linking neutrino-mass generation to the observed dark-matter abundance.

1.2.3 Weakly Interacting Massive Particles

The *WIMP* paradigm postulates a stable, neutral particle with weak-scale mass and couplings. In the early Universe, such particles were in thermal equilibrium with the radiation bath via annihilation and creation processes,

$$\chi + \bar{\chi} \leftrightarrow f + \bar{f}, \quad (1.4)$$

where f denotes Standard-Model fermions. Their co-moving density evolves according to the Boltzmann equation [11, 12],

$$\frac{dn_\chi}{dt} + 3Hn_\chi = -\langle \sigma v \rangle (n_\chi^2 - n_{\chi,\text{eq}}^2). \quad (1.5)$$

In Eqs. (1.5)–(1.6), H is the Hubble expansion rate; n_χ and $n_{\chi,\text{eq}}$ are the (physical) and equilibrium number densities of χ ; $\langle \sigma v \rangle$ is the thermally averaged annihilation cross-section; the subscript f denotes evaluation at *freeze-out* ($x_f \equiv$

$m_\chi/T_f \approx 20\text{--}30$ for weak-scale χ); g_* is the effective number of relativistic degrees of freedom in the plasma at T_f ; and $M_{\text{Pl}} = 1.22 \times 10^{19}$ GeV is the (unreduced) Planck mass.¹ Numerically, $\Omega_\chi h^2 \simeq 0.12$ is obtained for $\langle\sigma v\rangle_f \sim 3 \times 10^{-26} \text{ cm}^3 \text{ s}^{-1}$ for $g_* \sim 80\text{--}100$. When the annihilation rate falls below the Hubble expansion rate, interactions freeze out and the relic abundance becomes fixed. Solving for the asymptotic yield gives [3, 11, 12]

$$\Omega_\chi h^2 \approx \frac{1.07 \times 10^9 \text{ GeV}^{-1}}{M_{\text{Pl}} \sqrt{g_*} \langle\sigma v\rangle_f}. \quad (1.6)$$

This reproduces the observed dark-matter density for a characteristic thermal cross-section $\langle\sigma v\rangle_f \sim 3 \times 10^{-26} \text{ cm}^3 \text{ s}^{-1}$, a coincidence linking the weak scale of particle physics with the cosmological abundance—the so-called *WIMP miracle* [13, 14].

Possible realisations include the lightest neutralino in supersymmetric models, inert Higgs doublets, Kaluza–Klein excitations in theories with compact extra dimensions, or singlet scalars interacting via the Higgs portal [3, 13]. Stability is generally ensured by a conserved discrete symmetry (e.g. R -parity or Z_2) preventing decay into lighter Standard-Model states. WIMP interactions may, however, be mediated by Standard-Model bosons or by additional heavy gauge fields, producing both annihilation signatures (for indirect searches) and elastic scattering with nucleons or electrons (for direct detection). These processes are governed by the same coupling constants that determine the relic density, yielding a unified cosmological and experimental framework.

The elegance and quantitative simplicity of this connection—where a weak-scale interaction naturally yields the correct relic abundance—have made WIMPs the benchmark dark-matter candidate for over three decades. Their well-defined mass range, calculable cross-sections, and testable couplings have driven an extensive experimental programme spanning collider production, indirect detection, and the global network of underground direct-detection experiments. Although null results have now challenged parts of the simplest parameter space, the WIMP framework remains the cornerstone against which alternative dark-matter scenarios are often compared.

Beyond the canonical WIMP, alternative scenarios have gained increasing attention. These include asymmetric dark matter, which mirrors the matter–antimatter asymmetry of the visible sector; axions and axion-like particles, motivated by solutions to the strong-CP problem; and freeze-in or feebly interacting candidates, where dark matter never attains thermal equilibrium with the early Universe. Such frameworks relax the coincidence between the weak and cosmological scales while remaining accessible to next-generation laboratory and astrophysical searches [15].

1.2.4 MOND and Beyond

While particle candidates remain the dominant explanation, alternative frameworks posit that the inferred mass discrepancy arises from a breakdown of Newtonian or general-relativistic dynamics at low accelerations. *Modified Newtonian Dynamics* (MOND) introduces an acceleration scale $a_0 \sim 10^{-10} \text{ m s}^{-2}$ below which the effective gravitational force transitions as

$$\mu\left(\frac{a}{a_0}\right) a = \frac{GM}{r^2}, \quad (1.7)$$

¹Using the *reduced* Planck mass $\tilde{M}_{\text{Pl}} = 2.435 \times 10^{18}$ GeV changes the numerical prefactor in Eq. (1.6) accordingly; the standard $1.07 \times 10^9 \text{ GeV}^{-1}$ form assumes M_{Pl} .

where $\mu(x)$ interpolates between Newtonian ($\mu \approx 1$) and deep-MOND ($\mu \approx x$) regimes [16, 17]. MOND successfully reproduces galactic rotation curves with a universal baryonic Tully–Fisher relation but fails to explain cluster dynamics, gravitational lensing, or cosmological structure without reintroducing unseen mass [18].

Relativistic extensions such as TeVeS (Tensor–Vector–Scalar) and emergent-gravity theories aim to reconcile MONDian behaviour with general relativity and the cosmic microwave background [16, 18]. Although these approaches capture certain galactic phenomenology, they remain less predictive than Λ CDM and have yet to provide a complete, self-consistent alternative to the particle dark-matter paradigm.

1.3 Searches for Particle Dark Matter

The properties of dark matter can be probed on three complementary fronts: (i) production of dark-sector states at high-energy colliders, inferred through missing transverse energy and momentum signatures; (ii) indirect detection via astronomical observations of photons, charged particles, and neutrinos from annihilation or decay; and (iii) direct detection of rare scatters with ordinary matter in ultra-low-background experiments. These approaches thus interrogate different legs (figure 1.3) of the same interaction and together provide coverage of distinct combinations of couplings, masses, and kinematics. Coordinated interpretation across the three is essential, as the leading systematics and astrophysical assumptions differ, and the resulting sensitivities are strongly complementary.

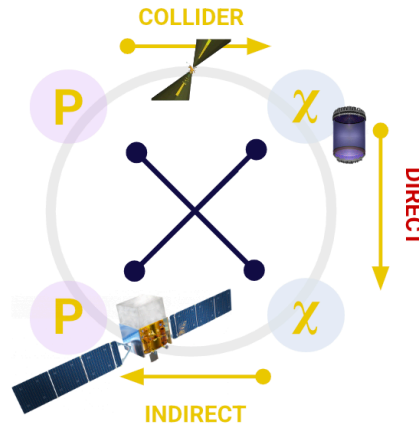


Figure 1.3: The three search frontiers for dark matter and the umbrella interactions they probe: production in collider searches (“make it”), detection of decay or annihilation signatures from distant astrophysical bodies such as dwarf galaxies (“break it”) and (typically) low-cross-section scattering of dark matter with ordinary matter targets “shake it”. Dark matter particles are represented as χ and Standard Model particles by P .

1.3.1 Collider Searches

At colliders, dark matter can be produced in high-energy particle collisions if kinematically accessible and sufficiently coupled to Standard-Model fields. Since dark-matter particles escape detection, their presence is inferred through an apparent imbalance of transverse energy or momentum. Typical analyses at the LHC thus search for events with large missing transverse energy (MET) recoiling against a visible object such as a jet, photon, or vector boson—the so-called

mono- X signatures [19]. These signatures are interpreted using simplified models in which dark matter couples to quarks or gluons via a mediator of mass m_{med} and coupling strength g_{DM} . Null results from Run 2 constrain such mediators to lie above the TeV scale for $\mathcal{O}(1)$ couplings, corresponding to effective limits on the WIMP–nucleon cross-section near 10^{-46} – 10^{-45} cm^2 , depending on mediator spin and coupling structure [20]. Crucially, visible mediator searches—dijet and dilepton resonance searches when the mediator decays back to quarks or leptons—often provide stronger exclusions on m_{med} and g_q than mono- X channels for sizeable, visible branching fractions [21]. Higgs-portal searches (invisible Higgs decays and $\text{VBF}+E_T^{\text{miss}}$) provide complementary coverage at lower masses and small couplings [21]. Together, these channels tightly constrain collider-accessible WIMP scenarios within the simplified-model framework.

Beyond simplified models, supersymmetric and extended Higgs-sector searches continue to test concrete WIMP candidates such as neutralinos, Higgsinos, and inert doublets. No excess has yet been observed, but the complementarity of collider bounds and direct-detection limits is crucial: collider results constrain low-mass and large-coupling regimes where scattering cross-sections fall below current detector thresholds, while direct searches dominate at higher masses and weaker couplings. Run-3 (proposed to continue data-taking until 2026) and proposed high-luminosity upgrades at the LHC will further extend these searches to multi- TeV mediators and probe sub-percent couplings in simplified models [20, 22].

1.3.2 Indirect Detection

Indirect searches probe the possible annihilation or decay products of dark matter accumulated in astrophysical environments. If dark matter self-annihilates or decays into Standard-Model particles, the resulting gamma rays, positrons, antiprotons, or neutrinos can be sought from regions of high dark-matter density such as the Galactic Centre, dwarf spheroidal galaxies, and galaxy clusters [23]. Space- and ground-based instruments—including *Fermi*-LAT, AMS-02, PAMELA, H.E.S.S., MAGIC, and IceCube—have provided increasingly stringent constraints on annihilation cross-sections and decay lifetimes across many final states.

An early excess of high-energy positrons observed by PAMELA and later confirmed with greater precision by AMS-02 was initially interpreted as a possible signature of WIMP annihilation into leptonic channels [24, 25]. However, the cross-sections required to explain the observed flux exceed the canonical thermal-relic scale by several orders of magnitude and are now more plausibly attributed to nearby pulsars or other astrophysical accelerators [26, 27]. This illustrates a central challenge of indirect detection: many potential dark-matter signals are degenerate with poorly constrained astrophysical foregrounds, making robust interpretation intrinsically difficult. For annihilation into heavy quarks or gauge bosons, current upper limits from *Fermi*-LAT dwarf-spheroidal analyses reach

$$\langle\sigma v\rangle \lesssim (1\text{--}3) \times 10^{-26} \text{ cm}^3 \text{ s}^{-1},$$

consistent with the canonical thermal relic expectation [28]. No unambiguous excess consistent with dark matter has yet been confirmed: the Galactic-centre gamma-ray excess remains debated [29, 30], and tentative X-ray features (e.g. at 3.5 keV) lack firm attribution [31, 32]. Constraints from antiprotons and cosmic-ray positrons are similarly compatible with secondary production in astrophysical sources.

Collectively, these null results exclude a wide range of WIMP and decaying dark-matter scenarios while complementing collider and direct-detection efforts through their sensitivity to annihilation and decay dynamics rather than elastic scattering.

1.3.3 Direct Detection

Direct searches seek to observe the rare elastic scattering of Galactic dark-matter particles off atomic nuclei or electrons in terrestrial targets. The expected differential recoil spectrum falls approximately exponentially with recoil energy,

$$\frac{dR}{dE_R} = \frac{\rho_\chi}{m_\chi m_T} \int_{v_{\min}}^{v_{\text{esc}}} f(\mathbf{v}) v \frac{d\sigma_T}{dE_R} d^3\mathbf{v}, \quad (1.8)$$

where $\rho_\chi \simeq 0.3 \text{ GeV cm}^{-3}$ is the local dark-matter density, m_T the target-nucleus mass, and $f(\mathbf{v})$ the dark-matter velocity distribution in the Galactic halo, typically described by a truncated Maxwellian with dispersion $v_0 \sim 220 \text{ km s}^{-1}$ and escape velocity $v_{\text{esc}} \sim 550 \text{ km s}^{-1}$ [33]. The minimum speed required to produce a nuclear recoil E_R is given by

$$v_{\min}(E_R) = \sqrt{\frac{m_T E_R}{2 \mu_T^2}}, \quad \mu_T = \frac{m_\chi m_T}{m_\chi + m_T}, \quad (1.9)$$

where μ_T is the WIMP–nucleus reduced mass. Recoil energies of only a few keV and interaction rates below one event per tonne-year demand ultra-low backgrounds, radiopure materials, and powerful discrimination between nuclear and electronic recoils. A wide range of detector technologies has been developed to meet these challenges (Fig. 1.4). Cryogenic calorimeters such as SUPERCDMS [34] and CRESST [35] measure both phonon and scintillation or ionisation signals, enabling sub-keV thresholds and discrimination between nuclear and electronic recoils. Dual-phase noble-liquid TPCs—including LUX–ZEPLIN (LZ) [36], XENONNT [37], and PANDAX-4T [38]—combine prompt scintillation (S_1) and electroluminescence (S_2) to reconstruct the energy and three-dimensional position of each interaction, providing self-shielding and world-leading sensitivities. Superheated-liquid detectors such as PICO [39] distinguish nuclear recoils from electron recoils via the differing energy deposition densities (dE/dx), rather than through an acoustic phase transition, while low-pressure gas TPCs such as CYGNUS [40] aim to measure recoil directions, offering the potential for a definitive Galactic signature.

Scattering formalism and connection to limits

For spin-independent (SI) interactions, the nuclear cross section factorises into a per-nucleon term and a finite-size nuclear form factor:

$$\frac{d\sigma_T^{\text{SI}}}{dE_R} = \frac{m_T}{2 \mu_N^2 v^2} \sigma_N^{\text{SI}} [Z f_p + (A - Z) f_n]^2 F_{\text{SI}}^2(E_R), \quad (1.10)$$

where μ_N is the WIMP–nucleon reduced mass, Z and A are the atomic and mass numbers, $f_{p,n}$ the effective couplings (usually taken equal, $f_p \simeq f_n$), and $F_{\text{SI}}(E_R)$ is the Helm form factor [33]. The total rate thus scales approximately as A^2 , motivating heavy targets such as xenon. Spin-dependent (SD) scattering, by contrast, probes the nuclear spin content and is governed by the proton and neutron spin expectation values $\langle S_{p,n} \rangle$ and the total nuclear spin J [41], rather than a simple A^2 enhancement, with the nuclear response encoded in the SD structure function/form factor [42, 43]. The exclusion curves shown later in Fig. 1.5 represent 90% confidence upper limits on σ_N^{SI} (or σ_N^{SD}) obtained

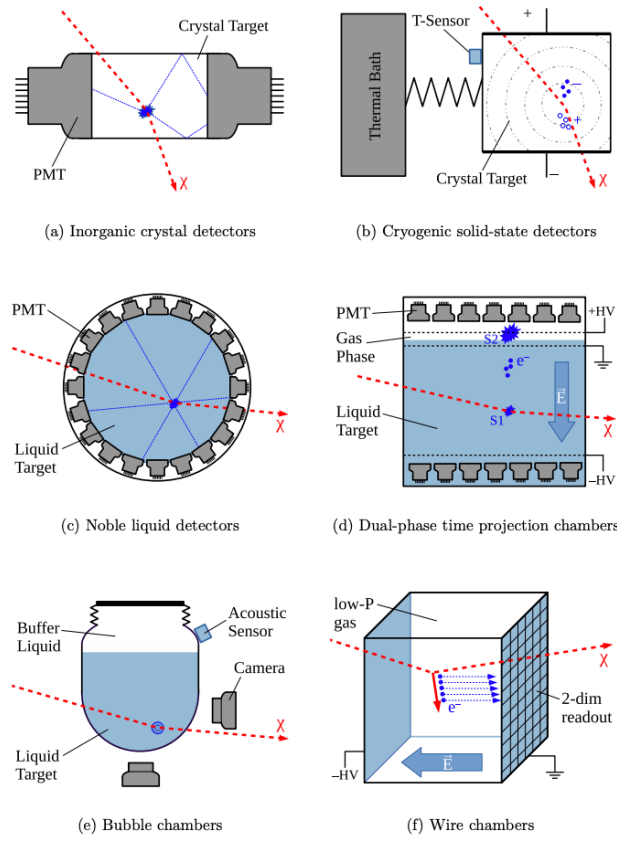


Figure 1.4: Representative classes of direct-detection experiments and their target media. Techniques include (a) scintillating crystal detectors, (b) cryogenic solid-state detectors, (c) single-phase noble-liquid detectors, (d) dual-phase time-projection chambers, (e) bubble chambers, and (f) low-pressure gas TPCs. Each aims to identify scatters from a hypothetical dark-matter particle χ (red dashed line) through some combination of ionisation, scintillation, or phonon readout. Fig. from [2].

by fitting the recoil rate of Eq. (1.8) under the Standard Halo Model. At low WIMP masses, sensitivity falls steeply as $v_{\min}$ approaches the tail of the velocity distribution, while at high masses the rate scales as $1/m_\chi$, producing the characteristic U-shaped behaviour. Finite-size effects through $F^2(E_R)$ suppress the high-energy tail, and as experiments approach the so-called “neutrino floor,” coherent neutrino–nucleus scattering defines the discovery limit [44].

Experimental landscape

The essential observables—ionisation, scintillation, and phonon production—span complementary regions of parameter space. Phonon readouts excel for light-mass candidates ($m_\chi \lesssim 1$ GeV), while ionisation and scintillation dominate at higher masses up to the TeV scale. Across all technologies, present experiments now approach cross-section sensitivities near $6 \times 10^{-48} \text{ cm}^2$ at $m_\chi \sim 30$ GeV, excluding large regions of supersymmetric parameter space. Next-generation instruments such as SUPERCDMS SNOLAB, Skipper-CCDs, and extended xenon and argon detectors will probe deeper into the sub-GeV regime via electron-recoil and phonon-assisted channels, pushing direct detection toward the neutrino fog. Together with collider and indirect probes, these efforts form the triad of complementary search frontiers introduced in Fig. 1.3, constraining the mass, couplings, and interaction dynamics of the dark sector.

1.4 On the Horizon for Dark Matter Searches

Over the past two decades, dark-matter searches have shifted from exploration to precision. Across the collider, indirect, and direct frontiers, sensitivities now exclude large regions once favoured for canonical WIMPs and beyond, while technological advances - from quantum-sensor readouts at eV scales to ultra-quiet cryogenic and noble-liquid detectors - have broadened discovery reach. Given this thesis's focus on direct detection for $m_\chi \sim GeV - TeV$ (traditionally associated with WIMPs), the present multi-experiment projections and xenon “neutrino-fog” contours are succinctly summarised in figure 1.5.

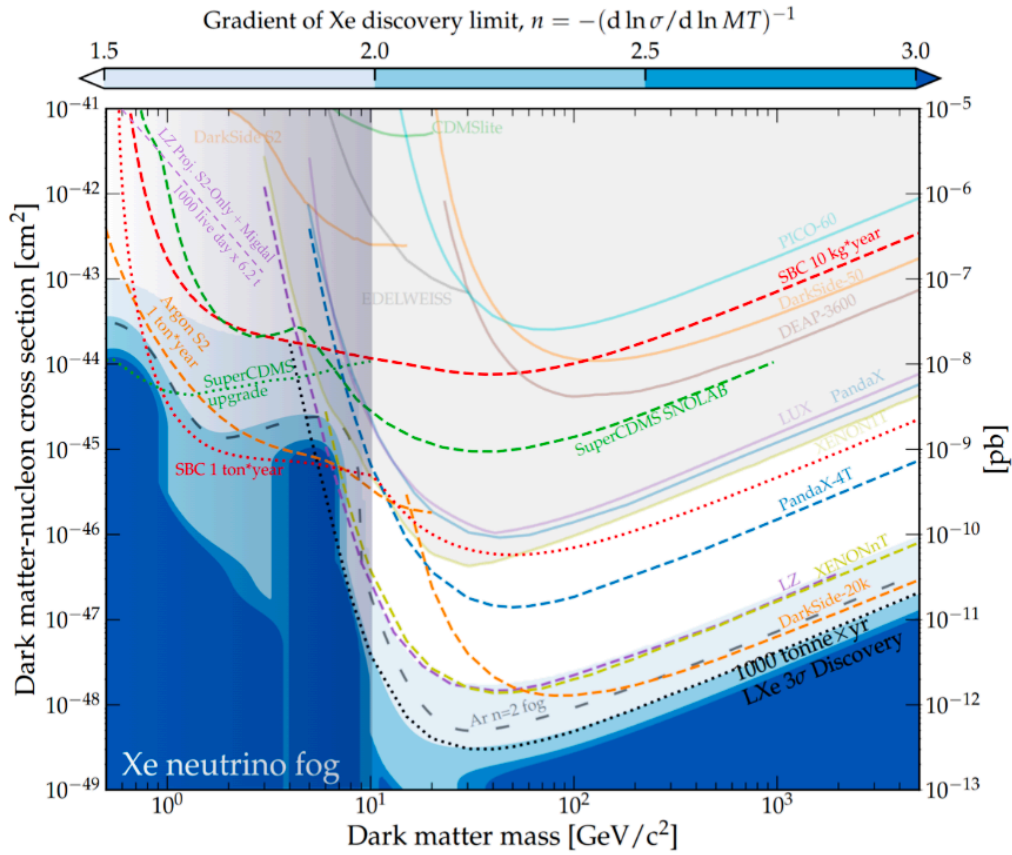


Figure 1.5: Spin-independent dark-matter–nucleon cross section projections versus mass modified from the most recent Snow-mass direct detection review (2021) [45]. Parameter space excluded (all results up to 2021) is shaded grey; dashed curves show projected 90% CL sensitivities from upcoming experimental exposures. The blue contours indicate the xenon “neutrino fog”. The figure has been modified with a magenta dashed line (top-left corner) for the LZ S2-only + Migdal projected sensitivity [46], evaluated for an exposure of $17 t \cdot yr$. The shaded band identifies the sub- GeV region, where cryogenic solid-state detectors (especially SuperCDMS) are particularly competitive. Comparisons between curves should be made with care, as statistical treatments and target media differ across experiments.

Within direct detection, coherent-neutrino backgrounds are no longer viewed as a hard discovery floor, but instead as a sensitivity regime that transitions from being statistics-limited to systematics-limited as exposure increases [47]. At the boundary where statistical and systematic uncertainties become comparable (corresponding approximately to the $n = 2.0$ contour in Fig. 1.5), further improvement is driven primarily by control of neutrino-flux systematics rather than by additional exposure. With sufficiently well-constrained systematics, spectral, timing, and prospectively

directional information can still be used to discriminate signal from background. At sub- GeV masses, ionisation-only searches in noble-liquid TPCs compete with cryogenic solid-state experiments such as SuperCDMS [34, 45]. Longer exposures in xenon TPCs also enable analyses that exploit the Migdal effect [48] - where a nuclear recoil can occasionally unbind an atomic electron; although rare ($\lesssim 10^{-5}$ per recoil) and not yet observed in a dark-matter context, the resulting electronic recoil is detectable and extends reach into the $MeV - GeV$ regime (as demonstrated by the preliminary LZ S2-only + Migdal projection in Fig. 1.5 [46]).

Taken together, the field is maturing while expanding its discovery space. Multi-tonne xenon TPCs (LZ [49], XENONnT [50], PandaX-4T [51]) set the current benchmark, and community roadmaps (Snowmass [45]; APPEC [52]) motivate next-generation observatories such as XLZD [53] to push closer to the neutrino fog. The next chapter turns to LUX-ZEPLIN (LZ), where these developments cohere in a single, exquisitely sensitive instrument.

2

The LUX-ZEPLIN Experiment

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THE LUX-ZEPLIN (LZ) EXPERIMENT defines the state of the art in direct dark-matter detection. Operating at the 4850 *ft* level (≈ 1.5 *km* underground) in the Davis Cavern at the Sanford Underground Research Facility (SURF)¹, LZ is the culmination of decades of dual-phase xenon TPC technology development, combining ultra-low-background materials, a large self-shielding target, and refined signal-background discrimination capabilities. In its first WIMP search, LZ achieved unprecedented sensitivity to the spin-independent WIMP-nucleon cross-section of $9.2 \times 10^{-48} \text{ cm}^2$ after only ~ 60 live days [36]. In the latest combined WIMP search, world-leading constraints were set for masses $\geq 9 \text{ GeV}/c^2$, reaching a minimum excluded cross-section of $2.2 \times 10^{-48} \text{ cm}^2$ and a best median sensitivity of $5.1 \times 10^{-48} \text{ cm}^2$ at $40 \text{ GeV}/c^2$ [49]. Over its planned 1000 live days, LZ is projected to reach a sensitivity of $1.6 \times 10^{-48} \text{ cm}^2$ to the spin-independent WIMP-nucleon interaction at $40 \text{ GeV}/c^2$ [55], extending its reach even further, deep into uncharted parameter space. This regime is visualised in Fig. 2.1. The same low-background, high-resolution environment also supports a broad physics programme [55–58] - including neutrinoless double-beta decay ($0\nu\beta\beta$) [56] and sensitivity to solar ^8B neutrino interactions - pushing toward penetrating the “neutrino fog”,

¹SURF is located in the Homestake mine, the largest and deepest gold mine in the Western Hemisphere, and the site of the Homestake solar-neutrino experiment. It also hosted LZ’s predecessor, LUX (2012-2016) [54]

a challenging regime where signal and background become increasingly hard to distinguish [45].

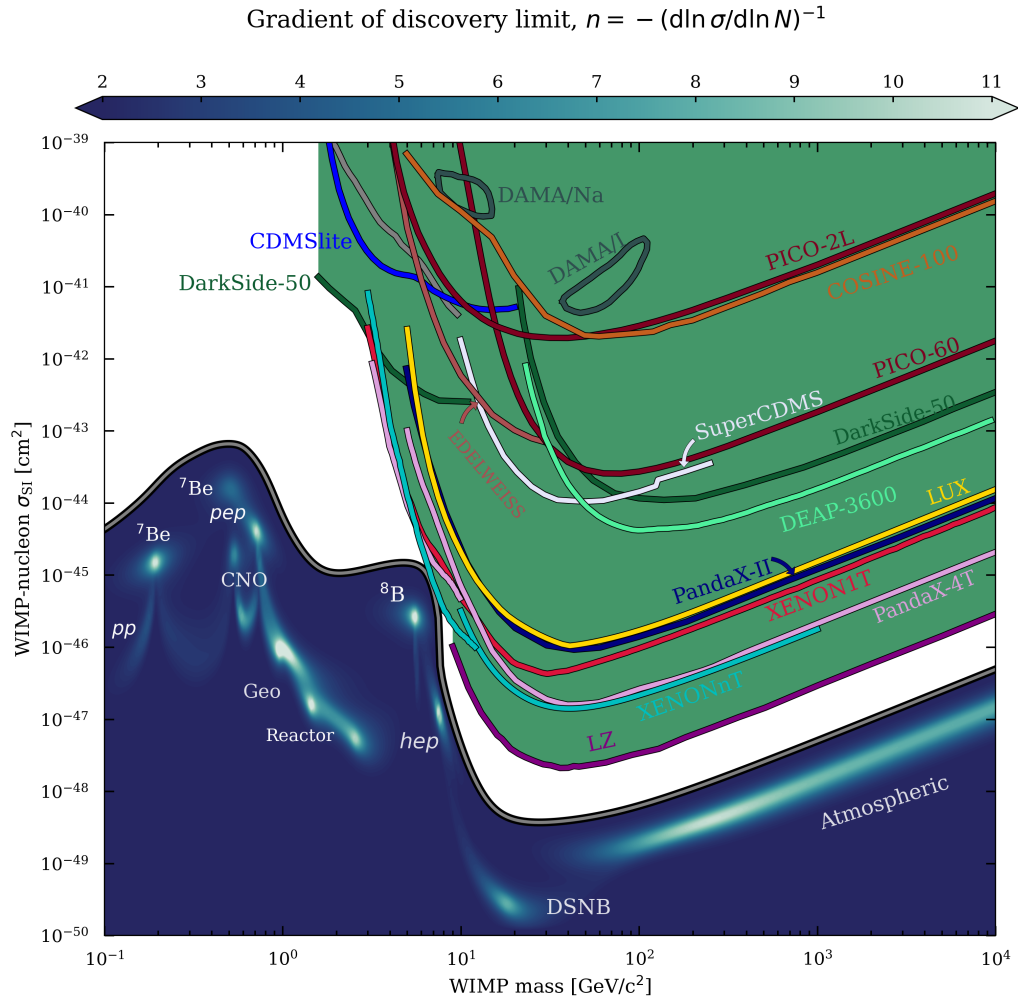


Figure 2.1: Spin-independent WIMP–nucleon cross-section limits (90% CL) as a function of WIMP mass. Recent results from XENONnT [59] and PandaX-4T [60] approach the ^8B solar–neutrino region, effectively skimming the onset of the “neutrino fog” where discovery sensitivity is governed by coherent neutrino scattering. LZ sets the leading constraints above $\sim 9 \text{ GeV}/c^2$, and parameter space excluded by complementary searches from argon, cryogenic semiconductors, and bubble chambers are also blocked out in green. The heatmap indicates the irreducible neutrino background that sets the so-called “neutrino fog,” with the colour bar showing the local slope of the discovery limit $n = -(d \ln \sigma / d \ln N)^{-1}$. Fig. reproduced using code from [61].

LZ’s sensitivities and limits are obtained with a frequentist two-sided profile-likelihood-ratio (PLR) framework evaluated in the corrected signal space of prompt scintillation and ionisation, (S_{1c}, S_{2c}) [36, 49, 62, 63]. This construction exploits xenon’s ability to distinguish electron recoils (ER) from nuclear recoils (NR)². Signal and background probability densities are built from detailed Monte Carlo and a tuned detector-response model; component normalisations are set by expected rates after selections, and nuisance parameters encode uncertainties in yields, efficiencies, and background contributions under external constraints. A scan over WIMP masses and cross-section hypotheses defines the 90% CL exclusion and the median expected sensitivity.

²Formal definitions and the underlying microphysics follow in §2.2; here we use the terms only to indicate the two populations separated by (S_{1c}, S_{2c}) , which will also be discussed at length.

The relevance here is straightforward: a powerful statistical engine only delivers credible results when its ingredients are trustworthy. Robust background models require a deep understanding of how a dual-phase TPC forms and reconstructs signals - fields, transport, gain, and calibrations - and that is precisely the focus of this chapter. We therefore survey the detector subsystems, operating principles, and analysis frameworks that underpin these results and set the stage for what follows. The subsequent chapters then turn to a single, pervasive ingredient, the electric field, which runs through the detector's behaviour like a quiet current, guiding charge, shaping signals, paving the way from design choices to discovery.

2.1 The LUX-ZEPLIN Time Projection Chamber

At the heart of LZ lies a dual-phase xenon Time Projection Chamber (TPC), the central instrument that converts faint particle interactions into measurable observables. Containing 7.7 t of liquid xenon in a cylinder 145.6 cm in both height and diameter [58], the TPC is suspended inside an ultra-radiopure titanium inner cryostat vessel (ICV) and enclosed by a vacuum-insulated outer cryostat vessel (OCV) that holds the detector near 175 K [36]. Between the field cage and the ICV wall sits the instrumented xenon “skin”, an active layer that rejects gammas and neutron activity from the detector's intrinsic radioactivity and also serves mechanical/HV roles (developed further in Chapters 4 and 6). Outside the cryostats, the near-hermetic Outer Detector (OD) surrounds the OCV with ten acrylic tanks containing $\approx 17.3\text{ t}$ of Gd -loaded liquid scintillator: thermalised neutrons capture predominantly on gadolinium, releasing a $7.9 - 8.5\text{ MeV}$ γ -cascade, while $5 - 10\%$ also capture on hydrogen yielding a single 2.2 MeV γ [64]. The system thus achieves $> 88\%$ neutron-tagging efficiency [65], efficiently rejecting a background which can otherwise masquerade as a WIMP interaction in the TPC. OD scintillation is viewed by 120 inward-facing 8” Hamamatsu R5912 PMTs on 20 ladders, with Tyvek lining to boost light collection, all submerged, together with the cryostat [58, 66], in the SURF Davis Campus water tank instrumented to moderate and tag residual gammas and neutrons.

Finally, underneath these layers of shielding, the field cage sets the electrostatic environment for transport with three fine stainless-steel woven-mesh electrodes - the cathode, gate, and anode - defining a 145.6 cm drift region (cathode-gate) and a precisely spaced 13 mm extraction region (5 mm of liquid above the gate and 8 mm of gas above the surface) [58]. Interlocking PTFE pieces form the TPC walls; with $> 97\%$ reflectivity at xenon-scintillation wavelengths [58, 67], this structure maximises photon collection toward the photosensor planes,³ while embedded titanium field-shaping rings linked by a resistive ladder preserve linearity at the boundaries. Two arrays of 3” Hamamatsu R11410-22 PMTs [68] (253 above and 241 below) observe the active xenon volume; level sensors near the extraction region can be used to gauge the surface and its alignment at the sub-millimetre scale; thermometers on the ICV and PMT structures track gradients; and loop antennae on the PMT trusses monitor transient electrostatic discharges [58]. The high-voltage (HV) configuration, electrode tolerances, and field-uniformity considerations are detailed in Chapter 4.

Together these elements realise a single, precisely tuned instrument: optically efficient, electrically uniform, and shielded at every boundary. Next, we outline how S_1 (prompt scintillation channel) and S_2 signals (ionisation/ secondary scintillation channel), in complementary strokes, render the detector's image of an interaction.

³PTFE's role runs deeper than optics: Chapter 4 examines how surface charge transport and trapping on PTFE subtly reshape bulk fields and influence charge drift.

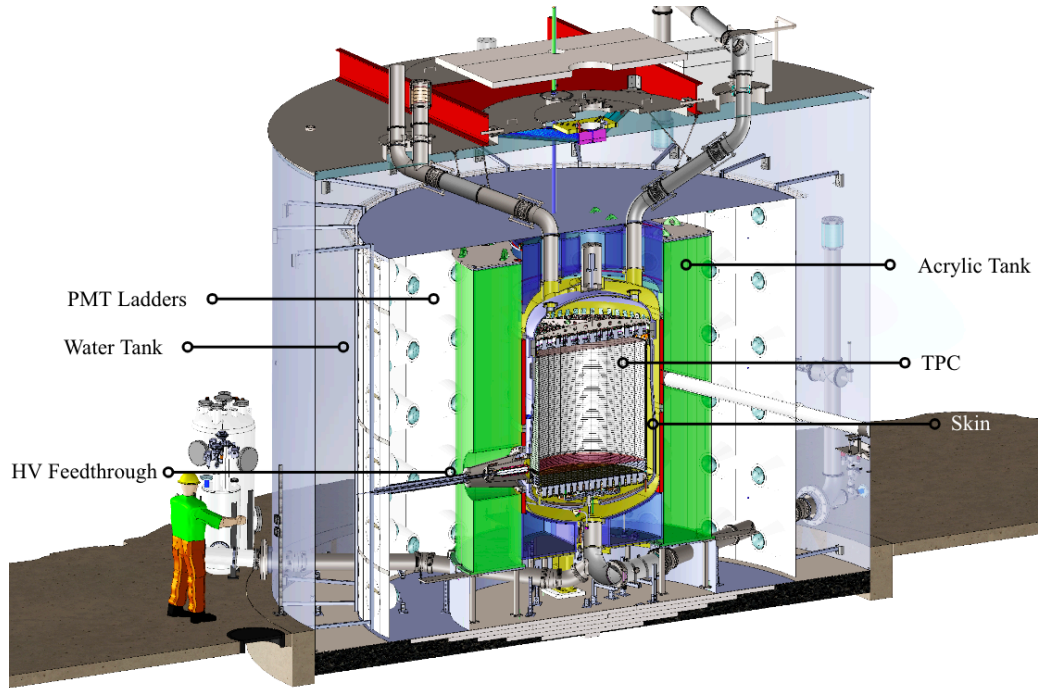


Figure 2.2: Cutaway rendering of the LZ detector. The LZ TPC, skin, OCV and GdLS-filled acrylic tanks are all shown submerged within the water tank. The deuterium–deuterium (DD) neutron-generator conduit, cable feedthroughs, and a glimpse of the calibration-source deployment (CSD) hardware are also visible showcasing the complexity of LZ’s subsystems.

2.2 Recombination and Interactions in Xenon

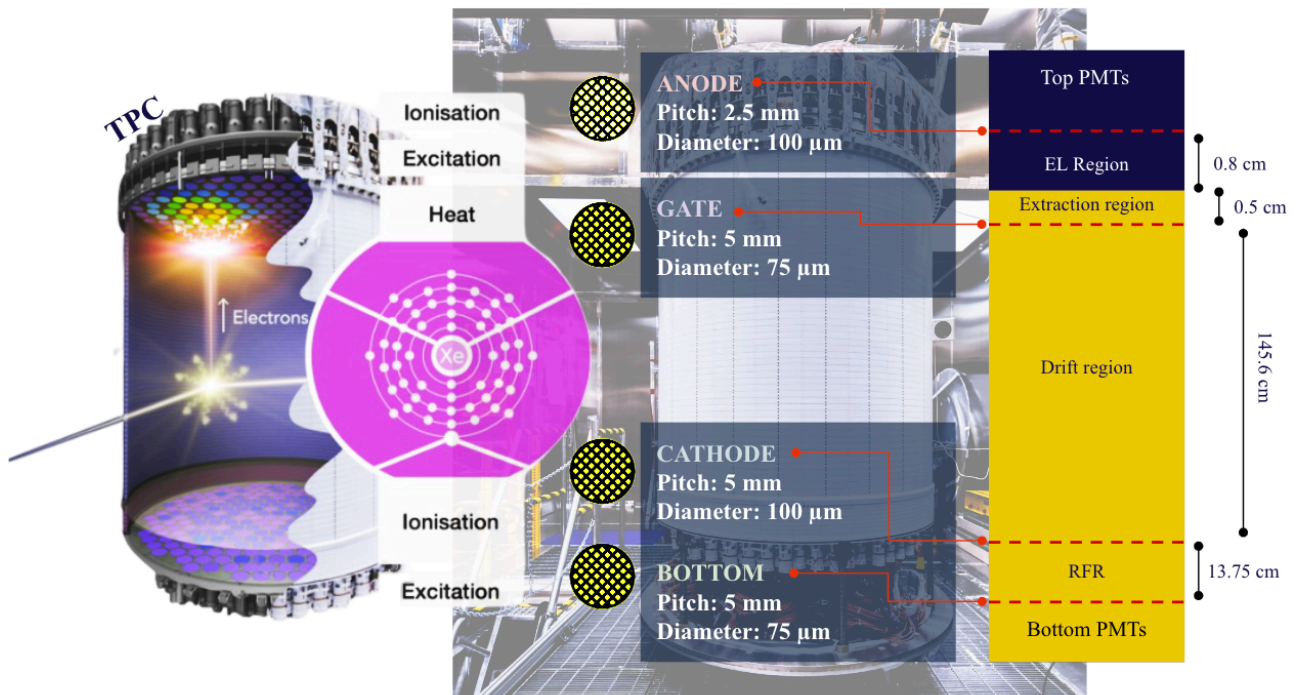


Figure 2.3: Schematic of the LZ TPC. The detector volume is bound by four electrostatic grids - anode, gate, cathode, and bottom - defining distinct field regions for drift, extraction, and electroluminescence (EL) in the gas. The cartoon visualises the scintillation and ionisation processes that occur when a particle interacts with the LXe bulk. Important dimensions are also labelled

When a particle interacts in liquid xenon, its deposited energy produces both excited and ionised atoms (with some energy dissipated as heat). Interactions with atomic electrons are termed electronic recoils (ERs), while elastic scatters on xenon nuclei are termed nuclear recoils (NRs). In WIMP searches, NRs are considered signal-like, whereas ERs are typically background-like. Excited atoms promptly form *excimers*⁴, yielding the primary scintillation signal (S_1), while ionisation electrons may either recombine locally or drift in the local field to form the secondary electroluminescence signal (S_2). The relative fraction of quanta partitioned into light and charge is described by the recombination probability $r(E)$, which depends on the local electric field and ionisation density (§4.2.2). A useful way to characterise the initial quanta is via the exciton–ion ratio $k \equiv N_{\text{ex}}/N_i$; in LXe, ERs have $k_{\text{ER}} \simeq 0.06$ [69], while NRs exhibit much larger k ($\mathcal{O}(\sim 1)$) [70]. This difference, together with nuclear-stopping losses encoded by the Lindhard factor for NRs $\mathcal{L}$, underpins the distinct S_2/S_1 response of ER and NR populations. In practice, $r(E)$ sets the field-dependent light and charge yields,

$$L_y = \frac{n_\gamma}{E}, \quad Q_y = \frac{n_e}{E}, \quad (2.1)$$

with n_γ and n_e the numbers of observable photons and electrons per unit deposited energy. A detailed discussion of the microscopic recombination mechanisms and their E -dependence is deferred to Chapter 4. Here we summarise how these quanta manifest as the measurable S_1 and S_2 channels in a dual-phase TPC. We begin with primary scintillation.

2.2.1 Primary Scintillation (S_1)

When an interaction deposits energy in xenon, it creates both excitations and ionisations [71]. Primary scintillation arises when short-lived xenon excimers (Xe_2^*) decay and emit VUV photons at ~ 175 nm. Two microscopic channels feed these excimers: (i) direct electronic excitation, and (ii) ionisation followed by electron–ion recombination. The total photon yield is [71]

$$N_\gamma = N_{\text{ex}} + r(E) N_i,$$

with N_{ex} excitons, N_i ion pairs, and $r(E)$ the field-dependent recombination probability. We denote electronically excited atoms by the superscript $(*)$ and vibrationally excited dimers by (ν) . The sequence of reactions in each channel is listed in Table 2.1.

Emission then proceeds via singlet $^1\Sigma_u^+$ and triplet $^3\Sigma_u^+$ excimer states with characteristic lifetimes of ~ 3 ns and $\sim 20 - 30$ ns, respectively; a field-dependent recombination component adds a slower tail. The convolution of these timescales produces the characteristic S_1 waveform [73] - a prompt, slightly skewed peak with an exponential-like tail. In dual-phase xenon TPCs the temporal overlap of components renders S_1 -only pulse-shape discrimination (PSD) comparatively weak, so ER/NR separation relies primarily on the S_2 – S_1 anti-correlation set by $r(E)$ and N_{ex}/N_i . By contrast, dual-phase argon TPCs exploit the much larger singlet–triplet separation to achieve strong PSD [74]. It is also emphasised that the amount of recombination is strongly dependent on the applied external electric field and the surrounding ionisation density [72]; with a higher field, the recombination probability decreases. The implications of this concept is explored further in Chapter 4.

⁴a molecule that is strongly bound in an excited state but normally has a dissociative ground state, with the excited state having a very short lifetime

Table 2.1: Microscopic pathways leading to S1 scintillation in liquid xenon [72] initiated by an electron (or ER).

Pathway 1: Direct excitation → excimer formation → vibrational relaxation → VUV		
Equations	$e^- + \text{Xe} \rightarrow \text{Xe}^* + e^-$	(impact excitation)
	$\text{Xe}^* + \text{Xe} \rightarrow \text{Xe}_2^*$	(excimer formation)
	$\text{Xe}_2^* + \text{Xe} \rightarrow \text{Xe}_2^* + \text{Xe}$	(vibrational relaxation)
	$\text{Xe}_2^*(s/t) \rightarrow \text{Xe} + \text{Xe} + \gamma (175 \text{ nm})$	(VUV emission)
Pathway 2: Ionisation → recombination → excimer formation → relaxation → VUV		
Equations	$e^- + \text{Xe} \rightarrow \text{Xe}^+ + e^- + e^-$	(impact ionisation)
	$\text{Xe}^+ + \text{Xe} + \text{Xe} \rightarrow \text{Xe}_2^+ + \text{Xe}$	(three-body molecular-ion formation)
	$e^- + \text{Xe}_2^+ \rightarrow \text{Xe}^{**} + \text{Xe}$	(dissociative recombination)
	$\text{Xe}^{**} + \text{Xe} \rightarrow \text{Xe}^* + \text{Xe} + \text{heat}$	(electronic/vibrational relaxation)
	$\text{Xe}^* + \text{Xe} + \text{Xe} \rightarrow \text{Xe}_2^* + \text{Xe} + \text{heat}$	(excimer formation + relaxation)
	$\text{Xe}_2^* \rightarrow \text{Xe} + \text{Xe} + \gamma (175 \text{ nm})$	(VUV emission)

2.2.2 Secondary Scintillation (S_2)

Ionised electrons that avoid recombination drift to the liquid–gas interface and, once extracted into gaseous xenon, are accelerated between the gate and anode. Collisions excite xenon atoms and dimers (Xe_2^*) that decay producing the proportional-scintillation signal S_2 .

For a single extracted electron traversing a gas gap of thickness h_g , the total proportional-scintillation yield (photons per electron) in saturated xenon vapour at cryogenic temperature is

$$N_{EL}^{e^-} = L_y = \left[(144 \pm 7) \frac{E_g}{P_g} - (136 \pm 11) \right] h_g P_g, \quad (2.2)$$

with E_g in $\text{kV}, \text{cm}^{-1}$, P_g in bar, and h_g in cm. These coefficients are from a recent re-fit to cryogenic, saturated-vapour data⁵.

The observed S_2 waveform is typically a $\mathcal{O}(\sim \mu\text{s})$ wide with an approximately Gaussian envelope: longitudinal diffusion during drift sets the core width, while small non-uniformities near the surface and occasional delayed emission at the interface can introduce slight asymmetry or low-amplitude tails; the electron transit time across h_g adds only a minor additional spread. The high electroluminescence yield in the gas phase, together with the stable and well-defined S_2 pulse shape, enables accurate (x, y) position reconstruction from the light pattern observed in the top PMT array and allows interactions producing only a small number of extracted electrons to be detected.

2.2.3 Corrected Signal Yields

Finally, the observed S_1 and S_2 signals are measured in units of photons detected (phd), calibrated according to the single-photoelectron response of each PMT [58, 75]. To remove position-dependent effects in light collection and

⁵see Appendix A for the dataset, method, and comparison to room-temperature fits.

extraction efficiency, they are corrected to their central-equivalent values as

$$S_{1c} = C_1(x, y, z) S_1, \quad S_{2c} = e^{t/\tau_e} C_2(x, y) S_2, \quad (2.3)$$

where C_1 and C_2 are empirical correction maps derived from dedicated calibration campaigns normalised to unity at the detector center ($x = 0, y = 0$), with the S_1 correction additionally referenced to the geometric center in z , and the S_2 correction referenced to the point of minimum drift time at the gate [36], t is the drift time and τ_e is the electron lifetime in liquid xenon. The corrected signals are related to the underlying numbers of emitted quanta, n_γ and n_e , through

$$S_{1c} = g_1 n_\gamma, \quad S_{2c} = g_2 n_e, \quad (2.4)$$

with g_1 the photon detection efficiency and $g_2 = \epsilon_e N_{\text{EL}}^{\text{GXe}} g_1^{\text{GXe}}$ the effective charge gain, incorporating the electron extraction efficiency ϵ_e , the electroluminescence yield $N_{\text{EL}}^{\text{GXe}}$, and the photon detection efficiency for light generated in the gas phase g_1^{GXe} .

Using these detector parameters, the total reconstructed energy can be written as

$$E = W \left(\frac{S_{1c}}{g_1} + \frac{S_{2c}}{g_2} \right), \quad (2.5)$$

where $W = 13.7$ eV [70] is the average work to produce a scintillation photon or an ionisation electron in xenon. For nuclear recoils, this expression must be modified by a Lindhard quenching factor such that

$$E^{\text{NR}} = \frac{W}{L(E^{\text{NR}})} \left(\frac{S_{1c}}{g_1} + \frac{S_{2c}}{g_2} \right), \quad (2.6)$$

reflecting the reduced fraction of energy partitioned into detectable quanta.

2.2.4 The Case for Liquid Xenon

Liquid xenon (LXe) has established itself as an excellent target for rare-event searches due to the conjunction of favourable nuclear, electronic, and operational properties. Its large atomic and mass numbers ($Z = 54$, $A \simeq 131$) provide strong coherent enhancement of the spin-independent WIMP–nucleon cross section, while the odd-neutron isotopes ^{129}Xe and ^{131}Xe ensure sensitivity to spin-dependent couplings [58]. Xenon’s isotopic composition also supports a broader programme in rare-event physics: in particular, ^{136}Xe is a leading isotope for neutrinoless double-beta decay ($0\nu\beta\beta$) searches [56, 76–78], with enrichment and deployment feasible within the same dual-phase TPC framework.

SELF-SHIELDING AND ATTENUATION

A key advantage of xenon is its high density ($\rho \simeq 3.0$ g cm $^{-3}$), which yields strong attenuation of external radiation. Photons of $\mathcal{O}(100)$ keV undergo photoelectric absorption within $\lesssim 1$ mm [58, 79], while higher-energy γ rays undergo Compton scattering on length scales of only a few centimetres [58]. Electrons are even more strongly contained, typically travelling < 1 cm before losing energy through collisions and bremsstrahlung [80, 81]. This pronounced self-shielding ensures that the inner detector volume can be rendered extremely quiet once an outer “skin” region is

excluded and a fiducial volume defined, enabling multi-tonne xenon TPCs to achieve backgrounds limited primarily by intrinsic or cosmogenic sources.

SIGNAL GENERATION AND ER/NR DISCRIMINATION

Xenon is both a bright scintillator and an efficient ioniser, with a scintillation yield of 63 photons per keV [82]. Interactions produce prompt VUV photons at $\sim 175\text{ nm}$ and ionisation electrons that drift over metre-scale lengths under fields of $\mathcal{O}(0.1 - 1)\text{ kV cm}^{-1}$ [36]. The recoil-type dependence of quanta partitioning between excitation and ionisation results in distinct S_2/S_1 distributions for electronic and nuclear recoils; analyses routinely achieve $> 99.5\%$ ER rejection in the WIMP region of interest at $\sim 50\%$ NR acceptance [36, 83].

HIGH-VOLTAGE COMPATIBILITY

Operational characteristics also favour xenon. LXe is chemically inert and compatible with continuous purification to part-per-trillion impurity levels; its boiling point (165 K at 1 atm) permits stable cryogenic operation with a robust vapour-liquid equilibrium, essential for maintaining a controlled extraction region. The dielectric constant of LXe ($\epsilon \simeq 1.85 - 1.96$ [84]) is closely matched to that of PTFE ($\epsilon \simeq 2.1$), the standard reflective field-cage material. This dielectric compatibility reduces field discontinuities at boundaries, mitigates localised regions of stress, and thereby protects the high-voltage system against breakdown. Together with xenon’s high intrinsic dielectric strength, these properties enable sustained dual-phase operation at tens of kilovolts without frequent sparking or gas discharge.

In aggregate, LXe offers great sensitivity to spin-independent scattering, robust ER/NR discrimination via S_2/S_1 , excellent self-shielding, favourable high-voltage behaviour due to dielectric matching and high breakdown strength, and versatility for additional rare-event programmes such as $0\nu\beta\beta$. LAr delivers unmatched economy and PSD-based background rejection, albeit with reduced self-shielding, intrinsic ^{39}Ar backgrounds, and lower spin-independent kinematic reach. The two media are therefore complementary, with xenon presently setting benchmark sensitivities for nuclear-recoil dark-matter searches.

2.3 Backgrounds

Achieving an unambiguous dark-matter measurement requires stringent control and modelling of detector backgrounds. In LZ, the detector design and material selection were driven by radiopurity; during operation, residual sources are constrained with component assays, in-situ tags (e.g. flow-state/radon), calibration data, and Monte Carlo within a global likelihood. Table 2.2 summarises dominant components for WS 2022 ($0.9\text{ t} \cdot \text{yr}$) and WS 2024 ($3.3\text{ t} \cdot \text{yr}$), showing the pre-fit constraints and post-fit yields. The subsections that follow provide a brief, targeted “birds-eye picture” of each dominant background class; comprehensive treatments are available in [85]. A discussion of accidental backgrounds is deferred to Chapter 5.

Table 2.2: Comparison of expected and best-fit counts for the principal background sources in the two LZ WIMP search datasets. WS 2022 [36] corresponds to an exposure of 0.9 t·yr (60 live days), and WS 2024 [49] to 3.3 t·yr (220 live days). Pre-fit expectations are derived from material assays, calibration tags, and Monte Carlo inputs, while the fit results reflect the posterior estimates from the global likelihood including all control samples.

Source	WS 2022 (0.9 t·yr, 60 days)		WS 2024 (3.3 t·yr, 220 days)	
	Expected	Fit Result	Expected	Fit Result
β decays + det. ER	215 ± 36	222 ± 16	743 ± 88	733 ± 34
Solar ν ER	27.1 ± 1.6	27.2 ± 1.6	102 ± 6	102 ± 6
^{127}Xe EC	9.2 ± 0.8	9.3 ± 0.8	3.2 ± 0.6	2.7 ± 0.6
^{124}Xe DEC	5.0 ± 1.4	5.2 ± 1.4	19.4 ± 2.5	20.4 ± 2.4
^{136}Xe $2\nu\beta\beta$	15.1 ± 2.4	15.2 ± 2.4	55.6 ± 8.3	55.9 ± 8.2
^8B CE ν NS / ν NRs	0.14 ± 0.01	0.15 ± 0.01	0.06 ± 0.01	0.06 ± 0.01
Accidental coincidences	1.2 ± 0.3	1.2 ± 0.3	2.8 ± 0.6	2.6 ± 0.6
Detector neutrons ^a	$0.0^{+0.2}_{-0.0}$	$0.0^{+0.2}_{-0.0}$	$0.0^{+0.2}_{-0.0}$	$0.0^{+0.2}_{-0.0}$
WIMP signal	—	$0.0^{+0.6}_{-0.0}$	—	$0.0^{+0.6}_{-0.0}$
Total	273 ± 36	280 ± 16	1210 ± 91	1202 ± 41

^a Neutron expectations derived from veto-tagged samples and profiled as nuisance parameters in the likelihood, not added as standalone counts.

2.3.1 Cosmogenic

Cosmogenic backgrounds in deep-underground detectors arise from (i) activation of detector or shielding materials during above-ground exposure and (ii) residual muon-induced interactions at depth. In LZ’s LXe bulk, the principal cosmogenic isotopes are ^{127}Xe and ^{37}Ar , produced via spallation while the xenon is stored, purified, or transported on the surface [85]. These decay via X-rays and Auger electrons in the keV range (with lines at ~ 1.2 , 5, and 33 keV for ^{127}Xe) and can intrude into the WIMP ROI. An additional external component⁶ arises from gamma rays emitted by radioisotopes in the cavern walls; these have been characterised in situ in the Davis Cavern with a sodium-iodide detector [86].

Depth provides substantial protection. The muon flux measured in the Davis Cavern is $(5.31 \pm 0.17) \times 10^{-9} \text{ cm}^{-2} \text{ s}^{-1}$ [87], suggesting a $\sim 10^6$ reduction relative to surface rates. Residual muons that do penetrate can still produce neutrons, gamma rays, and spallation in the surrounding rock, but most are moderated or captured in the water tank and efficiently vetoed by the OD, which tags neutron captures and correlated gamma cascades [36, 58, 85]. Cosmogenic contributions are time-dependent and, after cool-down and vetoing, are subdominant during steady science operation. The residual background budget is then dominated by radiogenics originating from detector materials, shielding, and cavern rock (e.g. $U/Th/K$ decays and (α, n) interactions) [58, 85].

2.3.2 Radiogenic

Radiogenic activity defines the dominant steady-state background in LZ and arises from long-lived isotopes embedded in detector materials as well as trace noble-gas contaminants within the xenon. The principal contributors are the ^{238}U and ^{232}Th decay chains, together with ^{40}K and ^{60}Co [88]. Their γ -ray emissions populate the electron-recoil (ER) band, while spontaneous fission and (α, n) reactions in construction materials generate neutrons that can mimic NR signatures. A comprehensive radioassay programme [58, 89] and the strong self-shielding of liquid xenon suppress

⁶Not cosmogenic, mentioned here for completeness.

these sources to negligible levels in the fiducial volume, though they dominate the high-energy ($> 100 \text{ keV}$) regime.

Within the xenon target, ^{222}Rn (from the ^{238}U decay chain) and its progeny constitute the most persistent intrinsic background. Short-lived daughters such as ^{218}Po , ^{214}Pb and ^{214}Po generate MeV -scale α and β emissions, while long-lived ^{210}Pb ($T_{1/2} = 22 \text{ yr}$) can plate-out on PTFE and electrode surfaces, producing delayed ^{210}Po decays long after emanation has ceased [58, 89]. These progeny are introduced during material exposure to air or during construction, and their subsequent decay on detector boundaries gives rise to distinct α populations on the gate, cathode, and wall. Although α tracks are easily identified, their emission in fluorinated materials can also induce (α, n) reactions, yielding untagged neutrons. Elevated ^{210}Po activity near the PTFE is therefore problematic for low-energy searches: it limits the usable fiducial volume and forms a dominant background for S_2 -only analyses, where cathode events can closely resemble signal-like S_2 s (Chapter 5). At the same time, these well-localised populations offer valuable spatial anchors for position reconstruction and microphysics calibration—helping to map the true detector boundaries and electron-transport response (see Chapters 4 and 5).

Additional diffuse contaminants include ^{85}Kr and ^{39}Ar , both reduced to subdominant levels through gas-phase charcoal chromatography and purification [58]. Together, these internal β emitters, external γ rays, and (α, n) neutrons comprise the radiogenic background budget constrained in the global likelihood fits of WS 2022 and WS 2024 [88].

2.3.3 Physics

Beyond radiogenic and cosmogenic sources, the final class of backgrounds we discuss arises from rare but well-understood Standard Model processes intrinsic to xenon itself. These include the two-neutrino double-beta decay ($2\nu\beta\beta$) of ^{136}Xe and the two-neutrino double electron capture ($2\nu\text{DEC}$) of ^{124}Xe , which contribute a small rate of low-energy, quasi single-site events within the WIMP ROI. The $2\nu\beta\beta$ decay, with a measured half-life of $(2.17 \pm 0.08) \times 10^{21} \text{ yr}$ by KamLAND-Zen [90] and EXO-200 [91], produces a continuous energy spectrum extending to the 2.46 MeV endpoint, while the $2\nu\text{DEC}$ process, observed by XENON1T [92] and LZ [93], releases a few-10 keV of de-excitation energy following electron capture on inner shells.

Neutrinos from solar, atmospheric, and diffuse supernova sources add further irreducible contributions. Elastic ν - e scattering from solar pp , ^7Be , and CNO neutrinos yields low-energy ERs [94], while coherent elastic ν -nucleus scattering ($\text{CE}\nu\text{NS}$) - first observed by the COHERENT collaboration [95] - produces genuine NRs in a domain coincident to that of low-energy WIMPs. In xenon TPCs, $\text{CE}\nu\text{NS}$ from ^8B (and hep) solar neutrinos populates the low-NR region already probed by PandaX-4T [60] and XENONnT [59] and forms a key forthcoming analysis in LZ [94]; at higher energies, $\text{CE}\nu\text{NS}$ from atmospheric and diffuse supernova neutrinos contributes additional, rarer NRs [94]. Accurate modelling of these channels is essential for both the standard $S_1 + S_2$ searches and S_2 -only analyses, ensuring rare Standard Model interactions are cleanly separated from potential signals and enabling LZ to push sensitivity further into the sub- GeV regime. Though subdominant in current datasets, these physics backgrounds underscore LZ's broader reach: the same sensitivity that drives its dark matter search could also enable the study of some of the rarest measurable processes in nature.

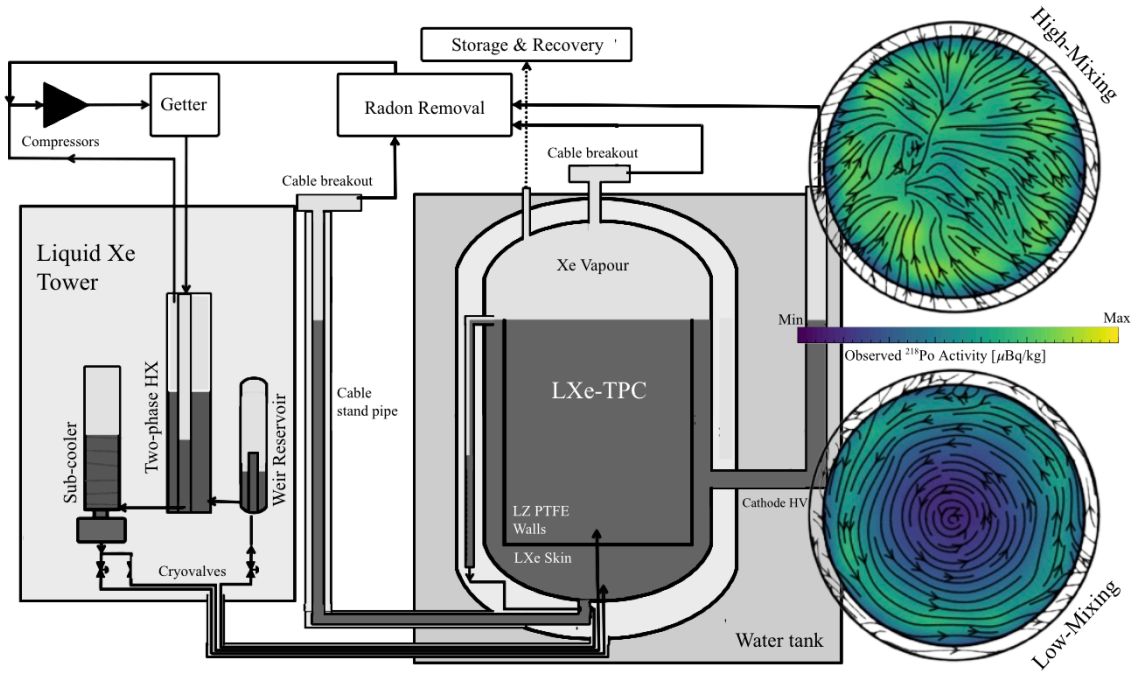


Figure 2.4: (Left) simplified schematic of the online xenon circulation and purification in LZ. Liquid xenon drains via weirs to the LXe tower, is evaporated in a two-phase heat exchanger, purified in a hot zirconium getter (with radon-removal available for gas in the conduits when required), then re-condensed and returned to the cryostat. Adapted from [96]. (Right) reconstructed bulk-flow patterns in two operating states, “high-mixing” and “low-mixing”, inferred from spatial-temporal correlations of ^{222}Rn – ^{218}Po pairs (credit: N. Angelides). Arrows indicate flow direction; the colour scale denotes observed ^{218}Po activity, with annotated panels indicating the mean flow speed.

2.4 Detector Operation and Calibrations

Having set out the principal backgrounds and their controls, we turn to the operational choices that keep the detector quiet and predictable. The full 10-tonne xenon inventory is circulated continuously through the online purification loop (Fig. 2.4): vapour drawn from the surface passed in series through dual hot-zirconium getters, removing non-noble molecular contaminants (O_2 , N_2 , H_2O , CO_2 , CH_4), were re-condensed in the external tower, and returned to the vessel; radon in warm gas lines was mitigated by the in-line radon-reduction system. This maintained electron lifetimes to above 5 ms , ensuring high S_2 -electron survival across the 1.5 m drift and supporting stable charge collection over the run. The same loop governs the liquid hydrodynamics: under a controlled thermal gradient of the returned liquid, the xenon settles into one of two well-defined modes — high-mixing with vigorous vertical convection, or low-mixing with flow largely circular, at least in lower half of the volume. Their imprint appears directly in delayed-coincidence ^{222}Rn – ^{218}Po α maps (Fig. 2.4), which trace convective streamlines and show reduced central activity during low-mixing periods. Small, correlated variations in temperature and pressure accompany these modes and feed through to reconstruction, most visibly the z -mapping; the microphysics is treated in Chapter 3. The same circulation and purification architecture also underwrites the calibration programme: injected sources remain well-mixed and diagnostically useful without compromising WIMP data, and, in practice, their concentrations are driven back towards baseline by continuous circulation and the purification train (e.g. staged CH_3T injections with measured removal on $\sim\text{day}$ timescales).

Calibration campaigns anchor the detector response and supply the position- and time-dependent corrections used throughout this thesis. A summary of a select few calibration sources are provided in table 2.3 [58, 75, 96]. Internal injections such as $^{83\text{m}}\text{Kr}$ and CH_3T homogenise coverage of the central volume: $^{83\text{m}}\text{Kr}$ maps (x, y, z) non-uniformities in S_1 and S_2 , while CH_3T sets the low-energy ER band down to threshold. Deployed sources around the cryostat via the calibration source deployment (CSD) system extend the dynamic range: γ lines (e.g. ^{57}Co , ^{228}Th) probe linearity and inter-detector timing; AmLi , lowered via CSD tubes outside the TPC, provides a broad sub- MeV neutron spectrum ($E_n \lesssim 1.5 \text{ MeV}$) for NR-band characterisation (Fig. 2.5); and a deuterium–deuterium generator delivers monoenergetic 2.45 MeV neutrons, with reflector modes covering mid- and low-energy NRs [58]. Taken together, these data define the ER and NR bands, provide the position-dependent corrections used later, and calibrate the detector response to signal-like (NR) and background-like (ER) interactions. Details of the skin calibration sources and their deployment are given in later in Chapter 4 (§4.8).

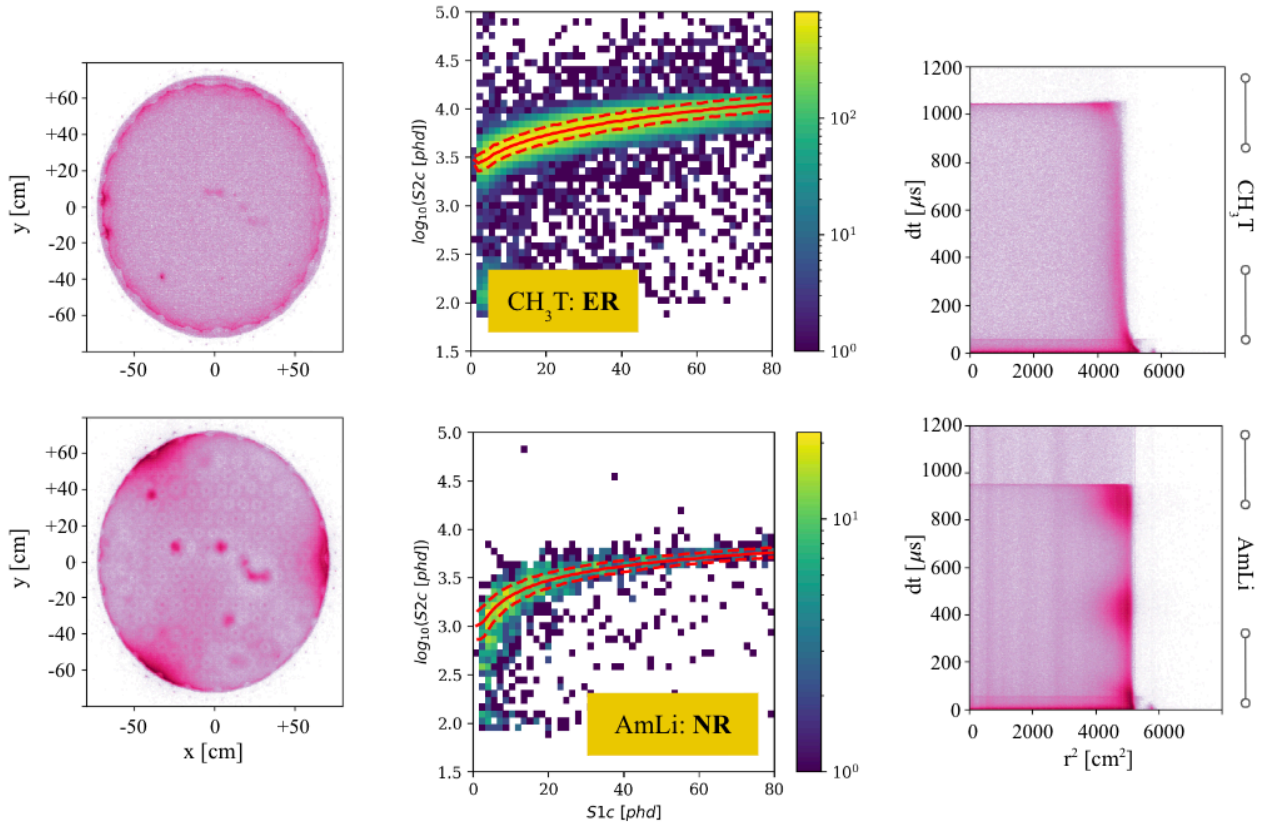


Figure 2.5: Injected vs deployed calibrations. Event distributions for AmLi (bottom) and CH_3T (top): (x, y) maps (left) and r^2 – dt occupancy (right), with the heatmaps/ z representing arbitrary counts. No analysis cuts have been applied to this data. CH_3T is well-mixed across the active volume, while AmLi interactions cluster at the CSD deployment locations. Bright central features coincide with regions beneath off-PMTs. **(Middle)** Finally, we see explicitly how ER and NR bands can be calculated using calibration data (red lines denote the official WS 2024 bands).

2.5 Simulations

Accurate simulation is indispensable to LZ, as it is for most modern physics experiments. The detector’s geometric and material complexity, together with the extremely low expected event rates, precludes an exhaustive first-principles treatment at analysis scale. LZ therefore adopts a modular Monte-Carlo framework in which a high-fidelity geometric

Table 2.3: Selected calibration sources used in LZ (not exhaustive [58, 75, 96]), limited to those relevant for context in this thesis. “CSD” denotes deployment in the vacuum space between the ICV and OCV; “DD” is the external deuterium-deuterium neutron generator.

Category	Source	Interacting particle	Half-life	Purpose
Internal	Tritium (^3H)	β ($Q = 18.6$ keV)	12.3 y	ER band (low energy)
Internal	$^{83\text{m}}\text{Kr}$	32.1 keV γ + 9.4 keV γ	1.83 h	TPC (x, y, z) corrections
Internal	$^{131\text{m}}\text{Xe}$	163.9 keV cascade	11.8 d	TPC (x, y, z) checks
External	^{88}YBe	152 keV n	107 d	Low-energy NRs
External	$^{124}\text{SbBe}$	22.5 keV n	60.2 d	Low-energy NRs
External	DD (direct)	2.45 MeV n	—	NR yields / monoenergetic NRs
CSD	$^{241}\text{AmLi}$	≤ 1.5 MeV n	432 y	Broad NR spectrum; NR band
CSD	$^{241}\text{AmBe}$	≤ 11 MeV n	432 y	NR band / efficiency checks
CSD	^{57}Co	122 keV γ	0.74 y	Skin threshold / low- E reference
CSD	^{22}Na	2×511 keV γ	2.61 y	Detector synchronisation
CSD	^{228}Th	2615 keV γ , etc.	1.91 y	High- E γ scale

model generates energy depositions from putative signals and known backgrounds; these depositions are then mapped, via calibrated microphysics and detector-response models, to the same reduced quantities (RQs) derived from data. In this arrangement, simulations (i) provide forward models for signal hypotheses, (ii) yield background expectations and probability density functions for inference, and (iii) support design, reconstruction, and selection studies under controlled conditions. The simulation chains available within LZ are illustrated in Fig. 2.6. Consistency of formats and calibrations across data and simulation is thus a design requirement rather than a convenience.

2.5.1 NEST

The Noble Element Simulation Technique (NEST) [97] supplies the semi-empirical description of scintillation and ionisation in liquid xenon used throughout LZ [97]. As an ever-evolving package, NEST encodes the dependence of light and charge yields on recoil type, energy, and electric field, and captures *global* behaviour such as the anti-correlation between channels and the field-induced partitioning of quanta (extensively discussed in chapters 4 and 6). These baseline models are subject to targeted re-tuning to reflect the dynamic detector-specific conditions and calibrations throughout LZ’s operation⁷.

2.5.2 Full-Chain Simulations

The full-fidelity workflow begins with BACCARAT [100] (**B**asically **A** Component-Centric Analogue **R**esponse to **A**nyThing), LZ’s GEANT4-based implementation of the as-built geometry and materials. Primary and secondary particles are generated, transported, and their interactions recorded as energy depositions; optical photon ray-tracing and electron transport can then be simulated explicitly in compliance with a detailed manual of microphysics and geometric profiles intrinsic to detector operation and hence, directly feeding into detector response. The resulting hit-level information is further processed by the **D**etector **E**lectronics **R**esponse (DER), which emulates the data-acquisition chain, including photomultiplier response (quantum efficiency, double-photoelectron emission, dark noise, after-pulsing), shaping and digitisation, and trigger behaviour. DER produces output in the same format as raw detector readout, enabling processing by the standard reconstruction (LZAP) to yield RQs directly comparable to data. This

⁷An example is the refinement of scintillation yields presented in appendix A of this thesis. A comprehensive account of LZ-specific updates to NEST-based inputs and their propagation into LZ’s own custom GEANT-4 [98, 99] package (BACCARAT) [100] and varying operation configurations will be provided in an upcoming thesis by N. Fieldhouse (Oxford).

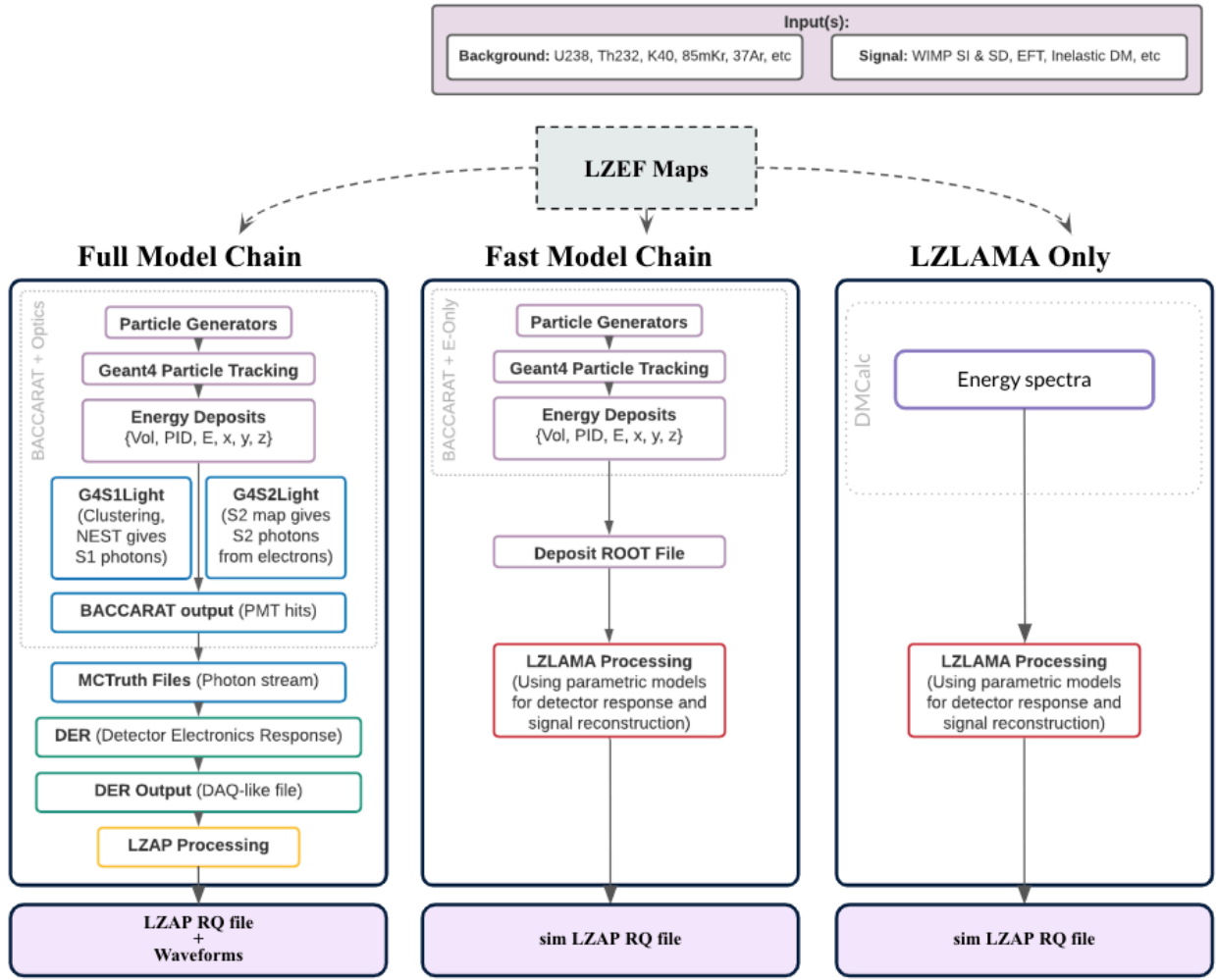


Figure 2.6: LZ’s custom simulation framework is extensive; the diagram illustrates the various pathways and their respective outputs. The LZEF field maps discussed in §4 can be used as an input to any one of these chains, constituting a fundamental piece of the complete detector response modelling puzzle within LZ.

chain maximises realism at substantial computational cost and is reserved for studies requiring waveform-level fidelity (as is the case for validations or tuning of fundamental physics parameters like those employed within NEST or to diagnose/ reproduce the topologies of pathological events) or detailed optical systematics.

2.5.3 Fast-Chain Simulations

For large-volume production, LZ also employs a fast workflow. BACCARAT [100] is run to the stage of recording energy depositions in active volumes; these depositions are then converted to light and charge quanta using NEST and passed to LZLAMA (**LZ** Light Analysis Monte-Carlo Application), which applies a parameterised detector-response model to produce RQs without explicit optical photon tracking or full electronics waveform synthesis. The fast chain preserves the observables relevant to most analyses while reducing CPU and storage requirements by orders of magnitude. Consequently, it serves as the primary simulation pathway during LZ science runs and underpins the simulation-based studies in this thesis, particularly for comparisons against calibration data⁸.

⁸The exception is the LZEF electrostatic modelling used to generate electric field maps (chapter 4), which are supplied as inputs to LZLAMA.

2.5.4 Event Reconstruction & Processing

Any quantitative measurement based on TPC waveforms relies on accurate energy and vertex reconstruction and on a faithful characterisation of pulse morphology. Simulations predict how energy depositions should manifest, but they are only testable once waveforms are converted into calibrated, position-corrected observables. Thus, with the simulation workflows defined, reconstruction is applied identically to data and Monte Carlo. LZAP [101], implemented in the GAUDI framework [102], executes an ordered chain of modular algorithms over data objects held in a shared transient store; run-/time-dependent calibrations are supplied by the conditions database, and outputs are persisted as ROOT ntuples of “reduced quantities” (RQs), which absorb pulse-level and event-level information into high-level variables for downstream analysis. This architecture standardises formats across data and simulation, enables parallel development, and localises computational bottlenecks to specific modules.

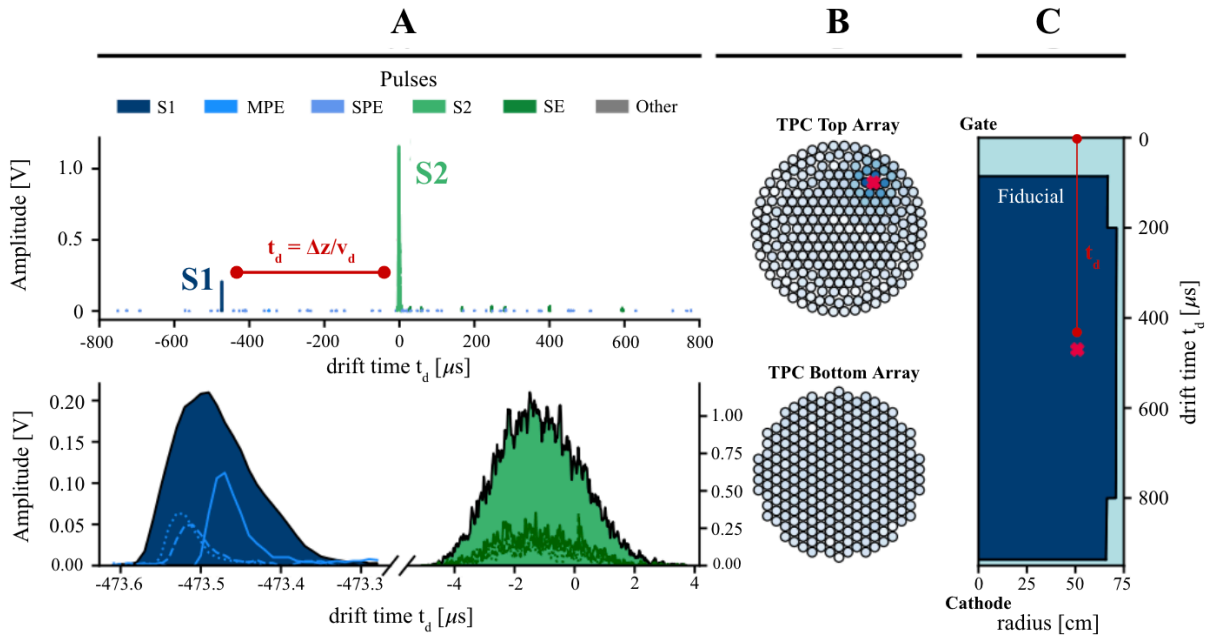


Figure 2.7: Reconstruction of a single-scatter event. **(A)** Digitised PMT waveform with LZAP pulse classification. The time separation between S_1 and S_2 gives the drift time t_d ; the depth follows $z = v_d t_d$. Insets show the summed waveforms which form S_1 (scaled by $\times 10$ for clarity) and S_2 pulse shapes (scaled by $\times 2$). **(B)** Transverse position from MERCURY: the maximum-likelihood (x, y) (star) is obtained by matching the observed S_2 hit pattern to light-response functions of the top array. **(C)** Event location in (r, dt) space with the fiducial contour and hardware boundaries (gate, cathode) achieving 3D reconstruction. Fig. modified from [103], original by A. Baker.

Operationally, LZAP ingests digitised PMT waveforms (from the data acquisition (DAQ) or, in full-chain simulations, from DER/BACCARAT), performs time-alignment, baseline restoration, and gain calibration to photons detected (*phd*), then segments and parametrises pulses. A lightweight classifier labels pulses as S_1 , S_2 , single electron (*SE*), single photoelectron (*SPE*), multiple photoelectron (*MPE*), or “other” (Fig. 2.7), with merge/split logic to resolve overlaps⁹. Events are formed by enforcing drift-time ordering between one S_1 and one or more S_2 s, yielding single

⁹This is an ever-evolving process and a product of the work of several people within the collaboration throughout the course of LZ’s operation.

scatter (SS) or multiple scatter (MS) labels. Depth is obtained from the S_1 - S_2 time difference, encoding drift time¹⁰; transverse position is then reconstructed with MERCURY, a maximum-likelihood-based estimator that compares the observed S_2 hit pattern to a smooth light-response model (derived from calibration), solving for (x, y) and signal intensity [104]. Parameter uncertainties follow from the curvature of the likelihood surface. As a reference for transverse granularity, MERCURY achieved $\sim 13 \text{ mm}$ (S_1) and 1.6 mm (S_2) FWHM¹¹ spatial resolutions in its original ZEPLIN-III deployment [104]; these figures set a useful scale for interpreting S_2 -width-limited performance and the diffusion studies in 3. Using the reconstructed (x, y, z) , LZAP then applies position- and time-dependent corrections, forming $S_{1c}(x, y, z)$ and $S_{2c}(x, y, z)$ folding in electron lifetime, extraction efficiency, geometry, optics and channel response, so that combined-scale energies are directly comparable across data and simulation. Taken together, this reconstruction process and subsequent corrections establish the foundation for all LZ measurements: they provide a uniform RQ basis for data–simulation comparison, from fiducialisation and diffusion studies to the signal and background modelling that underpins the success of the WIMP searches.

2.6 Outlook

This chapter set the stage for LZ: its principal subsystems and the physics that turn energy depositions into the signals we chase in rare-event searches. The through-line is simple: measure, model, mitigate - and build. With a concise picture of the background landscape and the simulation and analysis tools at our disposal, the next chapters dive into the specifics: (i) the microphysics governing charge transport in liquid xenon and its intimate connection to electrostatics (Chapters 3 & 4); (ii) the *in situ* reconstruction of electric fields and its impact on reconstruction, fiducial definition, and stability (Chapter 4); (iii) an S_2 -only analysis (Chapter 5) that targets the low-mass WIMP regime, develops controls for dominant backgrounds (including wall activity and grid radiogenics), and evaluates how far thresholds can be pushed into the sub- GeV domain; and (iv) the implications of these lessons for the design and realisation of next-generation dual-phase xenon detectors such as XLZD (Chapter 6).

¹⁰The $S_1 - S_2$ pair in a single scatter effectively behave like a stopwatch. The S_1 (or prompt scintillation) starts the clock when an interaction takes place, ionisation electrons then start their journey upwards to the extraction region, where after this t_d , produce the secondary scintillation pulse (S_2), stopping the clock.

¹¹Full width at half maximum of a pulse.

“No man ever steps in the same river twice, for it is not the same river; and he is not the same man.”

— Heraclitus

Part II

The Physics of Charge in Liquid Xenon

3

Electron Transport in Liquid Xenon

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LIQUID NOBLE DETECTORS play a pivotal role in searches for WIMPs and neutrinoless double beta decay, while also contributing to a wide range of low-background physics investigations, including ^8B and pp solar neutrino detection, supernova neutrino studies, and other nucleon decay lifetime measurements. However, achieving the necessary sensitivity to the distinct signatures associated with these searches imposes stringent technological requirements. This is particularly relevant for analyses that forgo the primary scintillation (S_1) signal to exploit the enhanced detection efficiency of S_2 -only searches, which can probe nuclear recoils down to the keV scale.

Without S_1 information, reconstructing the interaction depth (z-coordinate) becomes significantly more challenging, and the conventional discrimination methods using the S_2/S_1 ratio to differentiate between background and signal are no longer available. In this scenario, the diffusive processes associated with a swarm of charged particles drifting in a neutral liquid under the influence of an electric field becomes a crucial tool. If the drift and diffusion properties of an electron cloud is well understood, the shape of the S_2 signal can be used to approximately recover the z-coordinate, thereby enhancing the background rejection capability and improving the viability of such an analysis. Fig. 3.1

illustrates this idea.

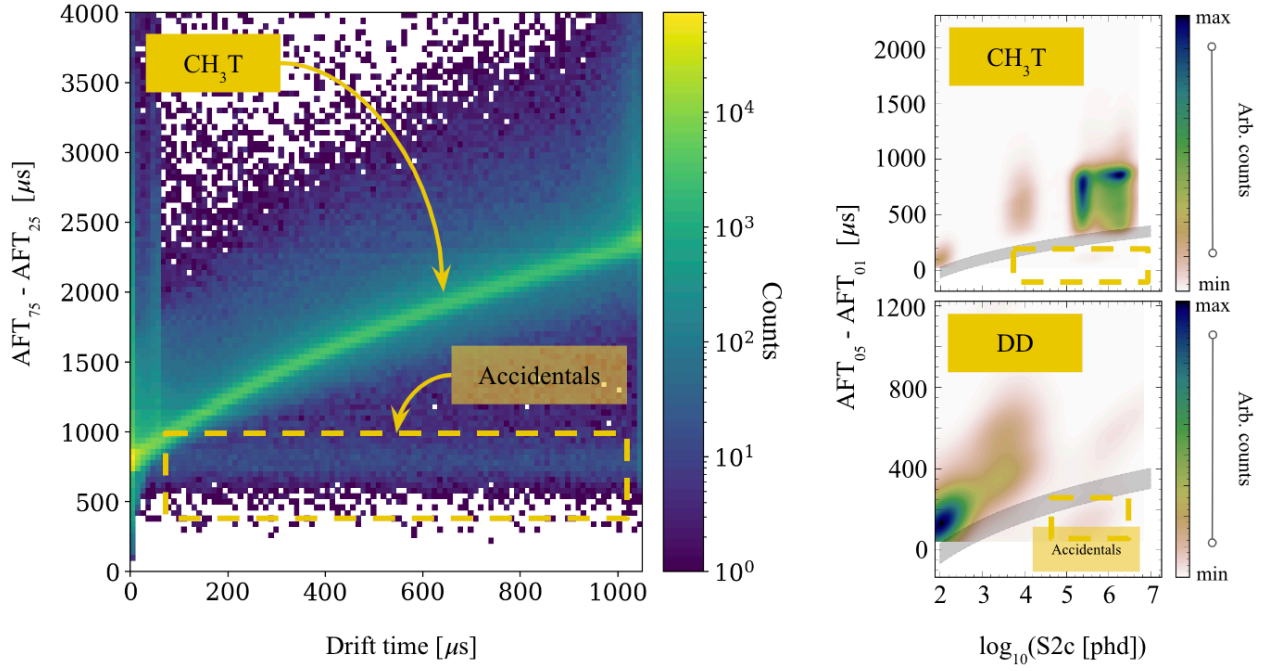


Figure 3.1: The S2 pulse width, defined here as $AFT_{75} - AFT_{25}$ [ns], as defined in Eq. 3.18, exhibits a clear dependence on drift time. This trend is physically well-motivated; as an electron cloud traverses the TPC drift region, is extracted, and subsequently generates secondary scintillation light, it undergoes diffusion. This diffusion leads to a characteristic broadening of the S2 signal with increasing drift time. Events falling outside a physically expected envelope of S2 widths as a function of drift time are identified as accidental coincidences (enclosed in yellow dotted boxes) - instances where uncorrelated (isolated) S1 and S2 signals are mistakenly paired. A similar example is given for area-dependence of the “rise time” ($AFT_{05} - AFT_{01}$) of a pulse allowing isolated S2 pulses (§5.1.1) to be identified and rejected. These typically arise from various instrumental effects and represent a class of backgrounds that can be difficult to model through other means. This highlights the utility of simple S2 shape-based observables for background discrimination, a topic explored further in Section 5.1.1.

It is clear that rare event searches require exceptional energy resolution and robust spatial reconstruction capabilities to efficiently identify signal events while suppressing background interactions spanning several orders of magnitude in energy. A thorough understanding of the underlying physics governing spatial reconstruction and resolution in detectors like LZ is therefore essential. This knowledge not only optimises analysis techniques and background mitigation strategies in current experiments but also informs the design of next-generation detectors. Advancing our understanding of dark matter, neutrino physics, and the microphysics of ion and electron transport in liquid noble detectors is at the heart of this pursuit, forming the primary motivation behind the discussions presented in this chapter.

Our only window into the interactions within the detector are the waveform-outputs of the DAQ. In particular, the S2 signal and drift time offer rich insights into the motion of electrons within both the liquid and gaseous xenon volumes in the TPC, as they are directly shaped by the paths and interactions of the electron cloud drifting through the xenon bulk volume. Since the S2 signal is an aggregate of individual electron pulses, the single electron pulse shape also plays an important part in this story. However, at drift lengths up to ~ 1500 mm in the LZ TPC, diffusion presents

a considerable challenge, becoming the dominant factor influencing the observed S2 width. Electron diffusion in high electric fields is inherently anisotropic [105], therefore it is necessary to measure the longitudinal (along the drift field) and transverse diffusion separately. Typically, the longitudinal diffusion coefficient is smaller than its transverse counterpart, owing to the confinement along the field direction. In the following sections, we will provide a detailed discussion on modelling both the drift velocity and longitudinal diffusion as functions of the electric field within the TPC. Due to existing literature on the transverse diffusion coefficient in conditions similar to LZ but also lack of resolution [58, 101], an explicit measurement of transverse diffusion as a function of field is not performed, although a small discussion will be included in §3.3 for completeness with a single estimate. Other important but mostly subdominant factors that contribute to the systematic uncertainties in the measurement of the longitudinal diffusion coefficient and the average drift velocity of an electron cloud will also be discussed. This comprehensive understanding is essential for deconvolving the various elements that shape the overall S2 pulse and enable more accurate event reconstruction, ultimately underscoring its intimate connection to the TPC geometry and high-voltage design choices.

3.1 Drift Velocities in Liquid Xenon

The LZ experiment has conducted multiple grid optimisation campaigns throughout its operation. In these campaigns, the bias voltages applied to the gate and cathode grids were modified to study consequences on phenomena such as spurious electron emission from the grids. The data from these campaigns enable a controlled exploration of how variations in the drift field throughout the detector volume impact the average drift velocity of electron clouds within the liquid xenon bulk. These measurements not only refine our understanding of the detector's time response and provide a critical baseline for subsequent studies of longitudinal diffusion, but could also offer insight into the momentum transfer cross section under different electric fields [106]. A robust understanding of these fundamental properties opens the door to innovative applications, such as doping liquid xenon with other gases to enhance sensitivity to low-mass dark matter, and lays the groundwork for future developments in detector technology.

3.1.1 Methodology

Within the liquid xenon volume contained between the cathode and gate grids, electron motion is commonly modelled as having a constant drift velocity. This assumption can be derived from first principles. Starting from Newton's second law and incorporating a relaxation-time model with a damping term to represent the effect of frequent collisions (parametrised by τ as the mean relaxation time), we obtain the equation of motion:

$$m \frac{dv}{dt} = eE(z) - \frac{mv}{\tau} \quad (3.1)$$

, where m is the effective electron mass, v is the drift velocity, t is time, e is the electronic charge and $E(z)$ is the electric field, which may vary as a function of the z -coordinate. Indeed, field uniformity is a central design objective for TPCs. In experiments such as LZ, a network of meticulously calibrated field-shaping rings and resistor chains is employed to minimise distortions, thereby ensuring that the electric field within the fiducial volume is highly uniform. Fig. 3.2 illustrates this. Consequently, assuming a uniform electric field should not only be reasonable but also valid to first order, as any residual non-uniformities should typically be more on the order of second-order effects that have minimal

impact on the overall detector performance. Under this assumption, the electron's equation of motion simplifies to a first-order linear differential equation, which admits the exact solution,

$$v(t) = \frac{eE\tau}{m} \left(1 - \alpha e^{-t/\tau}\right). \quad (3.2)$$

Equation 3.2 clearly demonstrates that, as $t \rightarrow \infty$, the electron's velocity asymptotically approaches the terminal drift velocity $v_\infty \rightarrow \frac{eE\tau}{m}$ independent of its initial velocity (α is determined by the imposed initial conditions). In liquid xenon, the relaxation time τ is $\mathcal{O}(10^{-12}s)$ ¹. For example, if $\tau \sim 10$ ps, then after $t \approx 50$ ps (or 5τ) the exponential term reduces to less than 1% of its initial value effectively ensuring that the electron reaches its equilibrium (terminal) drift velocity. This rapid attainment of steady state under a constant drift field validates the common assumption that, within the fiducial volume, electrons effectively experience a constant drift velocity. In other words, the transient dynamics occur on a timescale that is negligibly short compared to the overall drift times encountered in time projection chambers.

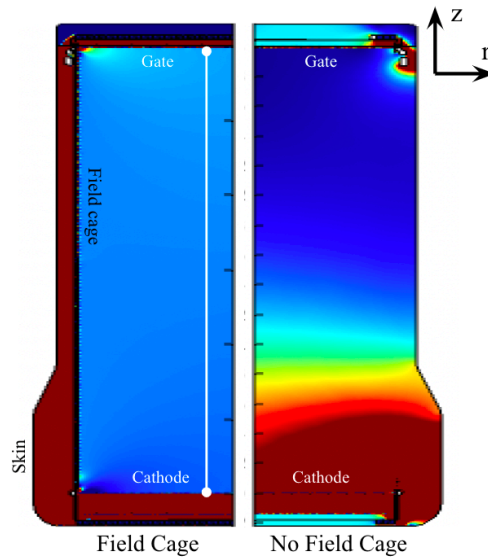


Figure 3.2: Demonstration of the importance of the field cage in maintaining field homogeneity within the TPC. Two scenarios are presented: a configuration without a field cage, and the performance of a fully optimised field cage. In both cases, field streamlines are shown to highlight the resulting charge flow patterns, reinforcing the point that without a well-designed field cage, TPCs would be unable to reliably support rare event searches.

In Chapter 4 we demonstrate that, depending on the electrode grid voltage configuration, the assumption of a perfectly uniform drift field is not always justified. In fact, due to the geometry of the TPC field cage, a small but significant linear gradient $\mathcal{O}(10 - 30\%)$ in the drift field may be present,

$$E(z) = E_0 + \beta z \quad (3.3)$$

, where E_0 is the field at $z = 0$ (typically at the cathode) and β characterizes the magnitude of the linear gradient as one moves toward the gate. Under this scenario, the electron's equation of motion (Equation 3.1) can be generalised

¹Though direct measurements of this do not exist, we can use past mobility measurements from swarm experiments in LXe [107, 108] to approximate this value using $\mu = e\tau/m$ and $v_d = \mu E$.

as a coupled inhomogeneous system. This can be expressed in matrix form as,

$$\frac{d}{dt} \begin{pmatrix} z(t) \\ v(t) \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ \frac{e\beta}{m} & -\frac{1}{\tau} \end{pmatrix} \begin{pmatrix} z(t) \\ v(t) \end{pmatrix} + \begin{pmatrix} 0 \\ \frac{eE_0}{m} \end{pmatrix}. \quad (3.4)$$

The general solution for the electron's motion can be expressed as the sum of a particular solution, $(z_P(t), v_P(t))^T$, that satisfies the full inhomogeneous system, and a homogeneous solution, $(z_H(t), v_H(t))^T$, which accounts for the transient dynamics. In practice, particularly in liquid xenon where the relaxation time τ is extremely short (on the order of picoseconds), the particular solution rapidly dominates. For a linearly varying electric field given by $E(z) = E(0) + \beta z$, the particular solution for the electron drift velocity is,

$$v_P(z) = \mu(E(0) + \beta z), \quad (3.5)$$

, with the mobility defined as $\mu = e\tau/m$. Thus, after a brief transient period, the electron velocity reaches the local terminal value determined solely by the local field. The full solution of the coupled system can be written as:

$$\begin{pmatrix} z(t) \\ v(t) \end{pmatrix} = \begin{pmatrix} z_P(t) \\ v_P(t) \end{pmatrix} + C_1 \mathbf{u}_1 e^{\lambda_1 t} + C_2 \mathbf{u}_2 e^{\lambda_2 t}, \quad (3.6)$$

$$\lambda_{1,2} = \frac{-\frac{1}{\tau} \pm \sqrt{\frac{1}{\tau^2} + \frac{4e\beta}{m}}}{2},$$

with $\lambda_{1,2}$ describing the eigenvalues of the homogeneous system, while their corresponding eigenvectors $\mathbf{u}_{1,2}$ characterise the transient response. Under typical conditions in LXe, the term $1/\tau^2$ overwhelmingly dominates over $\frac{4e\beta}{m}$, yielding one eigenvalue of approximately $\sim -10^{12} \text{ s}^{-1}$, indicating that any transient deviation from equilibrium is damped on a picosecond timescale, while the second eigenvalue is close to zero. This near-zero eigenvalue reflects the relatively slow, steady evolution of the electron's spatial coordinate z once the velocity has equilibrated.

This rapid relaxation is a hallmark of the “cold electron regime” [109], where electrons do not accumulate significant kinetic energy between collisions. Instead, they remain closely thermalised, with their energy distribution governed predominantly by the ambient temperature rather than by the energy imparted by the electric field [109, 110]. Consequently, once thermalisation occurs, the electron drift velocity is effectively given by the steady-state relation in Equation 3.5. More generally, if the electric field is an arbitrary function $E(z)$, the electron will rapidly reach a local terminal velocity given by $v(z) = \mu E(z)$. While this steady-state expression is often used to describe electron transport in liquid xenon, the mobility μ itself arises from a complex interplay of microscopic processes [109, 111]. Experimental studies have shown that the electron drift velocity can exhibit saturation at fields around 100 V/cm in liquid argon, krypton, and xenon [112–114], highlighting the non-linear behaviour that can occur at higher fields, which may also be exhibited at lower fields depending on the particular conditions of the dielectric medium. This can be observed in LZ data as will be discussed in Section 3.1.4. Moreover, ab initio calculations and comparative studies of the gas and liquid phases demonstrate that reduced mobility and transverse characteristic energy can vary over several orders of magnitude, with inelastic and elastic scattering processes playing a significant role [109, 110, 112–114]. In liquid xenon, the cold electron regime ensures that electrons remain largely thermalised due to frequent collisions, but subtle dependencies on temperature, density, and scattering cross sections still lead to non-negligible variation in μ . Consequently, although writing $v(z) = \mu E(z)$ succinctly captures the equilibrium drift velocity, it conceals a

rich microphysics wherein μ depends on both the local field and the underlying collisional dynamics. As such, robust modelling of LXe detectors requires empirical or semi-empirical formulations of μ that incorporate measured drift velocities, ab initio scattering data, and temperature-dependent cross sections, thereby ensuring that the final drift-velocity predictions accurately reflect the actual conditions in the detector.

Continuing in this generalised picture, the overall drift time across the detector is obtained by integrating the inverse of the local velocity:

$$t_d = \int \frac{dz}{\mu E(z)}. \quad (3.7)$$

Consequently, one can readily determine the average drift velocity using the simple relation

$$v_d = \frac{\Delta z}{t_d} \quad (3.8)$$

, where Δz is the known separation between two well-defined reference positions in the TPC, and t_d is the measured time required for electrons to traverse that distance. Finally, this calculation is repeated for various different field configurations. The methodology employed to compute the average electric fields is detailed in Chapter 4, based on simulations that have been rigorously validated using experimental data.

3.1.2 Establishing Fiducial Anchors in Z: The Gate and Cathode as Standard Candles

In dual-phase xenon TPCs like LZ, the vertical position of an interaction is determined by the drift time of ionisation electrons between the S1 and the S2 for a single scatter event. To convert drift time into an absolute distance (and therefore measure the electron drift velocity), it is crucial to have reference points at known z -positions within the detector. The gate and cathode electrode planes naturally serve as such fiducial anchors in z : serving as effective “standard candles” for the drift coordinate. These mesh electrodes are fixed in place, defining the top and bottom of the active drift region, respectively, with a well-known physical separation. Thus, any distinctive signals originating from the gate or cathode provide unambiguous markers of the drift endpoints. By measuring the time separation between an event at the cathode and one at the gate, one directly probes the full drift length, and hence the average drift velocity, without relying on external calibration sources. In LZ, the gate and cathode “alpha peaks” fulfill this anchor role: they appear at the extreme ends of the drift-time spectrum and can be used to calibrate and monitor the z position reconstruction. As the gate and cathode are rigid and held at constant high voltage, these anchor signals remain at fixed true positions regardless of modest variations in the drift field or xenon conditions, providing a stable reference frame for drift velocity measurements. Crucially, anchoring the drift-time to these electrodes allows any time-dependent changes in drift speed (due to temperature, density, or field fluctuations as in Fig. 3.3) to be identified as shifts in the gate/cathode peak separation, and corrected in the analysis. In effect, the gate and cathode form immutable “bookends” of the TPC’s active volume, ensuring that the mapping from drift time to z is grounded in physical reality.

The reason the gate and cathode produce distinctive signals in the first place is the presence of alpha-emitting radionuclides from the radon decay chain that deposit on these surfaces (Fig. 3.4). During detector construction and operation, trace amounts of radon gas (^{222}Rn from the ^{238}U decay series, as well as ^{220}Rn from ^{232}Th) can infiltrate

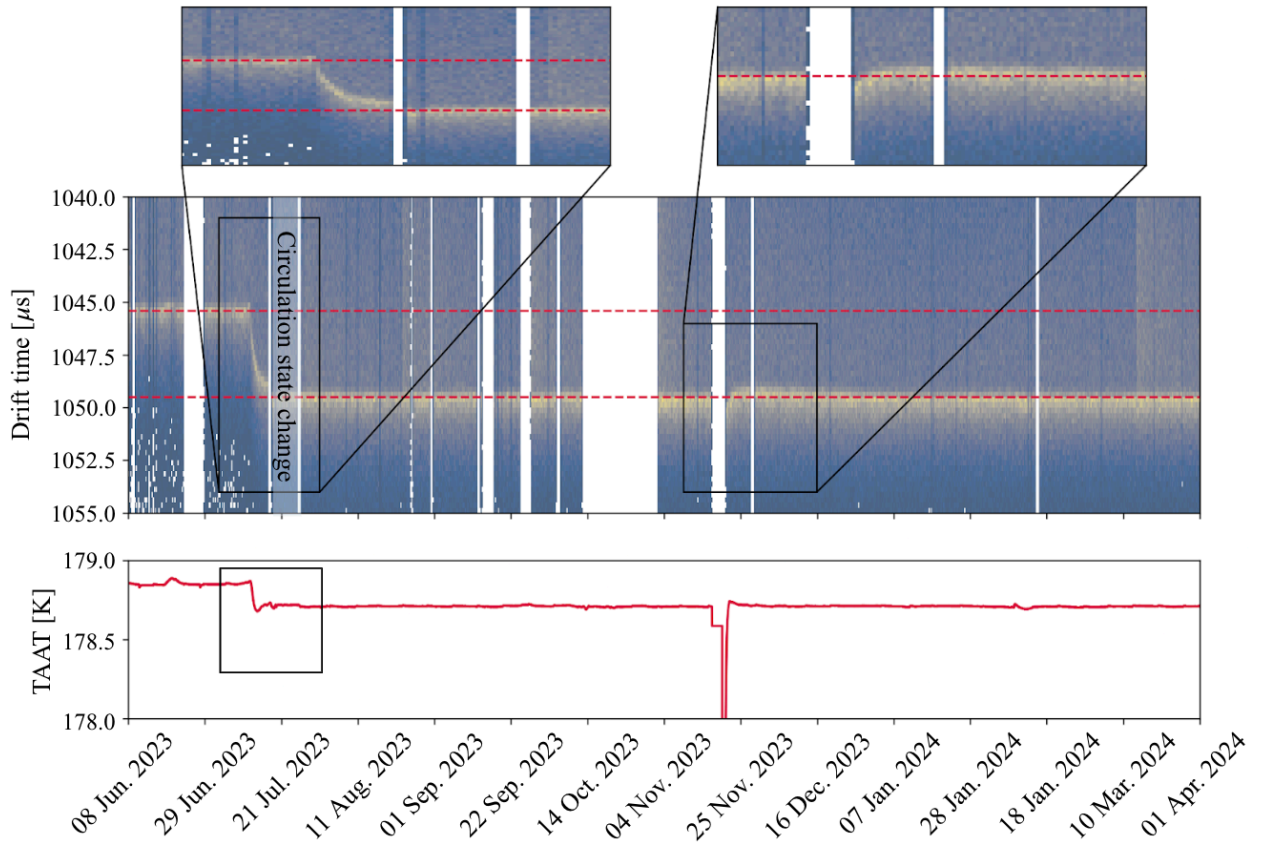


Figure 3.3: Evolution of the LZ TPC maximum drift time over the course of WS 2024, as identified by the visibly elevated rates due to the cathode α populations. The bottom panel displays the top-array average xenon temperature, showing a clear correlation between thermal fluctuations and modulations in drift velocity and z-reconstruction. As a reference, variations of the order of $\pm 1 \mu\text{s}$ correspond to $\simeq \mathcal{O}(1 \text{ mm})$ shifts in reconstructed z . Fig. reproduced and modified using code from A. Musalhi.

the xenon or emanate from materials. Radon is chemically inert and can diffuse throughout the detector, but its short-lived daughters (such as ^{218}Po , ^{214}Pb) tend to electrostatically adhere or “plate out” onto available surfaces such as electrode wires [58, 67]. The most important progeny in this context is ^{210}Pb , which has a 22-year half-life and thus accumulates over time on surfaces exposed to radon. Once ^{210}Pb is embedded on a surface, it beta-decays to ^{210}Bi and then to ^{210}Po , which in turn emits a high-energy alpha (5.30 MeV in the $^{210}\text{Po} \rightarrow ^{206}\text{Pb}$ decay). Due to the long-lived nature of ^{210}Pb , any initial exposure to radon can lead to a long-term presence of ^{210}Po within the detector components, even long after the radon itself is gone. By the start of LZ operations, the decay chain from ^{210}Pb through ^{210}Po on detector materials is expected to be in secular equilibrium, meaning the activity of ^{210}Po alphas will be essentially constant and equal to that of ^{210}Pb . Despite stringent clean-room protocols to minimise radon exposure during fabrication, the LZ electrode grids inevitably accrued some ^{210}Pb [58]. Estimates based on the measured air exposure times suggest an order of $0.001 - 0.01 \text{ Bq}$ of ^{210}Pb on each grid (on the cathode: $\sim 116 \text{ mBq}$ in a low-to-high exposure scenario) [58, 67, 115]. This corresponds to an order of a few decays per minute emanating from each of the gate and cathode wire planes – a small rate in absolute terms, but readily observable above background. The key point is that these decays occur *at known locations*: on the surfaces of the gate (towards the top of the liquid xenon bulk) and the cathode (at the bottom). Thus, the alphas from these decays effectively turn the gate and cathode into built-in calibration sources that continuously illuminate those electrode planes with alpha events.

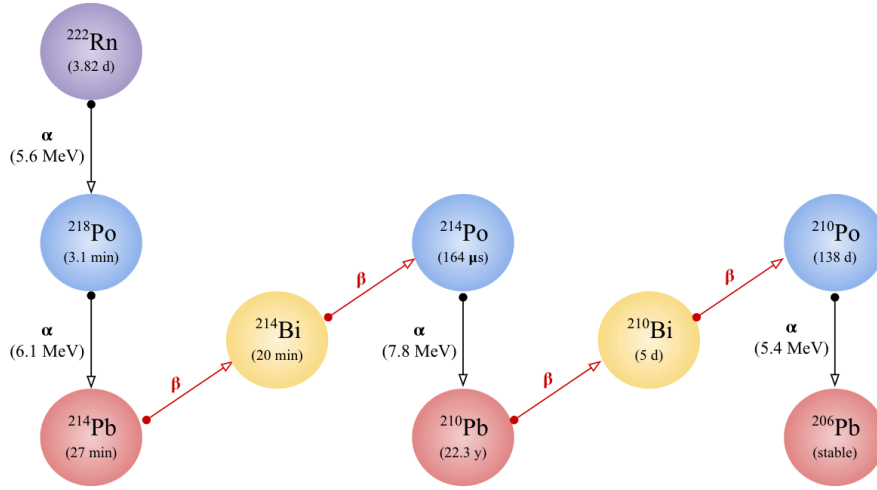


Figure 3.4: The ^{222}Rn decay chain.

Alpha particle interactions in liquid xenon also produce a very distinctive signature in the TPC, setting them apart from the keV -scale electron or nuclear recoils of typical dark matter events [75, 88]. A $5 - 7\text{ MeV}$ alpha deposits orders of magnitude more energy than a WIMP-like recoil, leading to a much brighter S1 flash and a correspondingly large ionisation signal. However, due to the dense ionisation along an alpha track, a substantial fraction of the charge recombines immediately, enhancing the S1 light at the expense of the S2. The net effect is that alpha events lie on a separate band in parameter space, with a high S1-to-S2 ratio (or equivalently, an anomalously low S2 given the S1 as compared to a standard single scatter event). In fact, radon-chain alphas in LZ produce “extremely large and readily identifiable S1 signals, far removed from those of other backgrounds” [88]. For example, an alpha decay in LZ might produce an uncorrected S1 of $\mathcal{O}(1000s\text{ phd})$, whereas a typical electron recoil in the MeV range would produce only a few hundred phd at most. The S1 is so bright that alpha interactions populate a distinct high-energy “alpha band” well above the electron recoil band in the $\log(S2)$ vs $\log(S1)$ parameter space. Even without using S2s, one can simply place a threshold on S1 area to select alphas: in LZ’s first science run, any event with $S1 > 30,000\text{ phd}$ was virtually guaranteed to be an alpha [36]. This makes identification of the gate and cathode alpha events straightforward in the data.

Another powerful identifier is the top-bottom asymmetry of the S1 light (S1 TBA). The fraction of S1 light seen by the top PMT array versus the bottom array depends on an event’s vertical position: interactions near the bottom (cathode) yield most of their light in the bottom PMTs, whereas events near the top (gate) produce more light in the top array. Alpha events on the cathode thus tend to have strongly negative TBA (since the scintillation occurs just above the bottom PMTs), while those at the gate have strongly positive TBA. In practice, plotting S1 vs TBA, as in Fig. 3.5, reveals clear bands corresponding to different alpha-emitter locations. LZ observed that without any position reconstruction, the alpha decays naturally form distinct loci in S1–TBA space: higher S1 (energy) combined with extreme TBA values marks out the surface populations (cathode, gate, walls) clearly. This is important because not every alpha event is a perfectly reconstructed single scatter with a well-formed S2. For instance, an alpha on the cathode that loses part of its ionisation signal might fail some SS selection criteria. Yet, even those can be identified

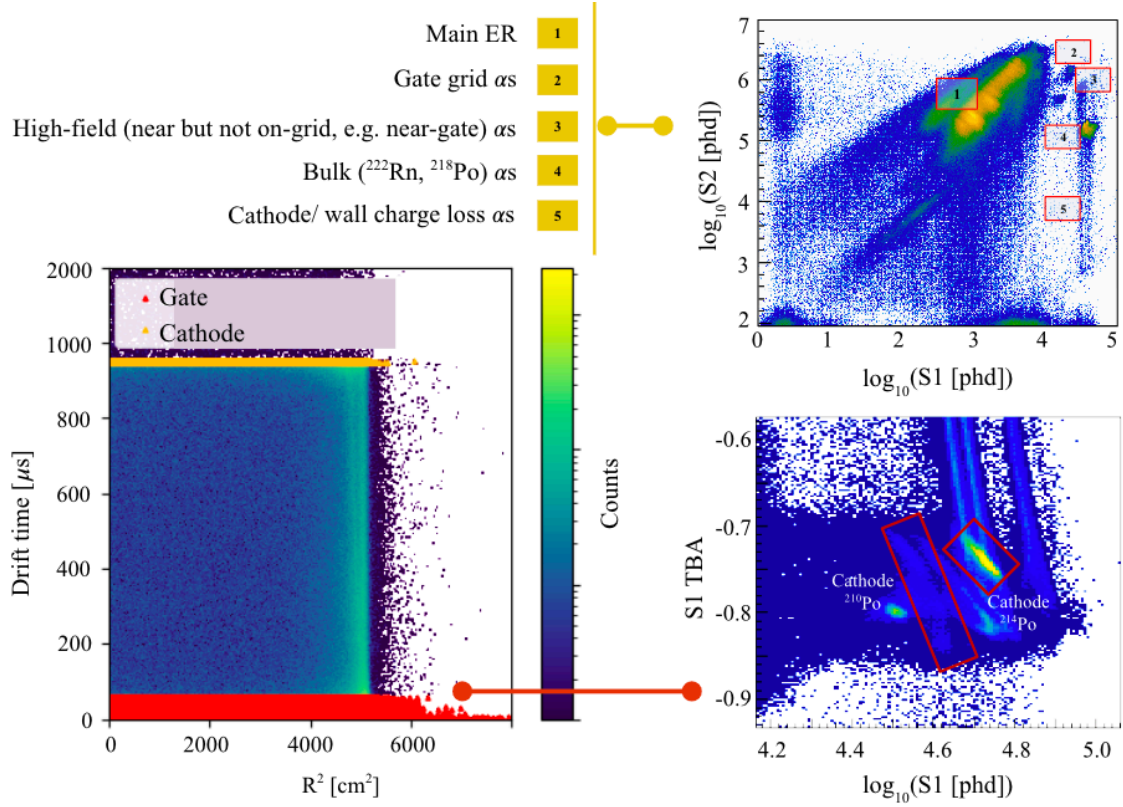


Figure 3.5: Alpha populations identified across complementary observables. **Top-right:** $\log_{10} S1$ – $\log_{10} S2$ for the full TPC (no cuts); boxes 1–5 mark the main ER band, gate-grid α s, near-gate high-field α s, bulk (^{222}Rn , ^{218}Po) α s, and cathode/wall-loss α s. **Bottom-right:** $S1$ –TBA after selecting cathode/RFR candidates; the cathode α bands are clearly visible, with remaining features from RFR α s of various isotopes. **Left:** Drift time vs R^2 confirms spatial localisation, with clusters at minimum and maximum drift time corresponding to the near-gate and near-cathode regions.

by their $S1$ and TBA alone. LZ can exploit this by performing an “agnostic” alpha analysis using all large $S1$ pulses, with cuts on TBA to reject events from the grids and below-cathode region (as in §5.1.3). In other words, one can cleanly separate the cathode and gate alpha populations from internal (radon) alphas by their light asymmetry. Once identified, these grid alphas show up as two sharp peaks in the drift-time distribution: one cluster at very short drift times (events originating from the gate), and one at the maximum drift time (events from the cathode). This dual-peak structure is essentially the “ruler” for the drift length (Fig. 3.5). It is worth noting that because of their high energy, alpha interactions in LXe are sometimes reconstructed using only the $S1$ signal. In XENON detectors, for example, the energy of an alpha can be determined “solely from the $S1$ ” because the $S2$ is comparatively small and can even be absent [116]. LUX likewise treated ^{210}Po alpha events at the detector boundaries with an $S1$ -only analysis, since those often suffered significant $S2$ losses. The fact that alphas are so easily distinguished and can be analysed independently means the gate and cathode peaks can be measured in situ with high precision, without confusion from other event types. In summary, the combination of an outlying $S1/S2$ ratio and extreme TBA value makes the grid alpha events stand out unambiguously as “calibration” populations.

While the gate and cathode alpha events are clearly identifiable, the details of their signals are influenced by the local electric field geometry at those electrodes. Both the gate and cathode are wire meshes that define the drift field boundaries: the cathode, at negative high voltage, creates the vertical drift field in the liquid xenon, with the gate just below

the liquid surface, defining the top of the drift region and the interface to the extraction field. Near these wire planes, the electric field is not perfectly uniform – it fringes and warps around the wires as the streamlines funnel from a lower-field region into the higher-field region of the extraction region as shown in Fig. 3.6. This has important consequences for how ionisation from alpha decays is collected, and introduces slight asymmetries in the observed signals.

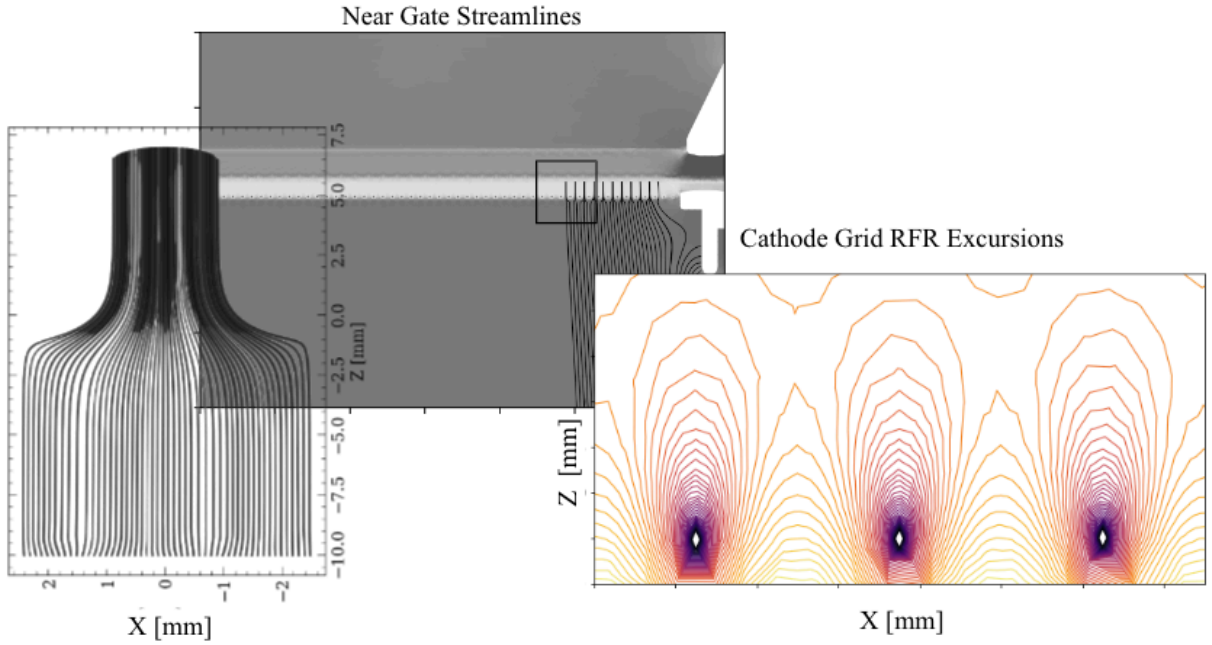


Figure 3.6: Electric-field structure near the wire planes. **(Left)** streamlines in the extraction region, funnelling from the lower-field drift region below the liquid–gas interface through the negatively biased gate toward the anode, illustrating fringing and local focusing near the wires. **(Right)** potential contours around the cathode grid showing reverse-field-region (RFR) excursions beneath the wires; the field concentrates at wire surfaces and relaxes between bays, producing a periodic modulation. Such non-uniformities can subtly alter charge collection and S2 pulse shapes for interactions occurring near these electrodes.

3.1.3 Other Considerations

Forward vs Reverse Field Regions

The cathode wire plane divides the TPC into two regions: a forward-field drift region above, where electrons drift upward toward the gate, and a reverse-field region below, where electrons are pulled downward into passive structures (Fig. 3.6). Thus, ^{210}Po decays on the cathode only contribute to the fiducial cathode peak if the α is emitted upward into the active LXe; downward emissions deposit energy below the mesh, yielding an S1 but little or no S2. This behaviour, first noted in XENON1T [117–119], is also visible in LZ as isolated S1s or suppressed S2s. The effective cathode anchor is therefore the subset of decays directed into the drift volume.

Field Focusing and Electron Collection Efficiency

On smaller scales, grid wires focus field lines into the metal. Electrons born very near a wire may terminate on it, reducing the S2. Simulations with COMSOL and Garfield++ confirm that this effect produces a modest low-energy tail in the alpha spectrum [88, 115], consistent with LZ’s observed asymmetric peak shape. These losses are percent-level and do not bias the timing of the anchor peaks, though they slightly broaden the energy distribution. Any effective source depth offsets (tens of microns of alpha range, sub-mm wire capture zones) are negligible compared to the ~ 1.5 m drift length, but are included in detailed field models [67].

Azimuthal Variations

Finally, the grid geometry and support structures can introduce weak azimuthal modulations in S1 or S2 amplitude. Partitioning LZ's alpha data by azimuth showed at most a few-percent variation in signal size, with no measurable timing shift [75, 115]. Thus, the cathode and gate anchors are isotropic for drift-time calibration.

Data Selection

CUT NAME	CUT DESCRIPTION
PRELIMINARY DATA QUALITY CUTS	
Single Scatters	Selects events with a correlated S1 and S2 signature occurring within a single event window; effectively rejects several bulk alpha events, which often induce multiple scatters.
Electron Train Veto	Electron trains, caused by delayed electron release from impurities or delayed extraction at the liquid surface, can generate additional pulses in the S2 region that obscure genuine alpha events. By applying this livetime-based cut, one ensures that these extra drifting electrons do not contaminate the timing or shape of the S2 signals, thereby yielding a cleaner, more reliable sample of gate and cathode alpha events for drift-velocity calibration.
Fiducial Radius	Removes charge loss events due to regions of higher field variation near the TPC PTFE walls (Chapter 4)
Stinger	Stingers arise when electrons initially drift upward through the anode wires before reaching the anode surface. In the extraction region, the electric field is sufficiently high to generate electroluminescence; however, electrons that pass through the interstitial gaps between the wires enter a zone with a much lower field, temporarily suppressing an S2 from being produced. When these electrons finally land on the anode wires, the field increases abruptly, causing a renewed and delayed burst of electroluminescence. The resulting temporal gap between the main single-electron or S2-like pulse and the subsequent "stinger" can mimic a genuine single-scatter alpha event. Such signatures are therefore rejected to avoid misidentification.
GATE SELECTION CUTS	
Drift Time	Drift-time tagging of the gate based on high-event rates: [1500, 3500] ns
S1 TBA	A cut in S1 TBA-log(S1) parameter space which allows further distinction between RFR S1-induced photoionisation events, ERs produced in the non-uniform high-field regions very near the gate wires and bulk ER events, vs gate alphas.
Above-Anode Gas Events	Above-anode gas events generate electroluminescence pulses with unusually high S2 TBA, potentially masking the signature of gate alphas in particular. By rejecting these events, one can effectively eliminate such gas-phase contributions and isolate a cleaner gate alpha sample.
CATHODE SELECTION CUTS	
Drift Time	Field-dependent selection to tag the maximum physical drift time of events occurring within the TPC: [949500, 954000] ns for WS 2022 & [1042000, 1055000] ns for WS 2024 (note that the two circulation states led to a $\sim 5 \mu s$ difference in maximum drift time). This will be discussed further in the context of systematics in the following section.
S1 TBA	A cut in S1 TBA-log(S1) parameter space which allows further distinction between RFR and bulk alphas vs cathode alphas.

Table 3.1: Summary of data quality and selection cuts used for isolating gate and cathode alpha events.

For single scatter events, a drift time selection effectively eliminates many non-grid events, yet it alone does not guarantee the purest sample of gate and cathode alphas. Following on from the discussions in the previous section, Table 3.1 summarises the complete set of selection cuts implemented to isolate the gate and cathode alpha populations. These cuts not only delineate the electrodes in drift time but also minimise particularly statistical uncertainties arising from radon progeny in the bulk and within the reverse field region, which typically broaden the drift time distributions.

3.1.4 Results & Discussion

By combining the data-driven calculations of the drift velocity with the simulated calculations of the average forward field region electric field, we can elucidate the relationship between the electric field strength and the drift velocity of electrons in liquid xenon. It is crucial that this relationship is correct as it directly impacts our understanding of the charge transport properties in the detector, constituting a fundamental parameter required to accurately simulate detector response; this will be described in more detail in Chapter 4. The results of the analysis, along with similar measurements taken by other dual phase xenon experiments, is shown in Fig. 3.7.

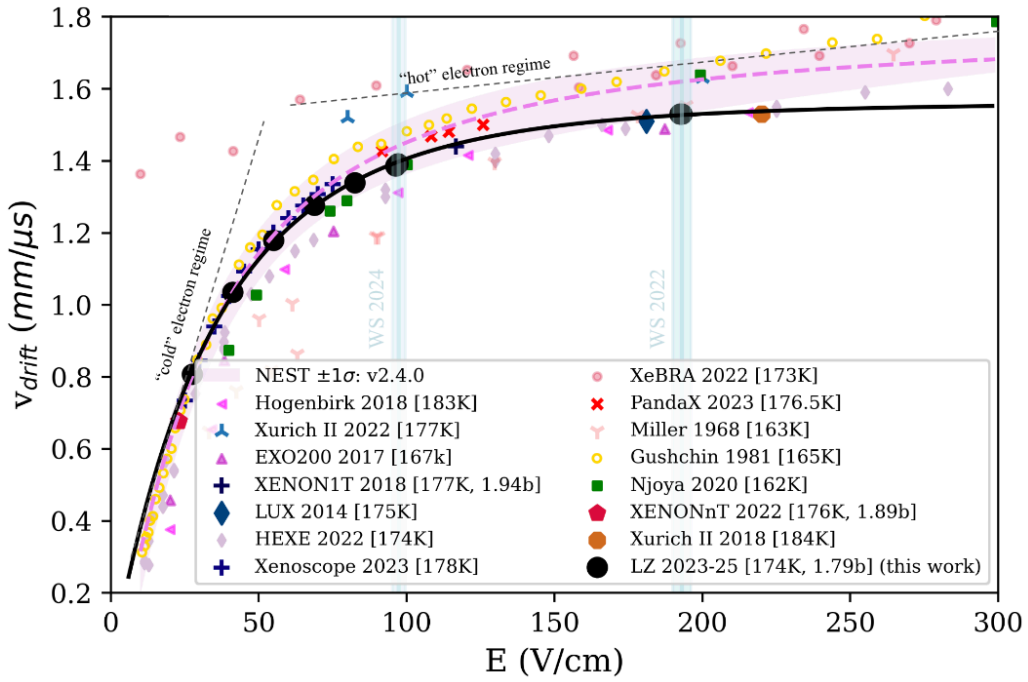


Figure 3.7: Electron drift velocity in liquid xenon versus electric field. Points show measurements from modern dual-phase TPCs and legacy studies; black circles are the LZ data at $T = 174$ K and $P = 1.79$ bar (this work). The solid black curve is a “pure-LXe” fit constrained to datasets with similar thermodynamic conditions and sub-ppb impurities; the shaded band is its 1σ uncertainty. The purple band shows the NEST v2.4.0 prediction. Three regimes are evident: (i) a low-field linear rise governed by the momentum-transfer mean free path Λ_1 ; (ii) a transition near $E \sim 40\text{--}100$ V cm $^{-1}$ where collective modes open and cool the electrons; and (iii) a high-field plateau with $v_{\text{sat}} = 1.48 \pm 0.02$ mm μs^{-1} at 174 K. Vertical shaded bands mark the average LZ drift fields in WS 2024 (~ 97 V cm $^{-1}$) and WS 2022 (~ 193 V cm $^{-1}$). Finally, black dashed lines derived from Cohen-Lekner theory for the two regimes are also overlaid for comparison [111, 120].

Along with the experimental data collected from various experiments in literature, Fig. 3.7 also illustrates the theoretically-derived cold & hot electron model curves from Cohen-Lekner theory [109] as explicitly summarised in both [120] and [111]. A few key features stand out. We will address these in turn in the context of theory.

When an electron travels through LXe, it can not only scatter off individual xenon atoms (elastic, momentum-transfer collisions) or excite electronic levels (inelastic, high-energy collisions), but can also excite low-energy density fluctuations. Each of these modes are also visible in Fig. 3.7 and will be discussed in the context of a few different regimes.

I - RAPID RISE AT LOW FIELD (THE COLD-ELECTRON REGIME)

At low field ($\lesssim 30 \text{ V/cm}$) the LZ data follow the common linear rise shared by all modern measurements. In this domain electrons remain thermalised with the liquid: the energy gained between successive momentum-transfer collisions is negligible, so the drift speed is fixed by the elastic mobility (see §3.1.1),

$$v_d \simeq \mu_0 E, \quad \mu_0 = \frac{e\Lambda_1}{m\langle v_{th} \rangle}, \quad (3.9)$$

where Λ_1 is the momentum-transfer mean free path and $\langle v_{th} \rangle$ is the thermal speed at $T = 174 \text{ K}$. Using the first three LZ points we find $\mu_0 = (4.0 \pm 0.1) \times 10^2 \text{ mm } \mu\text{s}^{-1} (\text{V cm}^{-1})^{-1}$. Small variations in temperature or pressure modify Λ_1 via the liquid's static structure factor, producing the $\pm(2 - 3)\%$ spread in the low-field slope seen among LZ, LUX ($T = 175 \text{ K}$), and XeBRA.

II - TRANSITION REGION ($\sim 40 - 100 \text{ V/cm}$)

Atrazhev & Iakubov's multi-term solutions [121] confirm that the drift-velocity curve is expected to transition gradually over roughly a factor of 3 in field, with the inflection point migrating toward higher fields as you refine the cross-sections and include collective-mode scattering. This is well in line with our observations. To demonstrate this, we start with Cohen & Lekner's 1967 theory of electron transport in dense fluids [109], where they introduced two characteristic lengths - Λ_1 (the momentum-transfer mean free path) and Λ_0 (the energy-transfer mean free path). As per this formalism, the crossover field E_t between “cold” and “hot” regimes should occur when the work done by the field over a distance Λ_1 is equal to the thermal energy of the electrons:

$$eE_t\Lambda_1 = \frac{3}{2}k_B T \quad (3.10)$$

However, for $T = 174 \text{ K}$ and $\Lambda_1 \approx 400 - 1000 \text{ \AA}$ [112], this yields a value $\mathcal{O}(\sim \text{kV/cm})$, far higher than the observed range of transitions. This large discrepancy has an explanation and is rather excellent evidence for LXe's dynamic structure factor. In a dense fluid like liquid xenon, atoms do not behave as isolated scatterers the way they do in a dilute gas. Instead, their motions are highly correlated, and collective excitations become visible: coherent, wave-like disturbances of the medium's density. These phonon-like modes, or more generally “collective modes”, represent the complex structure of LXe. As these modes lie at very low energies ($\mathcal{O}(10 \text{ s meV})$), they provide the first inelastic channel an electron can excite once it warms up. Below the field where those modes become accessible, electrons remain “cold” (no energy loss). Above that field, they start to lose energy into the collective modes, which tames further acceleration, hence the onset of the hot-electron plateau.

Collective-mode scattering is therefore the dominant inelastic, energy-loss mechanism in ultra-pure LXe until the

much higher thresholds for xenon’s atomic excitations ($\sim 9 \text{ eV}$) are reached. It controls exactly where and how quickly the drift-velocity curve bends over from the linear rise into the saturation plateau. We can modify our initial back-of-the-envelope calculation to take this effect into account as follows. Electrons will begin to lose energy to a collective-mode of energy $\hbar\omega$ once the work done by the field over one momentum-transfer mean free path $\Lambda_1 = \hbar\omega$:

$$eE_t\Lambda_1 \approx \hbar\omega \quad (3.11)$$

, such that below E_t these modes are “frozen out” (electrons remain cold), and above E_t they open as a cooling channel (gradual onset of hot behavior). In LXe the lowest “phonon”-like excitations lie around $1 - 10 \text{ meV}$ (from inelastic neutron-scattering data), resulting in a transition window of roughly $10 - 200 \text{ V/cm}$ ($20 - 100 \text{ V/cm}$ if we only consider the most probable values of $\Lambda_1 : \{2, 5 \text{ meV}\}$) in excellent agreement with the observed results across LZ and other experiments [80, 111, 122–128].

III - PLATEAU AT HIGH FIELD (THE HOT-ELECTRON REGIME)

Beyond $\approx 100 \text{ V/cm}$ the new LZ measurements cluster tightly about $v_{sat} = 1.48 \pm 0.02 \text{ mm } \mu\text{s}^{-1}$, defining the pure-LXe saturation velocity at 174 K and 1.79 bar . In this regime the power input eEv_d is balanced by inelastic energy loss, primarily to collective modes of the liquid; further increases in field raise the electron temperature but not their drift speed. Experiments with ppm-level molecular impurities (e.g. [123]) sit up to 15% above the LZ plateau, while ultra-pure data sets such as EXO-200 [125] lie a few per-cent below: consistent with the vertical spread expected from variations in the energy-transfer mean free path Λ_0 , since molecular impurities open additional inelastic energy-loss channels for drifting electrons.”.

In order to account for these differences across experiments, a new fit was generated using data only from experiments which share similar purification protocols and operate at temperatures close to LZ’s (174 K): XENON1T [117], XENONnT [37], LUX [129]. This approach significantly reduced the deviation in maximum drift time between data and simulation to just 0.78%. While the revised data-driven approach shows improvement, it highlights the sensitivity of drift velocity models to seemingly minor changes (coefficient fluctuations of $\lesssim 0.01$) in both functional form and coefficient, capable of shifting z -reconstruction by up to $\mathcal{O}(\sim 10 \text{ } \mu\text{s})$, especially in regions of higher field variation. Hence, the error bands in Fig. 3.7 are still not enough to achieve a one-to-one mapping of drift time measurement to z position within the TPC. We have confirmed the action and implication of the two mean free path model, tried to inspire and motivate their relationship with the observables in LZ and other TPC experiments, but an exact theory-derived dependence on pressure, temperature and impurity concentration remains unknown; without this information the error envelope on the $v_d - E$ relation cannot be narrowed further.

IV - VARIATION BETWEEN EXPERIMENTS

Having established the three canonical regimes, (i) cold electrons, (ii) the collective-mode transition, and (iii) hot-electron saturation, we can now account for the residual spread visible in Fig. 3.7. All departures from the “pure-LXe” parameterisation can be traced to modest perturbations of one (or both) of the two characteristic mean free paths: A

Table 3.2: Primary mechanisms that shift the drift-velocity curve.

Physics mechanism	Parameter	v_d - E impact	Typical experimental lever
Density / structure	momentum-transfer path Λ_1	low-field slope; secondary shift of E_t	temperature (± 5 K), pressure (1 – 2 bar)
Inelastic energy loss	energy-transfer path Λ_0	plateau height v_{sat} ; transition width	ppm-level molecular impurities; deliberate “doping” studies

vibrational or rotational mode of a dilute molecule (N_2 , O_2 , H_2O , CH_4) at 0.2 – 0.3 eV supplies a much more efficient sink for electron energy than LXe’s native collective modes. The steady-state energy balance is therefore:

$$eE v_d = \underbrace{m \nu_m(\varepsilon) v_d^2}_{\text{elastic (momentum) losses}} + \underbrace{\langle \varepsilon \rangle [\nu_E(\varepsilon) + \nu_{imp}(\varepsilon)]}_{\text{inelastic (energy) losses}}, \quad (3.12)$$

where the right-hand side contains (i) elastic losses at the momentum-transfer rate ν_m and (ii) inelastic losses: native xenon channels ν_E plus impurity-induced channels ν_{imp} , each removing approximately the mean electron energy $\langle \varepsilon \rangle$.

Adding only a few ppm therefore shortens Λ_0 , allowing electrons to stay “cold” out to higher fields and driving the plateau upward. This can be used to explain, for example, the data from Gushchin et al., operating with xenon purified to 1970s standards; the resulting ppm contamination could have raised v_{sat} to ≈ 1.7 mm μ s $^{-1}$. Similarly, EXO-200 recirculated xenon through hot getters to sub-ppb levels of impurities, effectively removing ν_{imp} and restoring the canonical ≈ 1.45 mm μ s $^{-1}$ plateau. As Λ_0 appears only in the energy-balance term, these vertical shifts leave the low-field (Λ_1 -controlled) slope essentially unchanged.

A modest thermodynamic adjustment, cooling the liquid by ≈ 5 K or raising the pressure from 1 bar to roughly 2 bar changes the xenon density by about 3 %. The denser medium shortens the momentum-transfer mean free path Λ_1 , driving the cold to hot inflection field upward by ≈ 10 Vcm $^{-1}$ and slightly suppressing the mobility along the entire drift-velocity curve. This density effect is visible in the data: LUX, operated at 175 K, exhibits a 2 – 3% reduction in both the low-field slope and the saturation plateau, exactly as predicted for a shorter Λ_1 . By contrast, the marginally warmer (and thus less-dense) xenon in XENON1T (177 K [117]) and XENONnT (176 K at 1.89 bar [37]) lengthens Λ_1 , yielding a steeper cold-electron rise and a plateau $\approx 2\%$ higher than the LZ baseline. This is not a conclusive relationship however, and studies characterising the impact of larger temperature variations is motivated throughout this chapter due to the significant gap in literature.

The residual cloud of points in Fig. 3.7 is therefore not noise but a diagnostic fingerprint of the two mean free paths (Table 3.2). Overlaying impurity-enhanced model curves (Yoshino-style) and temperature-shifted structure-factor calculations quantitatively reproduces the full envelope of measurements, lending strong support to the Λ_1/Λ_0 framework.

Errors & Systematics

As with any precision measurement, a complete uncertainty budget must accompany each determination of the drift velocity. The subsections that follow describe, in turn, the origin of every relevant systematic - thermodynamic state, electric field non-uniformity, geometric effects, timing calibration, residual impurity, and model choice - and explain how the size of each contribution is quantified. For reference, Table 3.3 consolidates these statistical and systematic terms for the WS 2022 data set, illustrating the relative weight of each source in the overall uncertainty assigned to the LZ drift velocity measurement.

THERMODYNAMIC STATE

Table 3.3: Systematic and statistical contributions to the WS 2022 drift-velocity uncertainty. Values refer to the LZ WS 2022 conditions ($T = 174$ K, $P = 1.79$ bar, full drift time $\Delta t \simeq 950$ μs , fiducial radius $r < 65$ cm). Totals represent per-point uncertainties on v_d for WS 2022.

Category	Source	$\Delta v_d/v_d$	Comments/mitigation
Thermodynamic	Temperature sensor (± 0.3 K)	0.5%	$\mu_0 \propto \rho^{-1}$; includes 2 K axial gradient.
	Absolute pressure (± 0.05 bar)	0.3%	Density scaling of Λ_1 .
Electric field	Field-map non-uniformity	1.0%	1% radial/axial variation inside $r < 65$ cm.
	HV read-back ($\pm 0.1\%$)	0.1%	Precision divider calibration.
Geometry	Gate/anode deflection	0.3%	0.4 mm central sag (upper edge of the model spread).
	TPC shrinkage (4.5 mm)	0.2%	Survey before/after cool-down.
	Liquid level (± 0.5 mm)	0.2%	Drift-length scale.
Timing chain	Clock stability (± 1 ppm day $^{-1}$)	0.0005%	100 MHz GPS clock; 1 ppm on 950 μs .
	Digitiser/trigger skew (± 1 sample = 10 ns)	0.001%	10 ns on 950 μs .
	S1-S2 t_0 offset ($\lesssim 1$ μs)	0.1%	Same definition in data & MC.
Purity	Residual impurity variation (ppb-ppm)	0.5%	Plateau shift via Λ_0 ; lifetime monitor.
Model/fit	Functional-form choice	0.7%	Spread between tanh, NEST v2.4, polyExp.
Statistics	Drift-time peak fitting	0.03%	Width of drift-time histograms.
Total (quadrature)		1.69%	Dominated by field non-uniformity and T/P systematics.

For each dataset, the eight PT100 sensors on the cryostat wall [58] and the two immersion probes provide pressure and temperature readings at 1-minute cadence. The average liquid temperature and its axial gradient are fed into the NIST xenon equation-of-state to obtain the density; the sensor calibration uncertainty (± 0.3 K) and the observed top-to-bottom gradient (1 – 3 K, field-dependent) propagate to the momentum-transfer mobility as $\delta v_d/v_d = |\partial \ln \rho / \partial T| \delta T$. Similarly, the gas system logs the absolute pressure with ± 0.05 bar accuracy; this is converted to a density-scale uncertainty in the same way.

ELECTRIC FIELDS

For every voltage configuration, a full EM simulation is conducted with LZEF, LZ’s custom field-simulation software

(Chapter 4). From these maps we extract the mean field $\langle E_z(r, z) \rangle_{r < r_{\text{cut}}}$ and its r - z RMS, σ_E ; the latter, typically 0.5–1.5% depending on the field, is propagated to a drift-velocity uncertainty via

$$\left. \frac{\delta v_d}{v_d} \right|_E \simeq \underbrace{\frac{\partial \ln v_d}{\partial \ln E}}_{S(E)} \frac{\sigma_E}{\langle E \rangle}.$$

Here $S(E)$ is evaluated from the LZ fit to $v_d(E)$ and is $\mathcal{O}(1)$ at low field, falling toward zero on the plateau; consequently, a 1% field non-uniformity contributes $\sim 1\%$ at $E \lesssim 50 \text{ V cm}^{-1}$ and $\ll 1\%$ near saturation.

GEOMETRY

Laser tracker surveys performed before and after cool-down show a uniform TPC contraction of $4.5 \pm 0.7 \text{ mm}$ over the original 1456.5 mm drift length; this translates to a 0.2% uncertainty. Electrostatic sag of the wire grids is parameterised as a function of extraction voltage in § 6.2.3 (full study in [130]²). The sag value at a given extraction field is applied as a drift length correction with an uncertainty equal to the model spread ($\sim 0.3\%$). Liquid-level sensors add $\pm 0.5 \text{ mm}$ (0.2 %) to the drift-distance scale.

TIMING CALIBRATION

All digitiser crates are phase-locked to the GPS-disciplined 100 MHz master clock; the daily drift ($\leq 1 \text{ ppm}$) and inter-crate skew ($\leq 10 \text{ ns}$) are entered directly into $\delta(\Delta t)/\Delta t$ contributing $< 0.002\%$ (negligible). Run-to-run variation of the S1/S2 time-zero definition is kept below $1 \mu\text{s}$ by enforcing a common leading-edge criterion; this residual offset propagates as $\delta v_d/v_d = \delta t/\Delta t$ and is typically $\leq 0.1\%$.

PURITY/ATTACHMENT

Electron lifetime is measured continuously with periodic dispersed source injections, for example $^{83\text{m}}\text{Kr}$. For each run we take the lifetime uncertainty and convert it to a plateau-velocity shift via the empirical Yoshino scaling $v_{\text{sat}}(\tau_e) \propto 1 - e^{-\Delta t/\tau_e}$.

MODEL DEPENDENCE

Each field is modelled with three smooth saturation forms:

- a two-parameter tanh model with $v_{\text{sat}} = 1.4913 \text{ mm}/\mu\text{s}$, $\mu_0 = 0.03060 \text{ mm}/\mu\text{s} (\text{V}/\text{cm})^{-1}$

$$v_d(E) = v_{\text{sat}} \tanh(\mu_0 E / v_{\text{sat}})$$

- a NEST v2.4.0-like Hill/Richards form with

$$A (\text{mm}/\mu\text{s}), k (\text{V}/\text{cm}), n = 1.5616544, 183.66199642, 5.30557223$$

$$v_d(E) = A[1 - (1 + E/k)^{-n}]$$

- a NEST v2.3.8-like poly-exponential with parameters

$$[-0.804, 2188, -0.4, 468, -1.4, 33.8, 2.6] \text{ in the following expression (for } c (\text{mm}/\mu\text{s}), a_i (\text{mm}/\mu\text{s}), b_i (\text{V}/\text{cm}))$$

$$v_d(E) = c + \sum_{i=1}^3 a_i e^{-E/b_i},$$

Here $v_{\text{sat}} = \lim_{E \rightarrow \infty} v_d$ and $\mu_0 = \partial v_d / \partial E|_{E \rightarrow 0}$.

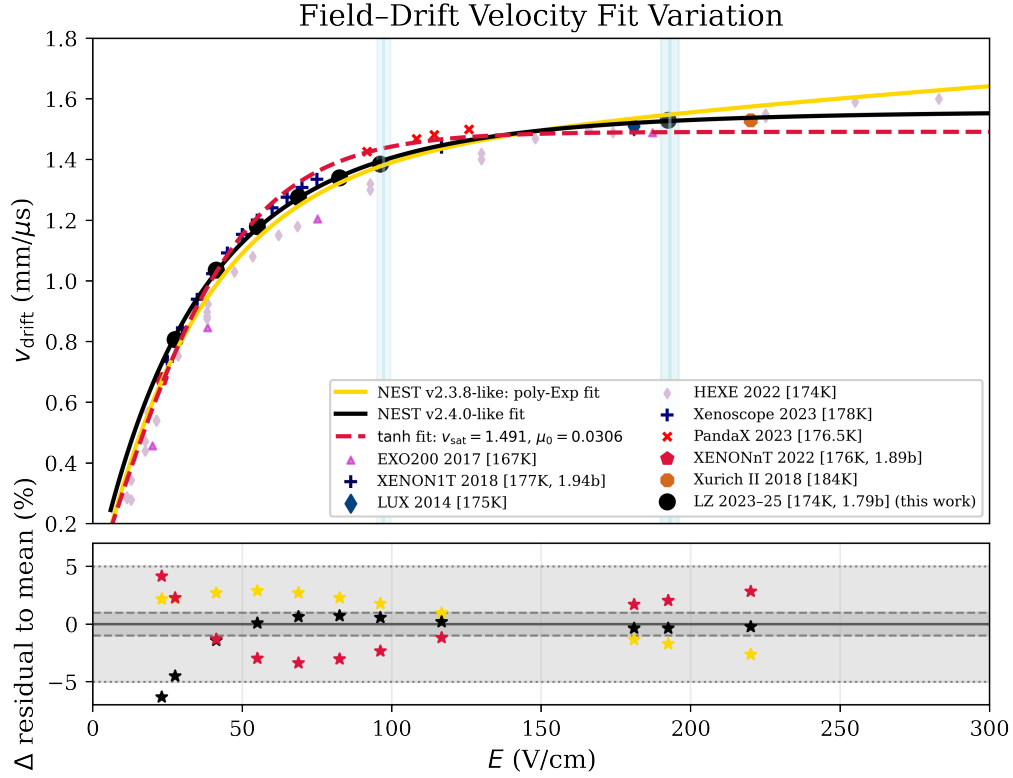


Figure 3.8: Fitting the electron drift velocity in liquid xenon as a function of the electric field. Curves show three smooth parametrisations: a NEST v2.3.8-like poly-exponential fit (gold), a NEST v2.4.0-like Hill/Richards form (black), and a two-parameter tanh fit (red dashed). The tanh curve yields $v_{\text{sat}} = 1.491 \text{ mm } \mu\text{s}^{-1}$ and $\mu_0 = 0.0306 \text{ mm } \mu\text{s}^{-1} (\text{V cm}^{-1})^{-1}$. Points include the LZ 2022–24 series at $T = 174 \text{ K}$, $P = 1.79 \text{ bar}$ (black), and selected other literature measurements. Vertical shaded bands mark the LZ drift fields for WS 2024 and 2022, respectively. **Bottom:** Percent residuals for the LZ measurements plotted as each model’s deviation from the model-mean at the same E ; grey bands indicate $\pm 1\%$ and $\pm 5\%$ inter-model spread. The figure demonstrates three conventional choices for the parametrisation of drift velocity as a function of E field and visualises the extent of deviation between the functional fits and experimental data.

The model uncertainty is taken as the full spread of the fitted plateau values v_{sat} across the three parametrisations and applied uniformly in E (typically 0.5–1.0%). Within the LZ operating range ($\sim 90\text{--}195 \text{ V cm}^{-1}$) the three forms agree to within a few percent; the residual panel in Fig. 3.8 visualises the inter-model spread with $\pm 1\%$ and $\pm 5\%$ guide bands.

STATISTICS

For every field configuration, the gate-cathode drift time distribution is fit with a gaussian or skew-gaussian; the statistical contribution to the error can be approximated by $\sigma_t / \sqrt{N} \langle \Delta t \rangle$, corresponding to typically $\sim 0.03 - 0.05\%$.

The Momentum Transfer Cross-Section

The electron momentum-transfer cross section, σ_{mt}^{eff} , quantifies the effective probability for an electron to scatter off an atom with momentum exchange. Unlike a simple elastic cross section, it weights collisions by $1 - \cos \theta$ (with θ the scattering angle), emphasising the degree of forward-momentum loss [121]. In this way, σ_{mt}^{eff} captures how efficiently collisions impede electron drift through a medium. This parameter directly governs macroscopic transport: the drift velocity v_d is roughly inversely proportional to σ_{mt} [121], while diffusion coefficients are likewise sensitive to its energy

²This is a dedicated technote written by the author addressing and modelling the impact of deflection.

dependence.

In gaseous xenon, $\sigma_{mt}(\varepsilon)$ exhibits the well-known Ramsauer-Townsend minimum near 0.5–1 eV: in gas, this is defined as the point where the cross section becomes exceptionally small, leading to a pronounced, localised peak in electron mobility [106]. In *liquid* xenon (LXe), however, dense-medium effects smear out such features: screening of the electron-atom potential and coherent scattering off neighbouring atoms suppress both the Ramsauer minimum and the forward-scattering peak. The result is a smoother, more uniform σ_{mt}^{eff} that is smaller in magnitude than in gaseous Xe across the sub- eV regime relevant to dual-phase TPCs [106, 121, 131]. This explains why electron mobility in LXe increases monotonically with field rather than exhibiting a distinct maximum³.

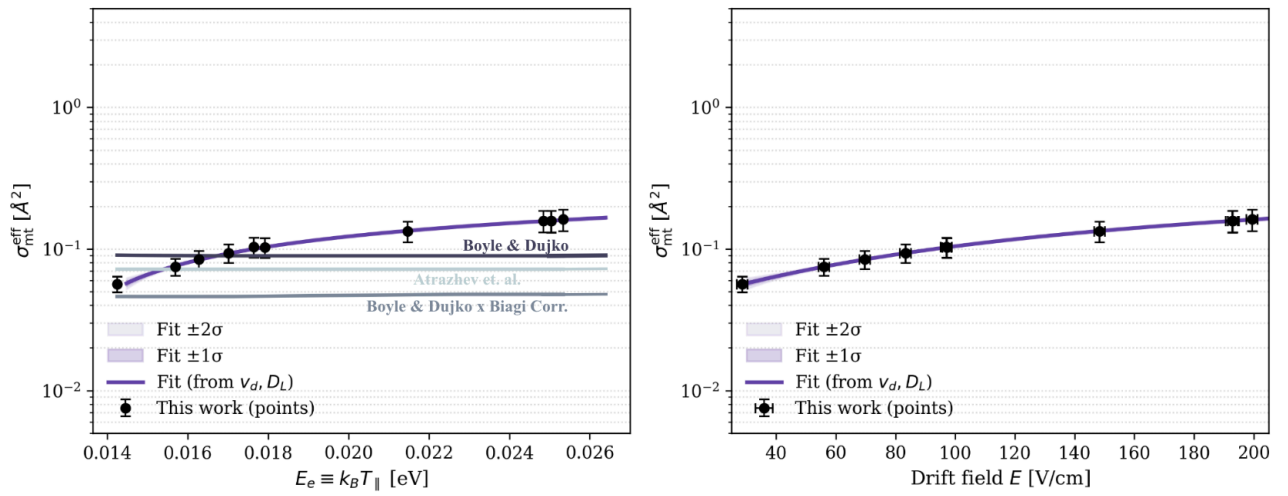


Figure 3.9: Effective electron momentum–transfer cross section in LXe. Black points with errors are calculated from v_d and D_L fits in this work; a 1σ band is also overlaid. Theory bands feature results from Boyle & Dujko, Biagi and Atrazhev [106]. Data then show the expected gentle rise/curvature ($\propto E/(v_d\sqrt{T_{\parallel}})$) and a small high-field ($\gtrsim 100$ V/cm) excess.

Although LZ’s operating regime spans only a narrow energy band near $E_e \simeq 0.02$ – 0.04 eV, it still allows comparisons to these models. From the measured drift velocity and longitudinal diffusion coefficient, an *effective* momentum-transfer cross section can be derived under the assumption of a Maxwellian electron-energy distribution function (EEDF)⁴. Starting from the momentum-balance equation and the Einstein relation [131],

$$m_e \nu_m v_d = eE, \quad (3.13)$$

$$D_L = \mu \frac{k_B T_{\parallel}}{e}, \quad \mu = \frac{v_d}{E}, \quad (3.14)$$

where D_L is the longitudinal diffusion coefficient (discussed in the next section), we write

$$\sigma_{mt}^{eff} = \frac{\nu_m}{n\langle v \rangle} = \frac{eE}{m_e v_d n \langle v \rangle}, \quad \langle v \rangle \simeq \sqrt{\frac{8k_B T_{\parallel}}{\pi m_e}}. \quad (3.15)$$

³By comparison, liquid argon has been mapped more directly via dedicated swarm measurements, whereas LXe has relied mainly on indirect inference from v_d and diffusion, motivating the model-based liquid treatments used below [107].

⁴I.e. electrons in thermodynamic equilibrium with the medium they are in. This is handy; the expression is valid for the “cold electron” regime by definition so any deviations in the expected behaviour will immediately hint at non-thermal conditions and the onset of a “hot electron” regime.

Here n is the xenon atom number density, and $T_{\parallel}$ is an effective electron temperature inferred from D_L , the longitudinal diffusion coefficient. This approximation provides a useful macroscopic-to-microscopic mapping, but may overestimate σ_{mt} once the EEDF departs significantly from the Maxwellian form at higher fields.

Fig. 3.9 shows σ_{mt}^{eff} inferred from LZ data versus both drift field and effective electron energy. Values lie in the range $0.05\text{--}0.18 \text{ \AA}^2$ ($5 \times 10^{-22}\text{--}2 \times 10^{-21} \text{ m}^2$) and track liquid expectations: within uncertainties the points overlap the *coherent-elastic* Boyle–Dujko calculation (structure-factor weighted), a *Biagi-rescaled* variant that maps gas cross sections to the liquid phenomenologically, and the *Atrazhev* pseudopotential treatment that embeds polarization and multiple-scattering effects [106, 121, 132].

Two brief comments. First, the data exhibits a gentle up-curvature while the theory bands are nearly flat. This follows directly from the mapping

$$\sigma_{mt}^{\text{eff}} \propto \frac{E}{v_d \sqrt{T_{\parallel}}},$$

so as E increases, $v_d(E)$ tends to saturate while $T_{\parallel}$ grows with the $\sqrt{\cdot}$, yielding an apparent rise in σ_{mt}^{eff} even for a featureless microscopic $\sigma_{mt}(\varepsilon)$ so one should be careful of this bias. Second, at $E \gtrsim 100 \text{ V/cm}$ the rise is slightly stronger than the (nearly flat) coherent-elastic curve, which is *consistent* with the onset of hot-electron transport discussed in §4.4.2: a modest elevation of T_e and quasi-inelastic coupling to collective modes (captured most naturally by Atrazhev, and mimicked by energy-dependent Biagi rescaling), rather than electronic inelasticity. A smaller contribution from mild Einstein-relation breakdown or additional weak momentum-loss channels thus cannot be excluded without higher- E/N data but cannot be confirmed either.

Overall, the inferred sub-eV σ_{mt}^{eff} agrees in scale and trend with liquid-phase expectations, with only a mild high-field rise. Results are compatible with coherent scattering and screening, and motivate broader measurements to clarify hot-electron contributions. We now examine $D_L(E)$ to track $T_{\parallel}$ and assess more directly the onset of Einstein-relation deviations.

3.2 Measurement of the Longitudinal Diffusion Coefficient in LXe

Electrons produced in liquid xenon drift under an applied field, while undergoing frequent elastic and inelastic collisions with the medium. These collisional random walks broaden the charge packet both along the field and across it. We quantify the axial component by the longitudinal diffusion coefficient D_L (the transverse component by D_T). In dual-phase xenon TPCs, D_L is the principal driver of the time-domain width of the S2 signal, and therefore feeds directly into z -reconstruction, pulse-shape modelling, and resolution.

For an initially compact packet that drifts for a time t_d at velocity v_d , the S2 time variance separates naturally into a drift-independent intercept and a drift-dependent diffusive term,

$$\begin{aligned} \sigma^2 &= \sigma_0^2 + \sigma_L^2 \\ &= \sigma_0^2 + \frac{2D_L}{v_d^2} t_d. \end{aligned} \tag{3.16}$$

Here, σ_0 is the zero-drift S2 width set by the detector geometry and light-production chain, chiefly the emission-time distribution at the liquid–gas interface, the finite thickness (and any vertical non-uniformity) of the electroluminescence region, photon time-of-flight dispersion, and PMT/electronics timing and reconstruction. The term $\sigma_L(t_d)$ is the diffusive growth arising from the random walk along the field; it increases strictly with drift time and encodes D_L . As the field drives motion along z while the liquid offers different channels to randomise momentum and dissipate energy in the axial and transverse directions, the transport is naturally anisotropic ($D_L \neq D_T$ [cm^2/s]).

This decomposition is practically useful. The pair (D_L, σ_0) sets an intrinsic S2 time-resolution floor and can be used to define a predictable diffusion band in σ as a function of t_d that genuine single scatters populate across the active volume. Events inconsistent with this band, accidental pile-ups, mis-classified edge pulses, or interactions in regions of strong field distortion, tend to sit systematically off-band and can be rejected at high efficiency. In S2-only analyses (chapter 5), the same relation could provide a z -proxy when S1 is absent; in standard WIMP searches it stabilises resolution modelling and improves background control [133]. More broadly, relating D_L to the local drift field gives a dynamic description of S2 broadening: small spatial/temporal field variations within a nominal voltage setting (see chapter 4), and changes of configuration between runs, map directly into changes of σ .

In the following, we perform a measurement of D_L throughout LZ’s operation, from the expected growth of σ^2 as a function of t_d , using a model-light width estimator on standard WS data, and compare with an independent waveform/IRF-based extraction that supplies an external intercept anchor. The methodology is outlined next; quantitative field-dependence and uncertainty budgets are then discussed.

3.2.1 Methodology

For drift–velocity we relied on grid alphas as bright, stable “standard candles”. For diffusion this would be unsafe. Alpha decays create compact, high–charge electron packets whose self–field induces an outward drift (Coulomb repulsion) in addition to stochastic broadening from collisions. Coulomb broadening is largest immediately after emission and decays roughly as $1/\omega_{\parallel}$ (the longitudinal width of the electron cloud along the drift direction) as the charge cloud expands. In the Njoya et. al. ODE picture, $d\omega_{\parallel}/dt = \beta E_{\parallel} + 2D_L/\omega_{\parallel}$ with $E_{\parallel} \propto Q/\omega_{\parallel}$; thus early–time Coulomb broadening can mimic an increased D_L [80, 124, 134], while at later times its contribution is effectively t_d -independent and can be absorbed into σ_0 . This analysis therefore excludes grid–adjacent slices and high–area (alpha-like or saturated) pulses from the broader selection of moderate–charge S2s drawn from the same WS and field–campaign data used in the drift–velocity calculation.

The longitudinal diffusion coefficient, D_L , is then extracted from the drift–time dependence of the S2 temporal variance (equation 3.16). In practice, the Gaussian width σ is not measured directly. Instead we use an area–fraction time (AFT) metric as a proxy⁵: the time at which a given fraction of the total integrated pulse area has arrived relative to its start time T_0 . For a Gaussian pulse,

$$R = \frac{1}{2} \operatorname{erf}\left(\frac{\text{AFT}_R - T_0}{\sqrt{2}\sigma}\right) + \frac{1}{2}, \quad \Rightarrow \quad \text{AFT}_R - T_0 = \sqrt{2}\sigma \operatorname{erf}^{-1}(2R - 1). \quad (3.17)$$

⁵This methodology has also been used in D. Hunt’s work [133] to define a drift-dependent S2-width-based cut to reject accidental coincidences across WS data. A complementary study of diffusion was also conducted by him as a result with different data selections.

The AFT width between two area fractions $a < b$ is therefore

$$w_{[a,b]} \equiv \text{AFT}_b - \text{AFT}_a = \underbrace{\sqrt{2} [\text{erf}^{-1}(2b-1) - \text{erf}^{-1}(2a-1)]}_{k_{[a,b]}} \sigma, \quad (3.18)$$

so that $\sigma = w_{[a,b]}/k_{[a,b]}$. We adopt symmetric AFT definitions (e.g. 25–75%, 10–90%, 5–95%) to suppress baseline and tail fluctuations; for these the scale factors are $k_{[25,75]} \simeq 1.349$, $k_{[10,90]} \simeq 2.563$, and $k_{[5,95]} \simeq 3.289$. This mapping is valid whenever the underlying S2 slices are approximately Gaussian; all selections below (moderate charge, non-saturated, away from grids and walls) are designed to enforce that regime.

Substituting $\sigma = w_{[a,b]}/k_{[a,b]}$ into $\sigma^2(t_d) = \sigma_0^2 + (2D_L/v_d^2) t_d$ leads to the working fit model in terms of the measured AFT width,

$$w^2(t_d) = w_0^2 + k_{[a,b]}^2 \frac{2D_L}{v_d^2} t_d, \quad w_0 \equiv k_{[a,b]} \sigma_0, \quad (3.19)$$

where the intercept encodes w_0 encodes the drift-independent broadening and the slope yields D_L . For our default 25–75% choice ($k_{[25,75]} = 1.349$) this reduces to

$$w^2(t_d) = w_0^2 + \underbrace{3.64}_{(1.349)^2 \times 2} \frac{D_L}{v_d^2} t_d, \quad (3.20)$$

providing the working expression used in the subsequent fits.

Finally, the extraction proceeds by fitting equation 3.19 (default form equation 3.20) in τ -bounded windows of drift time, excluding regions close to the grids. Cross-checks across AFT definitions for width, S2-area slices, and radial annuli define systematic envelopes, which are propagated into the final uncertainty budget (§3.2.3).

3.2.2 Field Dependence of Longitudinal Diffusion Coefficient

The measured longitudinal diffusion coefficients from LZ are shown in Fig. 3.10 and summarised in table 3.4. Our measurements span the transition between the low-field “cold-electron” regime and the high-field “hot-electron” plateau as described in §3.1.4, with a continuous description provided by a NEST-inspired fit. At the lowest drift fields ($< 50 \text{ V/cm}$), D_L rises steeply, reaching values of order $40 - 50 \text{ cm}^2/\text{s}$, while at higher fields ($E \gtrsim 150 \text{ V/cm}$) the coefficient declines to $\sim 20 \text{ cm}^2/\text{s}$ at $\sim 193 \text{ V/cm}$ exhibiting asymptotic behaviour. This field dependence reflects the competition between electron cooling via frequent elastic collisions with xenon atoms and heating from the applied drift field, as described in the Cohen–Lekner framework[109].

A central feature of our results is that the LZ measurements at $175 \pm 1 \text{ K}$ form the lowest set of diffusion points published to date. The closest comparison is XENON1T, which operated at 177 K and reports values within $1 - 2\sigma$ of our NEST-based fit across the accessible field range [80]. This consistency likely reflects the common dual-phase operating conditions: both experiments run close to the xenon saturation curve (at $175 - 177 \text{ K}$) with high electron survival ($\gtrsim 80\%$ over meter-scale drifts in LZ, $\sim 20 - 40\%$ over 97 cm in XENON1T). In contrast, the Xenoscope experiment, operated at 178 K and 2.05 bar , reported systematically higher values of D_L in the cold-electron regime

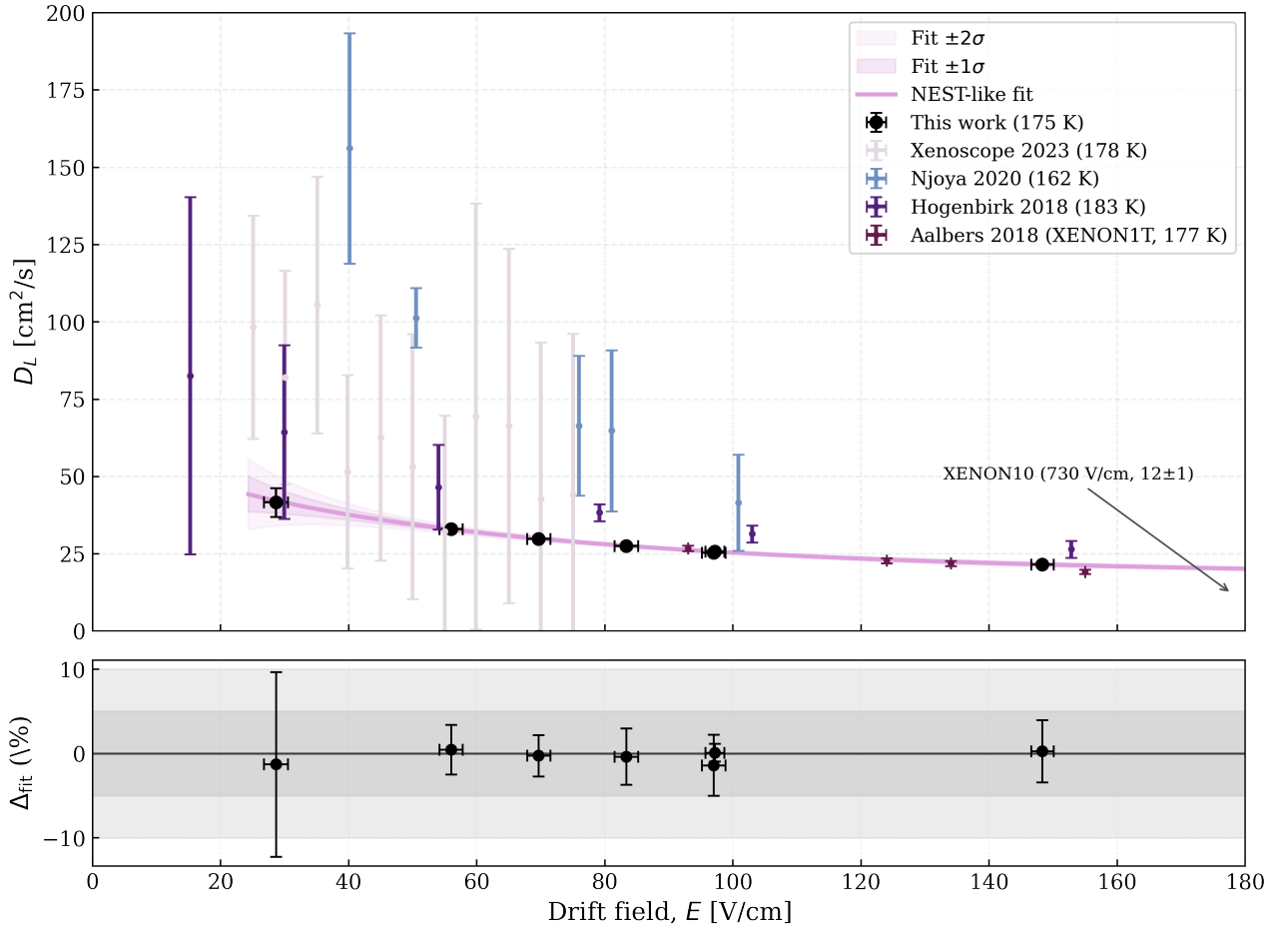


Figure 3.10: Longitudinal diffusion coefficient D_L as a function of drift field in LXe. Black points show this work (175 K), with the pink band indicating a NEST-inspired fit ($\pm 1\sigma$, $\pm 2\sigma$). External measurements are overlaid for comparison: Xenoscope (178 K, 2.6 m drift) [111], Njoya (162 K) [124], Hogenbirk (183 K) [122], and Aalbers (XENON1T, 177 K) [80]. LZ and XENON1T, both dual-phase detectors operating near the xenon saturation line with long lifetimes, yield the lowest D_L values, consistent with a hot-electron plateau of $\sim 20 \text{ cm}^2/\text{s}$. Higher diffusion observed in Xenoscope and earlier small-scale measurements is attributed to reduced electron survival, purity limitations, and analysis methodology, particularly in the cold-electron regime. The residuals panel shows fractional deviations of the measured D_L from LZ data in this work from the global fit, illustrating sub-percent agreement across LZ drift configurations. The XENON10 data point corresponds to a substantially higher drift field ($\sim 730 \text{ V/cm}$) than the range explored in this work and is therefore not included in the field-scan region of the figure, but is shown separately as an external reference.

[111]. With a drift length of 2.6 m but only a maximum $\tau_e \sim 600 \mu\text{s}$ [111], a less than 20% expected end-to-end electron survival rate makes the diffusion measurement more vulnerable to purity-driven biases and selection effects. This difference in survival probability provides a natural explanation for the divergence between LZ and Xenoscope at $E \lesssim 50 \text{ V/cm}$, while agreement is restored in the plateau regime where electron heating dominates over purity systematics.

Temperature-dependence remains the most open question. The Njoya et. al. study across 162 – 183 K concluded no clear correlation, with a weak upward trend at high temperature consistent with zero within uncertainties [124]. Nevertheless, the fact that LZ and XENON1T - at $\sim 175 - 177 \text{ K}$ - yield lower D_L than Hogenbirk et. al.’s 183 K results [122] suggests some residual T -dependence cannot be excluded. Reconciling this with Njoya et. al.’s conclusion may require attention to experimental details: Hogenbirk’s measurement employed shorter drift distances of $\sim 10 \text{ cm}$ (of

A/G/C Config	E (V/cm)	δE (V/cm)	D_L (cm ² /s)	δD_L	
				stat	syst
+1.5/-6/-10	28.6326	1.8607	41.6664	0.0315	4.6312
+1.5/-6/-14	55.9693	1.8171	33.0998	0.0177	0.9711
+1.5/-6/-16	69.6457	1.8162	29.8678	0.0127	0.7350
+1.5/-6/-18	83.3241	1.8249	27.5022	0.0098	0.9279
+1.5/-6/-20	97.0037	1.8417	25.4011	0.0098	0.9305
+1.5/-6/-34	192.7722	2.1392	19.6808	0.0064	0.5437
+3.5/-3.5/-25	148.2989	1.7667	21.6333	0.0149	0.7931
+2/-6/-34	192.8647	2.2119	19.8225	0.0315	0.7565
+3/-3/-32	199.4383	1.8348	19.4420	0.0138	0.9211
+4/-4/-32	192.9831	1.6853	19.8107	0.0139	0.4859
+3.5/-4/-18	97.1794	1.4845	25.7652	0.0020	0.2687

Table 3.4: Summary of longitudinal diffusion measurements. The systematic uncertainty on D_L is computed in quadrature from contributions due to AFT, area/acceptance, radial envelope, lifetime, and v_d systematics. Statistical uncertainties are the fit errors on the $w(t)$ slope.

which $\sim$ one-third was used for the actual fit) and a similar method to that used here to extract D_L . Along with this, varying definitions of the S2 width and potential biases from a pure NEST v_d model dependence, rather than a per-field in-situ determination, could amplify the impact of photon-flight-time spread and non-Gaussian tails, particularly at intermediate fields where the diffusion slope is shallow. Similar concerns apply to earlier measurements. Using our global fit, we predict $D_L(730 \text{ V/cm}) = 15.1 \text{ cm}^2/\text{s}$, about 25% above the XENON10 value $D_L = 12 \pm 1 \text{ cm}^2/\text{s}$ [105]. However, given the higher-field operating point, slightly cooler xenon, and analysis differences (short-drift leverage and deconvolution model), this level of tension is compatible with a modest downward trend expected in the hot-electron limit and residual systematics at very high field.

In summary, the LZ results extend the body of LXe diffusion measurements into the lowest statistical and systematic uncertainty regime achieved to date. They confirm the expected hot-electron plateau, highlight the experiment-specific biases that complicate the cold-field region, and underscore the need for controlled temperature-dependence studies to resolve the apparent inconsistencies across the 160 – 185 K range.

3.2.3 Systematics

Accurate determination of the longitudinal diffusion coefficient, D_L , demands a careful treatment of systematic effects. As the data selection and fitting strategy differ substantially from those used for the drift-velocity measurement, we evaluate the D_L systematics separately. The same set of effects is assessed at every drift-field setting using a common procedure. Table 3.5 summarises the source, treatment and typical size of each uncertainty, illustrated with results from the anode= +3.5 kV, gate= -4 kV, cathode= -18 kV (+3.5/ - 4/ - 18 kV) configuration (WS 2024). The individual contributions are described in detail below.

COULOMB REPULSION

Our working fit model in the τ -bounded window is

$$\sigma^2(t) \simeq \sigma_0^2 + \frac{2D_L}{v_d^2} t_d, \quad (3.21)$$

Table 3.5: Summary of D_L uncertainty sources and evaluation procedure. The rightmost column gives example absolute uncertainties (cm^2/s) for the $+3.5/-4/-18 \text{ kV}$ configuration (WS 2024), where $D_L = 25.765 \text{ cm}^2/\text{s}$.

Source	Column	What it captures	How it is estimated	Example
AFT choice	aft_sys	Global S2 shape variance: mapping of AFT width to Gaussian σ (sensitivity to non-Gaussian tails, electronics, EL/emission timing).	Repeat full extraction with symmetric AFTs (75–25, 90–10, 95–5); take half-range in D_L .	0.214
S2 area / Coulomb	area_sys	Charge-density (space-charge) broadening and acceptance/selection composition versus area.	Bin in S2 area; take half-range across area slices at fixed r .	0.155
Radial envelope	rad_sys	Combined effects that vary with radius: curved paths from E_r (path length bias), photon-TOF/instantaneous shape, and area mix.	Repeat extraction in radial annuli; take half-range across annuli.	0.041
τ window	tau_sys	Sensitivity to drift window boundaries (gate/cathode proximity; residual time-dependent intercept).	Scan $N_\tau \in [1.5, 3.0]$ in $t_{\text{lo,hi}}$; take half-range in D_L .	0.008
Drift velocity	vd_sys	Propagation from v_d used in $D_L = \frac{1}{2}bv_d^2$. Correlated per field.	First-order propagation $\delta D_L _{v_d} = 2(\delta v_d/v_d)D_L$ using in-situ v_d .	0.028
Statistics	stat	Fit uncertainty on slope b of $y(t) = (w/k)^2$ (per A/G/C field).	Linear fit uncertainty (per-slice averages) in the τ -bounded window.	0.002
Total (sys $\oplus$ stat, quadrature):				0.269

with all non-diffusive broadening absorbed into the intercept σ_0 . It is useful to view σ_0 as a combination of physically distinct, largely field-weak contributions:

$$\begin{aligned}
\sigma_0^2 = & \underbrace{\sigma_{\text{elec}}^2}_{\text{electronics shaping}} + \underbrace{\sigma_{\text{PMT}}^2}_{\text{PMT transit time spread}} + \underbrace{\sigma_{\text{TOF}}^2(r, z)}_{\text{photon flight paths}} \\
& + \underbrace{\sigma_{\text{emit}}^2(E_{\text{extr}})}_{\text{liquid emission time}} + \underbrace{\sigma_{\text{EL}}^2(E_{\text{gas}})}_{\text{EL production time}} + \underbrace{\sigma_{\text{rep}}^2(N_e)}_{\text{space charge}}. \quad (3.22)
\end{aligned}$$

Space-charge (Coulomb) broadening $\sigma_{\text{rep}}(N_e)$ arises when the cloud is dense near emission and saturates quickly as the cloud expands (self-field $\propto 1/\sigma^2$). Over our fit window the residual time-dependence is negligible, so we assume Coulomb acts as a *field-weak, t_d -independent* component of σ_0 and does not bias the slope b .

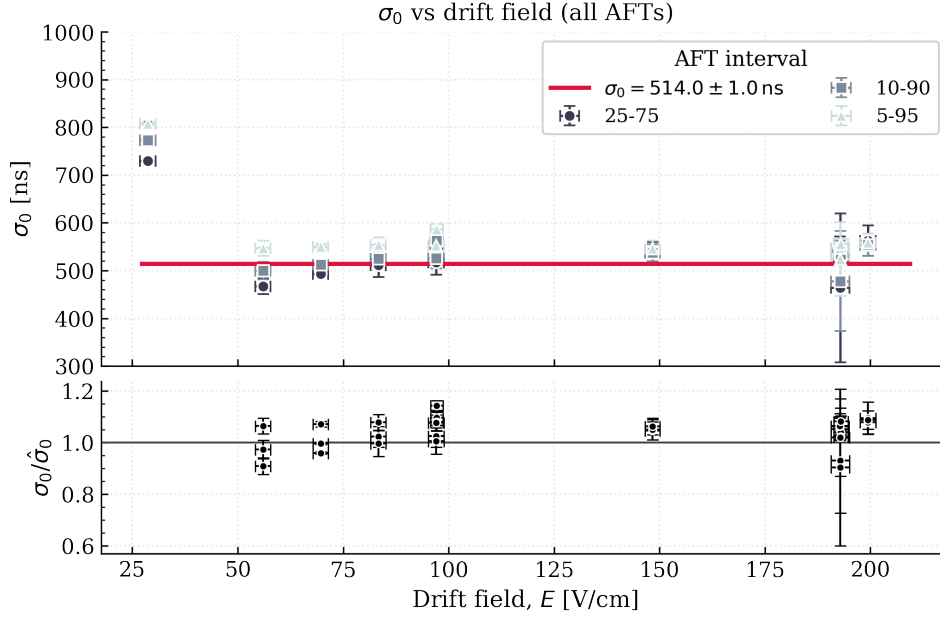
Two controls enforce this. First, we reject high-charge α S2s explicitly; a tag-and-veto spectrum (based on S1 TBA and area selections) check yields $< 1\%$ α contamination in every dataset. Second, we repeat the analysis in S2-area slices (proxy for N_e) and take the half-range of the resulting D_L values as the *area (Coulomb)* systematic. The near-linearity of $y(t) = (w/k)^2$ within the window and the absence of curvature corroborate that any residual $d\sigma_{\text{rep}}^2/dt$ is small. Fig. 3.11 further shows that σ_0 is consistent with a constant above $\sim 55 \text{ V/cm}$ (for similar extraction region voltages) across AFTs, supporting this treatment.

DRIFT WINDOW SELECTION

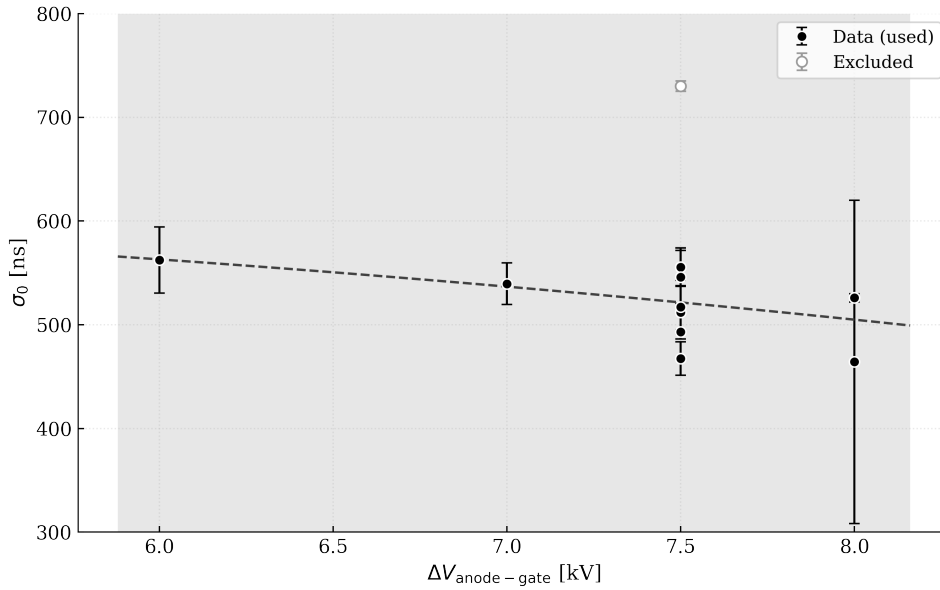
To avoid regions where the spectrum is shaped by extraction/EL microphysics (near the gate) or by RFR contamination/ general near-grid or cathode effects (near the bottom), we fit in a τ -bounded window,

$$t_{\text{lo}} = \mu_{\text{gate}} + N_\tau \sigma_{\text{gate}}, \quad t_{\text{hi}} = \mu_{\text{cath}} - N_\tau \sigma_{\text{cath}}. \quad (3.23)$$

Increasing N_τ reduces contamination from edge physics but shortens the lever arm in t ; decreasing N_τ increases lever arm but risks shape systematics. We scan $N_\tau \in [1.5, 3.0]$ and take the *half-range in D_L* as the τ window systematic. Since this variation probes a possible t -dependence of the intercept terms in equation (3.22), it is largely independent



(a) Fitted S2 widths extrapolated to zero drift, σ_0 , as a function of drift field for three symmetric AFT definitions.



(b) σ_0 versus anode-gate voltage difference, ΔV_{AG} .

Figure 3.11: σ_0 is stable above ≈ 55 V/cm, with the lowest-drift field bin excluded due to broadened, non-Gaussian slices. A mild dependence is seen, consistent with extraction/EL fields influencing the instantaneous S2 shape. A weak Gaussian fit is shown, as we expect electrostatic deflection to scale with the ΔV^2 , naturally translating to a shift in width (§6.2.3). While the drift field itself is not the dominant factor, leakage of near-gate field distortions at very low drift fields may further broaden S2s, reinforcing that σ_0 carries both extraction-region and drift-field contributions, amongst others.

of the radial and area systematics.

GLOBAL S2 SHAPE VARIANCE

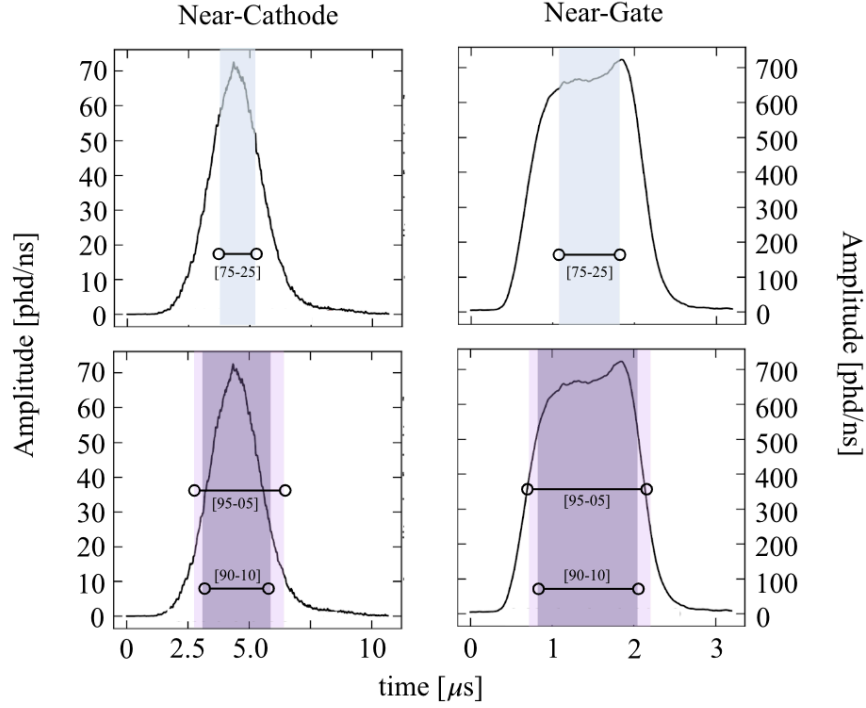


Figure 3.12: S2 width in near-cathode and near-gate slices using $AFT_{75} - AFT_{25}$ (top) and $AFT_{90} - AFT_{10}$, $AFT_{95} - AFT_{05}$ (bottom) - the shaded bands represent these intervals for clarity. $AFT_{75} - AFT_{25}$ is the most stable; wider spans aid morphology discrimination but increase sensitivity to pulse-shape systematics. This trade-off is an important consideration in studies where signal-background discrimination is particularly important as in Chapter 5.

Even within a “clean” selection window, the instantaneous S2 waveform is not perfectly gaussian and varies mildly with conditions (σ_{emit} , σ_{EL} , electronics⁶). Our fit uses AFT widths mapped to a gaussian σ via fixed factors k_{AFT} ; if the pulse deviates from a gaussian, the mapping can shift the intercept and, if it varies with t_d , induce a small slope bias. We bound this by repeating the full analysis with three symmetric AFT intervals (75 – 25, 90 – 10, 95 – 5 as in Fig. 3.12) and taking the half-range in D_L as the *AFT-choice* systematic. Fig. 3.11 shows that σ_0 is also consistent across these AFTs, while the lowest-field bin (excluded from the constant fit) exhibits broader, less gaussian near-gate slices (right panels), precisely where σ_{emit} and σ_{EL} dominate. This justifies the AFT-spread treatment and explains the isolated low-field deviation without affecting the D_L slope at higher fields.

DETECTOR CONDITION: DRIFT VELOCITY, TEMPERATURE, PRESSURE & RADIAL FIELDS

Looking back to the fit procedure described in the methodology section, our estimator for D_L was

$$D_L = \frac{1}{2} b v_d^2, \quad (3.24)$$

⁶Minor fluctuations of $\mathcal{O}(10\text{ s})$ ns in width have been seen to occur with time (within hour-long periods).

with b the slope of $y(t) \equiv (w/k)^2$ as a function of drift time t_d and v_d the drift velocity. A first-order propagation gives

$$\delta D_L|_{v_d} = |b| v_d \delta v_d = 2 \frac{\delta v_d}{v_d} D_L, \quad (3.25)$$

which we evaluate per field from the same runs (gate-cathode timing). This term is taken as *fully correlated* across radii and AFT choices at a given field. We also note that it is expected that electron lifetime will affect the S2 area more than the width-slope relation, and is therefore handled under the “area (Coulomb)” systematic.

Furthermore, near the wall the drift field acquires a radial component; charges follow slightly longer *curved* paths⁷. If the true path length is $\ell = L_z(1 + \epsilon)$ for a vertical drift L_z , both the measured slope and v_d scale as $t \rightarrow (1 + \epsilon)t$ and $v_d \rightarrow v_d/(1 + \epsilon)$. With $(w/k)^2 = a + bt$, the measured coefficient becomes

$$\frac{D_{L,\text{meas}}}{D_{L,\text{true}}} \approx \frac{1}{(1 + \epsilon)^3} \approx 1 - 3\epsilon \quad (\epsilon \ll 1). \quad (3.26)$$

Numerically, a 3 cm detour over $L_z \sim 146$ cm ($\epsilon \simeq 0.020$) would bias D_L down by $\sim 6\%$ in the outer annulus; 1 cm and 0.5 cm detours correspond to $\sim 2\%$ and $\sim 1\%$. WS 2024 shows the largest outer-annulus bias (Fig. 4.38), sometimes encroaching into the fiducial volume, whereas WS 2022 field maps suggest $\lesssim 0.5$ cm (and very localised near-wall). A conservative central-annulus estimate for the other configurations is ~ 1 cm.

At the same time, composition and shape systematics push in the opposite direction and can dominate in some runs: (i) S2 charge/light losses and acceptance effects reduce the area toward large r ; empirically, smaller S2 areas carry a larger fitted D_L (top panels of Fig. 3.13). If radial bins differ in their area mix, the outer annulus inherits a higher D_L even for identical microphysics. (ii) Photon time-of-flight and instantaneous S2-shape changes with r can produce small positive slopes of $w(t)$ that survive the AFT mapping. In LZ the tuned field maps show that E_z decreases with r near the wall (primarily from deflection). Since lower E_z increases the true/average D_L , a positive $D_L(r)$ can therefore include a genuine microphysics component. This balance explains the trends in Fig. 3.13: WS 2024 is more prone to a large charge-loss region than WS 2022, owing to stronger near-wall field distortions, ultimately leading to an inflated D_L . That said, detector/selection effects (S2-area composition and residual photon-TOF/EL shape) also push positive, so we treat the net radial trend conservatively as a systematic rather than a physics signal.

We therefore do not fit a universal radial slope. Instead, we repeat the full extraction in independent annuli and take the half-range across annuli as the radial envelope. This predominantly captures the combined impact of curved paths (see discussions in Chapter 4) and area/shape composition, is uncorrelated between annuli, and is treated as correlated across AFT choices at a fixed field.

Finally, thermodynamic variations enter in two ways: (i) through $v_d(T, P)$ - already covered by δv_d above - and (ii) through a genuine $D_L(T)$ dependence. In our data, a vertical gradient of $\sim 1.5 - 2$ K exists⁸ but within each τ -bounded fit window the effective span becomes smaller and we observe no curvature in $y(t)$ nor any N_τ -scan trend. Consistently, an IRF-based slope study featuring waveforms sampled with t_d , showed $< 1\%$ drift-time dependence

⁷Much more on this in §4.7.

⁸Higher at the top of the TPC, calculated from gas pressure vs temperature sensors at the bottom of the TPC.

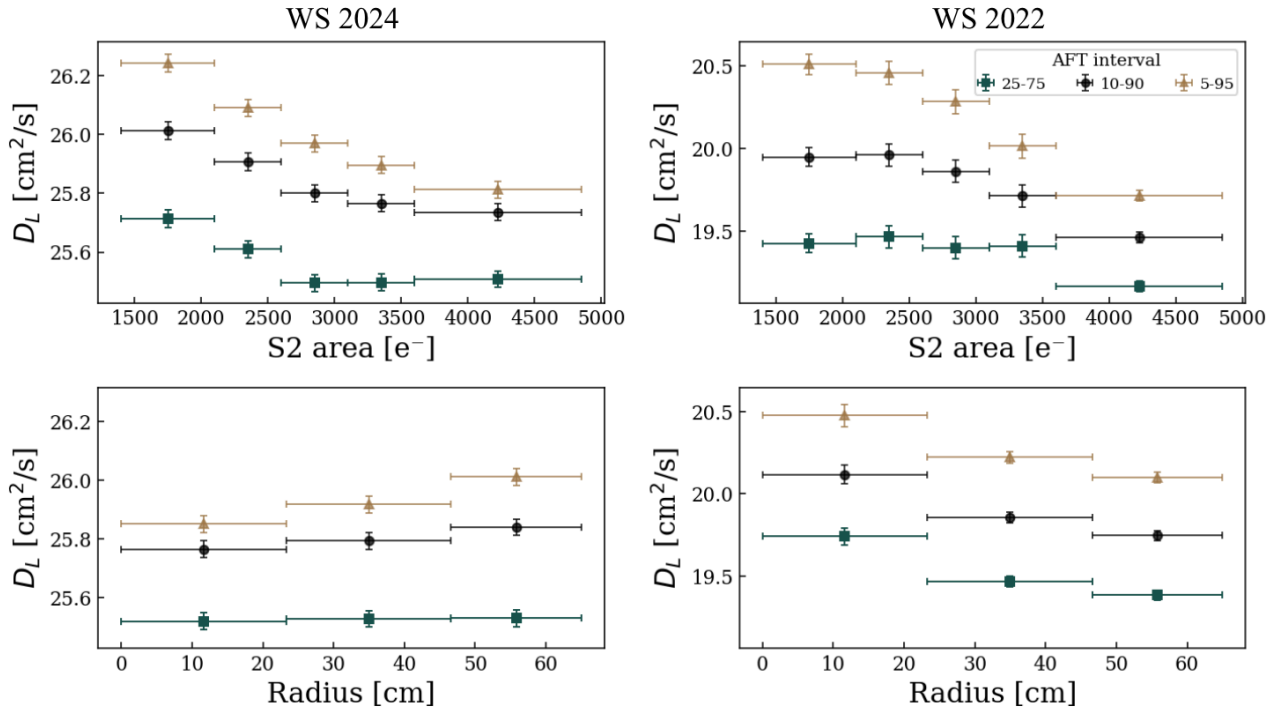


Figure 3.13: D_L stability checks at two representative fields. **Top:** D_L versus S2 area in fixed radial acceptance shows a consistent area dependence (smaller area $\rightarrow$ larger fitted D_L). **Bottom:** D_L versus reconstructed radius shows a run-dependent trend: WS 2024 rises with r (composition/shape/field effects dominate), whereas WS 2022 falls slightly with r (shape/curved-path effect dominates). Error bars are statistical; the systematic envelope from the half-range across annuli is used in the final budget.

attributable to temperature. Following the same methodology described, measurements of WS 2024 isolated vs mixed state runs also gave indistinguishable D_L at fixed field, granted only a sub-kelvin change. As a final note, there exists only one dedicated measurement of such temperature dependence in literature [124], where the authors concluded “no significant temperature dependence of D_L in LXe is found within the uncertainties of the measurements”. We therefore treat the thermal/pressure contribution as *negligible at our precision*.

THE ULTIMATE TEST: COMPARISONS AGAINST A WAVEFORM-TEMPLATE APPROACH (IRF)

In the diffusion analysis above, all detector effects in the extraction/EL region and the electronics chain that do *not* arise from in-drift longitudinal diffusion were absorbed into a single global intercept parameter, σ_0 , which we expect to be broadly field-independent. A more explicit treatment is possible by directly characterising the un-broadened S2 shape from data and then removing it from long-drift pulses. This is the *impulse response function* direct-waveform (IRF) approach⁹. As a final validation, the results of a complementary study conducted by E. Jacquet using this alternative methodology [135], is directly compared to the results achieved through the approach described in this chapter.

The IRF is built from events very near the gate ($4 \leq t_d \leq 6 \mu\text{s}$) where diffusion is negligible. Averaging and aligning these waveforms (with area-normalisation) yields a template that captures detector response (electronics bandwidth, PMT transit spread, photon time of flight) and production physics (electroluminescence timing in gas, liquid-to-gas

⁹This method will be discussed in detail in E. Jacquet’s forthcoming thesis and follows the spirit of ref. [124].

emission time). For each field/setting the template is re-aligned and used to model S2 pulses at long drift times. Any excess broadening beyond the template is attributed to longitudinal diffusion and mapped to D_L .

The two estimators are therefore complementary: the IRF method primarily constrains the *intercept* after removing a detailed pulse-shape model, while the width-slope method fits many time slices to determine the *slope* via equation 3.19, and is largely insensitive to the single-waveform topology. A comparison of the resulting D_L values is shown in Fig. 3.14.

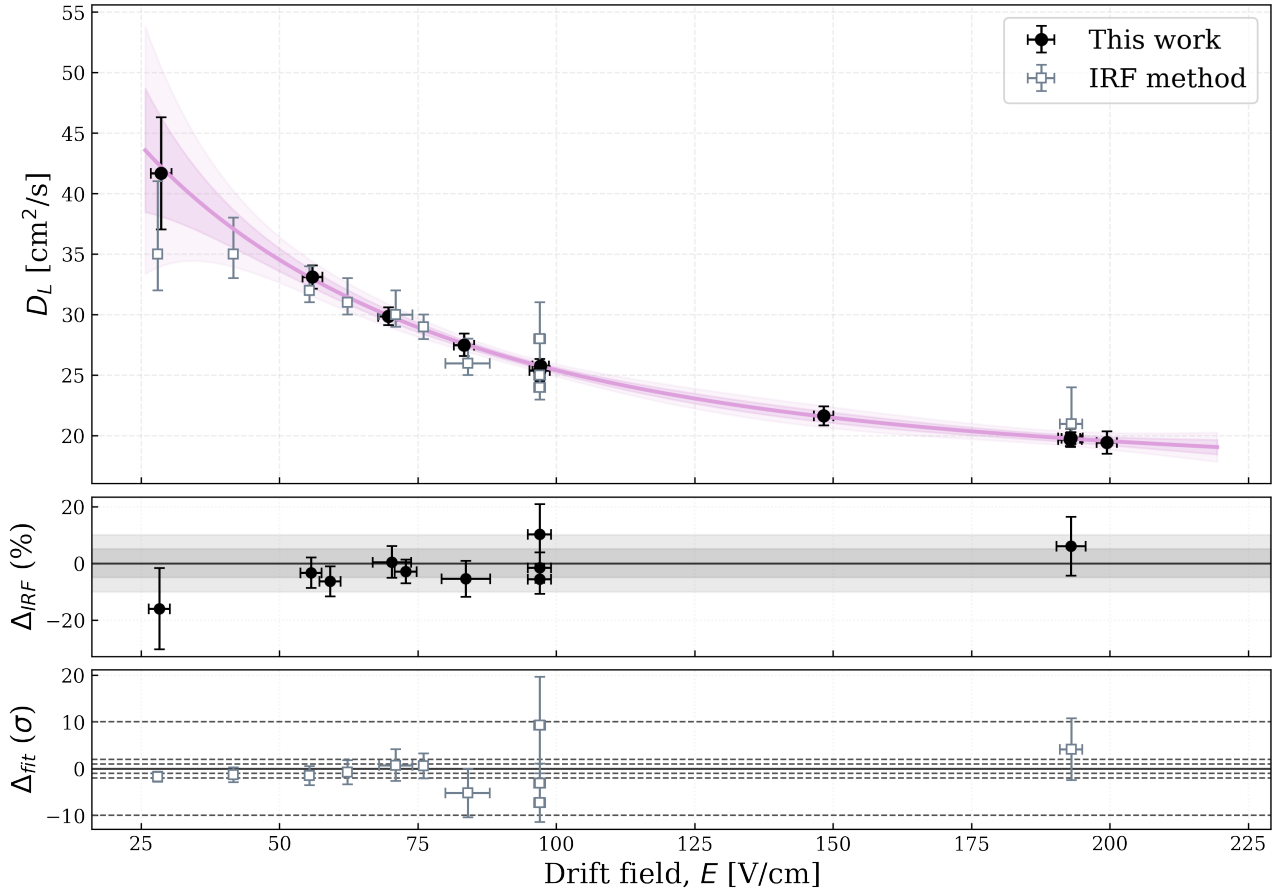


Figure 3.14: Comparison of longitudinal diffusion coefficients from the width-slope analysis (black) and the waveform-template IRF method (open). The band is the fit to the slope analysis. Agreement is generally within $1 - 2\sigma$; structured differences appear where each method is most sensitive (template systematics at low/mid field; percent-level timing vs radial/area effects at high field).

Overall, the two methodologies are in good agreement. We comment on the few structured deviations:

- Lowest field ($\sim 25 - 30 \text{ V/cm}$).

At low E the S2 is intrinsically broader (longer EL production time and longer emission time). The IRF procedure subtracts a *large* template width; a few-percent mismatch in the template can translate to $\mathcal{O}(1) \text{ cm}^2/\text{s}$ in D_L . By contrast, the width-slope method is anchored by an $\mathcal{O}(10^3) \mu\text{s}$ lever arm and is much less sensitive to this subtraction. A gate-referenced check also yields a non-zero early-time width, $\sigma_0(\tau = 2 \mu\text{s}) \approx (0.75 \pm 0.13) \mu\text{s}$, consistent with the broad/structured S2s at low field.

- Mid field ($\sim 90 - 100 \text{ V/cm}$; mixed grid settings).

Changing anode–gate–cathode (A/G/C) high voltages alters both the liquid extraction field (emission time) and the gas field (EL timing). Since the IRF is derived from near–gate waveforms, the template is *configuration dependent* and should be re-trained per run. If a template is reused across different A/G/C conditions, the deconvolution leaves a positive residual that mimics extra diffusion, explaining the elevated IRF point in this range.

- Highest field ($\sim 200 \text{ V/cm}$).

Here we are in the hot-electron/near-plateau regime where small absolute differences translate into larger fractional shifts. For the IRF method the diffusion width is obtained as the *difference of two small numbers* (data $\otimes$ template), so *ns*-level timing/response mismatches can move D_L by a few percent. For the width–slope method the statistical error is tiny but radial/area systematics and v_d propagation dominate at the $\sim 5\%$ level. The observed offset is therefore consistent with the combined method systematics.

In summary, across 25–200 V/cm the two extractions are largely consistent: most points lie within $1-2\sigma$ of a common, physically motivated $D_L(E)$ curve and typically within $\sim 5\%$ of each other. The structured differences appear exactly where each method is most exposed: at low- E to IRF template systematics; at mid- E to A/G/C–dependent emission/EL timing in the template; and at high- E to percent-level timing (IRF) versus radial/area and v_d systematics (width–slope). After accounting for these, both datasets are compatible with a single $D_L(E)$ curve anchored by cold-electron microphysics at low field and flattening toward the hot-electron plateau (see §4.4.2). Together, the combination of these complementary approaches provides one of the most rigorous, field-resolved determinations of long-drift longitudinal diffusion in LXe to date, while highlighting well-defined opportunities to refine per-run templates and shared calibrations.

3.3 Comments on the Transverse Diffusion Coefficient

Transverse diffusion, the lateral broadening of the electron swarm perpendicular to the drift field, is generally larger than its longitudinal counterpart. In liquid xenon, typical values are $D_T \sim 30-50 \text{ cm}^2, \text{s}^{-1}$ [124, 125, 136] for $E_d \approx 200-500 \text{ V/cm}$, versus $D_L \sim 10-30 \text{ cm}^2, \text{s}^{-1}$ over the same range. Even at meter-scale drifts, the impact of transverse diffusion on bulk XY resolution in dual-phase TPCs is modest. It acts only to broaden the lateral charge cloud at extraction; with the reconstructed width evolving as $\sigma_T^2 = \sigma_{T,0}^2 + 2D_T t_d/v_d$, the resulting spreads after meter-scale drifts are expected to be $\mathcal{O}(\text{mm})$. These values lie well below the readout segmentation scale and, in particular, contribute negligibly to the uncertainties in the light-response maps used by MERCURY relative to the 3-inch (7.62 cm) PMT face diameters that set the sampling granularity [58, 104].

In LZ, we can estimate the transverse diffusion coefficient directly from near-liquid surface calibrations. Using the measured $^{131\text{m}}\text{Xe}$ transverse width at $E_d = 193 \text{ V/cm}$ and $z = 31 \text{ cm}$, $\sigma_{\text{meas}} \simeq 1.35 \pm 0.13 \text{ mm}$ [137], and MERCURY’s optical-reconstruction floor $\sigma_{\text{opt}} \simeq 1.0 \pm 0.1 \text{ mm}$ (validated in LUX [58, 104]), the diffusion-only component is $\sigma_T = \sqrt{\sigma_{\text{meas}}^2 - \sigma_{\text{opt}}^2} \approx 0.9 \text{ mm}$. Propagating this with the LZ drift-velocity parametrisation (§4.4.2) gives

$$D_T(193 \text{ V/cm}) = \frac{\sigma_T^2 v_d}{2z} \approx 20.3 \pm 9.9 \text{ cm}^2/\text{s},$$

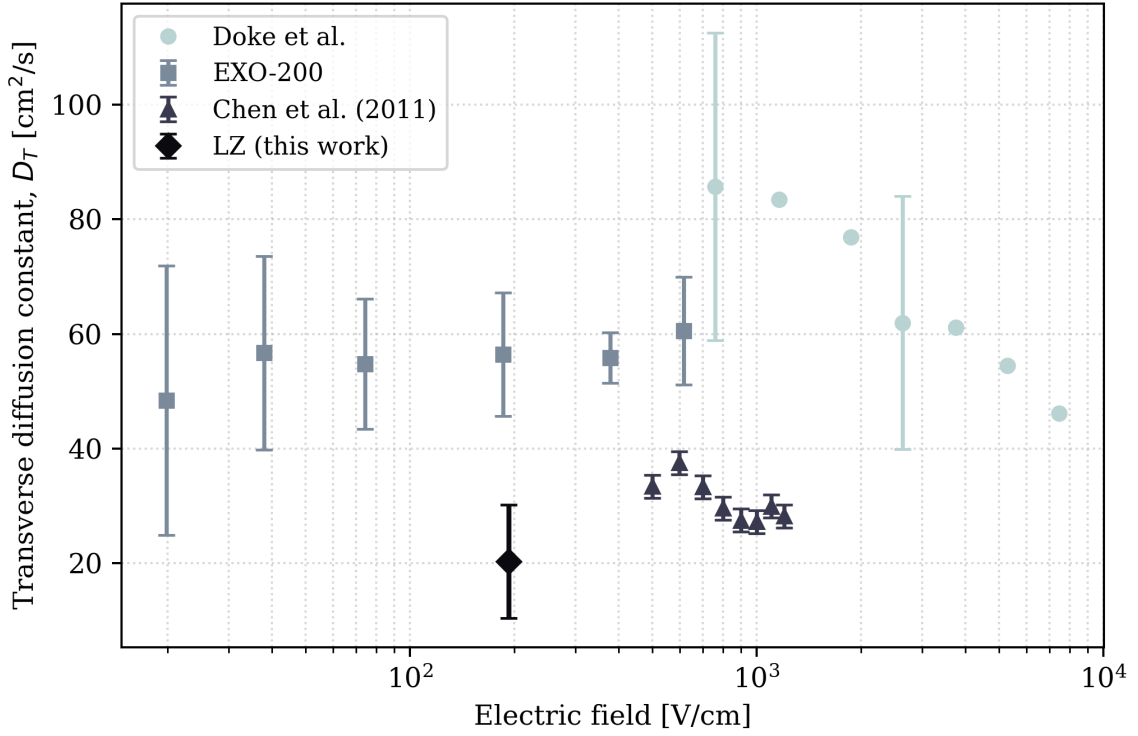


Figure 3.15: A compilation of the limited measurements available in literature of transverse diffusion (D_T) coefficients as a function of drift field [125, 136]. An approximate calculation for LZ is also overlaid.

Table 3.6: Pure transverse-diffusion RMS σ_T (mm) at four drift fields and three drift lengths, computed from $\sigma_T(z) = \sqrt{2D_T z / v_d(E)}$ using the $v_d(E)$ fit (see text). Entries are *intrinsic* diffusion only.

E (V/cm)	v_d (mm/ μ s)	σ_T (1.5 m)		σ_T (3.0 m)		σ_T (4.0 m)	
		$D_T=10$	$D_T \in [20, 55]$	$D_T=10$	$D_T \in [20, 55]$	$D_T=10$	$D_T \in [20, 55]$
25	0.7682	1.98	2.79–4.63	2.79	3.95–6.55	3.23	4.56–7.57
97	1.3970	1.47	2.07–3.44	2.07	2.93–4.86	2.39	3.38–5.61
193	1.5271	1.40	1.98–3.29	1.98	2.80–4.65	2.29	3.24–5.37
320	1.5543	1.39	1.96–3.26	1.96	2.78–4.61	2.27	3.21–5.32

Notes. $v_d(E) = A[1 - (1 + E/k)^{-n}]$ with $A = 1.56$ mm/ μ s, $k = 183.66$, $n = 5.31$. Values scale as $\sigma_T \propto \sqrt{D_T z} / \sqrt{v_d}$; recompute for other fields with the same formula and $v_d(E)$ fit.

consistent with expectations for LXe in the $\mathcal{O}(100 - 200)$ V/cm regime. For longer drifts, the intrinsic transverse spread grows as $\sigma_T(z) = \sqrt{2D_T z / v_d(E)} \propto \sqrt{z}$. Table 3.6 reports the *pure* diffusion RMS (no optics/reconstruction folded in) at four representative fields using the above $v_d(E)$ fit, giving both a literature bracket $D_T \in [20, 55]$ cm²/s and an LZ “best-case” reference $D_T = 10$ cm²/s.

Future xenon TPCs like XLZD (Chapter 6) are actively considering higher-granularity photosensors (smaller PMTs or tiled SiPM arrays) and improved optical modelling. As the sampling granularity and photon statistics push the optical-reconstruction floor below the millimetre scale, the intrinsic diffusion term will no longer be negligible in the (x, y) resolution budget at multi-metre drifts. In that regime, $\sigma_{XY}^2(z) = \sigma_{\text{opt}}^2 + \sigma_T^2(z)$ could become diffusion-dominated at depth, so accurate treatment of $D_T(E)$, its uncertainties, and depth dependence is required to avoid bias in position reconstruction and in the resulting uncertainties propagated to the light-response maps used by MERCURY-style algorithms.

3.4 Closing Remarks

We remeasured $v_d(E)$ and $D_L(E)$ in LZ and, from the same dataset, inferred a self-consistent $D_T(E)$ and $\sigma_{\text{mt}}^{\text{eff}}(E)$ consistent with Cohen-Lekner expectations. Transverse diffusion was verified to be millimetre-scale and sub-dominant for well-lit S2s, while the calibrated transport set $\{v_d, D_L, D_T, \sigma_{\text{mt}}\}$ now underpins the electric field modelling that follows - fixing the time-to- z map, depth scaling, and priors for assessing radial biases. Looking ahead, the same framework can inform longer-drift, higher-granularity designs like XLZD where explicit diffusion budgeting will matter for (x, y) resolution and light-response modelling.

4

Characterising & Modelling Electric Fields in the LZ Detector

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DUAL-PHASE XENON TIME PROJECTION CHAMBERS are, at their core, machines for choreographing the motion of charge in an otherwise invisible medium. From the first traces of ionisation to the eventual collection of electroluminescence light, every stage is shaped by the detector’s electric fields. The drift field ties drift time to an event’s vertical position; the extraction and electroluminescence fields set the size and uniformity of the S2 signal; and, everywhere in between, the local field magnitude dictates the recombination probability, knitting the S1–S2 anti-correlation directly into xenon microphysics. Precise knowledge of those fields is therefore the cornerstone of position reconstruction, energy calibration, electron/nuclear-recoil discrimination, and ultimately the discovery reach of any rare-event search.

Yet the very fields that so elegantly orchestrate the interactions and movement of charges in the TPC, are very fragile. Hidden beneath layers of cryogenic media, they are shaped by hundreds of wires, meshes, and dielectric (PTFE) panels - each rich in physics but also a potential source of inhomogeneity. A nanoscale burr on a gate wire can trigger a breakdown; the same static charge that lets a child’s balloon cling to a wall (order-of-magnitude $\mu\text{C}/\text{m}^2$) is large enough, once smeared onto the PTFE walls of the TPC, to warp the LZ field and slice centimetres from the fiducial volume as was dramatically demonstrated in LUX [81]. As we cannot peer into the detector and watch field lines bend, we must feel our way in the dark: infer distortions from calibration data and build ever more refined simulations until the picture clicks into place.

This chapter treats electric fields not as a peripheral detail but as the fundamental baseline on which LZ operates. Section 4.2 surveys the LZ geometry and the unmistakable footprints of field distortions: drift-time modulations, S2-wall shape evolution, and more. Section 4.3 establishes the axisymmetric field model on which all later work is built; Section 4.4 layers in finite-element simulations and a dedicated electron-drift suite tailored to LZ. Geometry alone proves insufficient (§4.5), prompting an investigation of PTFE wall charging (§4.6) and, ultimately, a relaxation of the axisymmetric assumption to accommodate observed azimuthal variations (§4.7). By iteratively adjusting surface-charge hypotheses we track the field’s month-to-month metamorphosis throughout the science runs. Section 4.8 tests consistency with observations in the skin, and the chapter concludes by summarising broader implications for next-generation TPC design.

4.1 The LZ Geometry

The LXe TPC at the heart of LZ is deliberately “simple” in geometry: a right-circular cylinder, $\sim 1.46\text{ m}$ in both height and diameter, its active volume is enclosed by interlocking PTFE panels, essential for high VUV reflectivity (Fig. 4.1). Set into radial slots in those panels are 57 titanium field-shaping rings, equally spaced at 25 mm pitch, which grade the potential between the upper gate grid and the cathode in order to maintain as homogeneous a field profile as possible while keeping field-lines from bending into the dielectric as far as possible [58]. In this chapter we assume the cylindrical symmetry implied by this layout as our zeroth-order boundary condition; every departure from perfect symmetry is treated as a perturbation to be quantified.

The liquid-gas column is enclosed by four woven-mesh electrodes as was shown in Fig. 2.3: the cathode at the base submerged in the liquid xenon, the gate $\sim 145.6\text{ cm}$ above it still within the liquid phase, the anode 8 mm above

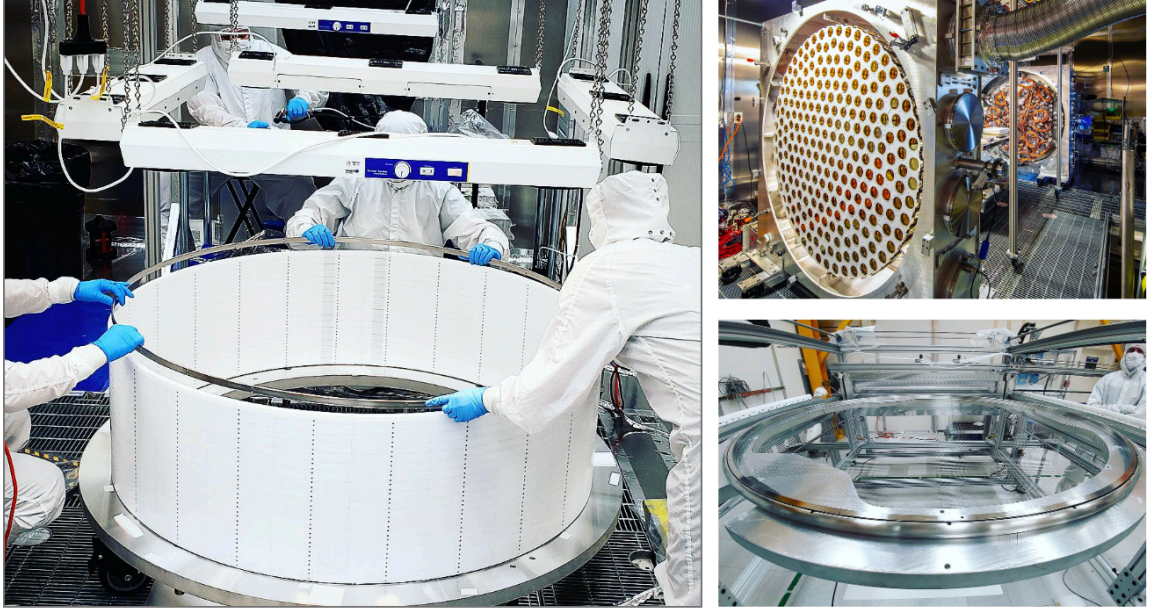


Figure 4.1: Assembly photographs of the LZ TPC: interlocking PTFE field-cage panels (**left**), top and bottom PMT arrays (**upper right**), and the grid electrodes (**lower right**). The cylindrical, quasi-axisymmetric layout defines the zeroth-order geometry used in this chapter.

the liquid surface in the vapour pocket, and a bottom “reverse-field” grid that shields the lower photomultipliers from large fields. The associated operational voltages (table 4.1) establish three working regions that the field model must reproduce: a drift field of $\sim 150\text{--}350\text{ V cm}^{-1}$, an extraction field of $\geq 3\text{ kV cm}^{-1}$ in the liquid, and a $\geq 6\text{ kV cm}^{-1}$ electroluminescence field in the gas¹. The mechanical realisation of these grids - including their $100\text{ }\mu\text{m}/75\text{ }\mu\text{m}$ wire diameters, $\sim 5\text{ mm}/2.5\text{ mm}$ wire pitches and sub-millimetre roughness/striation tolerances - is described in detail in Linehan et al. [67] and forms the basis of the μm -scale boundary conditions for any finite-element solution.

Although the TPC is nominally axisymmetric, several engineering necessities break that ideal:

- **High-voltage umbilical.** The stainless-steel/PTFE HV conduit enters the cryostat on a single azimuth, creating a localised bulge in equipotentials that is most pronounced in the LXe in the skin region.
- **Woven-mesh electrodes.** The cathode, gate and anode are woven stainless steel (SS) meshes rather than concentric rings; their orthogonal wire directions, $\sim\text{ mm}$ -scale “sag” (§4.3) and bars at discrete azimuths introduce small but non-negligible φ -structure to the fields in reality.
- **Photomultiplier arrays.** The top (253) and bottom (241) 3” PMTs are mounted in close-packed hexagonal lattices that are themselves rotated relative to each other; the PMT steel bodies, bases and cabling form metallic islands that slightly perturb the surrounding field.
- **Grid support hardware.** Cathode, gate and anode frames are tied to the field cage by PEEK pins and titanium tension rods that appear at discrete angles; these supports, together with the PTFE “ribs” that anchor them, break perfect cylindrical symmetry and provide sites where surface charge can accumulate.

¹More details on the motivation behind these fields are discussed later in chapter 6.

- **Weir overflow and level sensors.** The liquid-level weir and its capacitive sensors sit on one side of the TPC lid; when the detector is very slightly re-levelled, these features impose a sub-degree tilt that can modulate the gate–anode gap azimuthally.

Later sections show that these asymmetries along with various features of the geometry of the LZ TPC are sufficient to seed measurable distortions in event positions and even the build-up of negative charge on the PTFE barrel.

Table 4.1: Operational voltages applied to the primary LZ electrodes during the WS 2022 and WS 2024 science runs. The values reflect nominal high-voltage settings at the start of each campaign.

Electrode	WS 2022 Voltage [kV]	WS 2024 Voltage [kV]
Anode	+4.0	+3.5
Gate	−4.0	−4.0
Cathode	−32.0	−18.0
Bottom	−1.5	−1.5

The dielectric interfaces that matter most for electrostatics therefore group naturally into four classes:

- the PTFE–LXe boundary;
- the liquid–gas meniscus beneath the anode;
- the stainless-steel grid wires, whose microscopic protrusions may dominate peak fields;
- PTFE ribs and bosses that clamp the grids to the field cage and introduce tiny LXe-(PTFE or PEEK)–SS triple points.

Each interface enters the modelling chain twice: first as a geometric boundary in the static finite-element calculation, and again as a potential host for time-dependent surface charge movement. This will be discussed further in §4.3.

Finally, while the anode–gate differential has remained relatively similar, at $7.5/8\text{ kV}$, the cathode voltage has evolved from -32 kV in 2021 commissioning runs to -18 kV for the second (and latest) WIMP-search exposure. Tracking those changes is essential because the bulk drift field sets the scale of recombination, diffusion and z-position reconstruction.

In summary, the PTFE/Ti field cage provides an almost cylindrical starting point; the electrode stack fixes absolute potentials; and a shortlist of well-understood asymmetries and dielectric boundaries supplies a few of the perturbations that should potentially be investigated and then folded into any realistic electric-field map. The remainder of this chapter builds directly on that framework: §4.2 identifies the data signatures of field non-uniformity, and §4.3 onward develops progressively higher-fidelity models constrained by those observations.

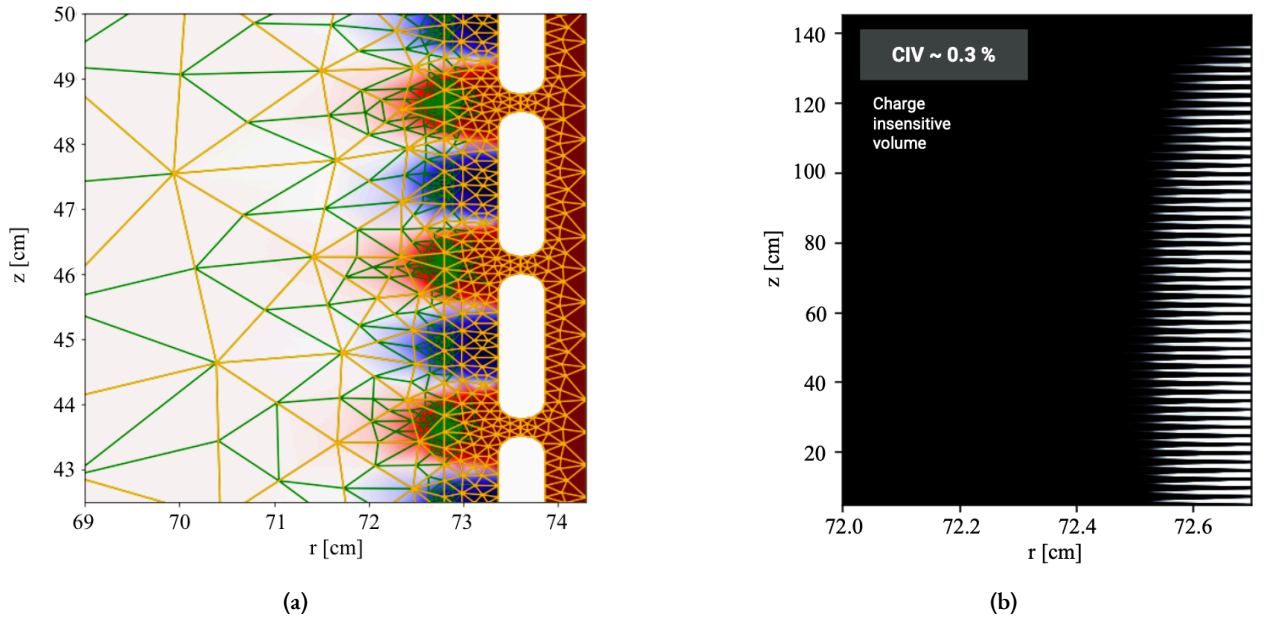


Figure 4.2: Electric field inhomogeneities and their impact on charge survival near the PTFE wall. (a) Finite-element calculation of the electric-field magnitude in the r - z plane, overlaid with the computational mesh, showing the local field modulation induced by the field-shaping rings. (b) Monte-Carlo estimate of the electron-attachment probability for the same region, showing a $\lesssim 3$ cm fluctuation region near the physical TPC boundary at $r \simeq 72.8$ cm where $P_{\text{attach}} > 99\%$. We term this the *Charge Insensitive Volume* (CIV) and for WS 2024 (no-wall-charge) this encapsulates $\sim 0.3\%$ of the maximum potential fiducial volume.

4.2 Tell-tale Signs of Field Effects in LZ Data

Even in a detector engineered for a perfectly vertical drift field, imperceptible twists and gradients in the electric field leave recognisable fingerprints in routine LZ event populations. This section gathers the key empirical clues - how charge disappears at the outer radius, how light-to-charge ratios drift with depth, how uniformly dispersed calibration lines truncate at slightly different radii, how electron-attachment lengths stretch with field, and how (particularly) the ER band warps under changing recombination. Taken together, these observables form a coherent, data-driven picture of the field that we will later confront with electrostatic simulations and triboelectric charging models. Our aim here is not to solve the field but to establish where and by how much it must deviate from ideal, providing the experimental benchmark for the modelling work in the remainder of the chapter.

4.2.1 The Wall

The radial wall is more than a mechanical edge of the LZ TPC; it provides the first high-level sanity check on every event we reconstruct. Pure geometry would place the wall where the PTFE panels terminate (at $\sim r_{\text{wall}} = 728$ mm). Analysis, however, relies on the S2 signal, so the operational boundary is the largest radial coordinate in S2 space at which drifting electrons still survive to reach the gas gap. Misidentifying this boundary biases our understanding of the fiducial mass and, therefore, the quoted WIMP exposure.

Close inspection shows that the drift field near the PTFE is inhomogeneous for a few intertwined reasons. The first is due to the expected scalloping from field-shaping rings: the discrete equipotential steps imposed by the resistor chain bend otherwise vertical field lines outward, forming shallow electrostatic wells along the circumference. The

scalloping and its impact on charge survival are illustrated in 4.2 for demonstration purposes using an arbitrary field configuration. Panel (a) shows equipotential contours from the finite-element solution; the sinusoidal modulation is evident. Panel (b) converts that geometry into a data-driven attachment probability, revealing a $\sim cm$ -thick skin where the survival probability falls below 50%. The observable implication of this is explicitly shown in §4.5. The second considers the long-observed but little-understood phenomenon of surface-charging of PTFE². The hypothesis originates from the idea that trace impurities and the intrinsic electronegativity of PTFE increase the probability that electrons travelling through this distorted region are captured before entering the gas gap, suppressing their S2 pulse. Sources of the excess charge may come from ionising radiation, depositing negative charge on the dielectric, warping the local potential (already distorted periodically due to the field-shaping rings) even further leading to an expected enhancement in electron attachment impacting real events within the TPC, signal and background alike.

These effects jointly define the effective S2 wall: the radius beyond which electrons are lost and the event becomes invisible in the S2 channel. In the remainder of this subsection we compare independent, data-driven techniques for locating this S2 wall, exploring also the concordance between the derived wall definitions, namely (i) charge-loss tails, (ii) breaks in the spatial uniformity of dispersed calibration sources like ^{83m}Kr & ^{131m}Xe , and (iii) intrinsic wall backgrounds like ^{210}Po α decays. These methods mostly agree to within $\mathcal{O}(mm)$; we adopt the charge-loss technique as the reference because it carries the smallest statistical uncertainty and is least sensitive to run-to-run purity variations, also deviating least from all other curves where the departure is greatest near-cathode, while maintaining consistency with the energy scale of the ROI. The resulting empirical wall serves as a benchmark for the electrostatic simulations described in §4.5 and beyond, and underpins the triboelectric-charging study in §4.6.

Figure 4.3 juxtaposes the five data-driven wall curves derived from the WS 2024 data set, which we will use an example. Four of them, namely the ^{83m}Kr percentile shoulder, the ^{131m}Xe percentile shoulder, the NR charge-loss side-band, and the ^{210}Po surface- α selection, lie within $\pm 0.25 cm$ of one another over the drift interval $71 - 900 \mu s$. Only the ^{83m}Kr charge-loss tail departs, drifting outward until it is about $1.5 cm$ beyond the common envelope in the final $\sim 150 \mu s$ where event vertices approach the cathode–field-cage interface.

All five techniques are implemented slice-by-slice in drift time. This work has been conducted by the wall group and will be referred to as a reference for the ensuing field studies. Inside a slice the radial distribution $N(R)$ is fitted with an analytic form that depends on the physics of the sample. :

- Dispersed sources (^{83m}Kr and ^{131m}Xe ³).

Two methods are explored. The first is an error function fit, following

$$N(R) = N_0 \frac{1}{2} \operatorname{erfc} \left(\frac{R - R_{wall}}{\sqrt{2} \sigma_0} \right), \quad (4.1)$$

where the wall position R_{wall} is defined by the half-maximum point of the $N(R)$ PDF. The second, non-parametric approach defines R_{wall} as the “50th”-percentile of the empirical erfc -shaped profile, which is numerically equivalent to the half-maximum of $N(R)$ for a sharp geometric boundary. In practice both methods yield consistent results owing to the steep fall-off at the physical edge of the TPC.

²I say “little-understood” as the underlying mechanism, rate and characteristics of the capture or surface charge transport mechanism is not clear and has not been explicitly studied. Experiments thus far have observed and simply corrected for its effects on fiducial volume.

³Also see §4.2.3 and §4.2.4 for more details on these specific sources.

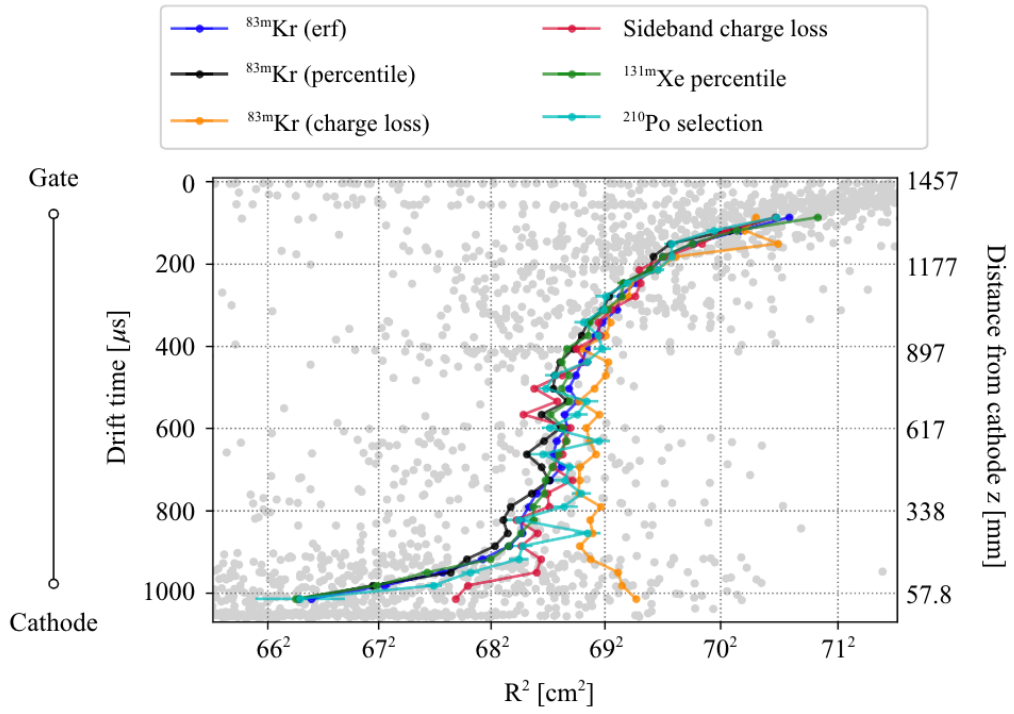


Figure 4.3: Reconstructed PTFE wall from multiple tracers: $^{83\text{m}}\text{Kr}$, $^{131\text{m}}\text{Xe}$, ^{210}Po surface- α selection, and an ER sideband charge-loss method. Curves are shown versus drift time (left axis) and the equivalent distance from the cathode z (right axis). Grey points are WS 2024 WIMP-search ROI events after all cuts. The methods agree closely across the drift range; the sideband charge-loss curve provides the most stable and complete estimate of the S_2 wall and is therefore adopted for fiducialisation. This figure has been reproduced and modified using plotting code provided by A. Musalhi, with respective curves derived by various members of the wall working group.

- Charge-loss population (NR side-band).

A Gaussian sitting on a falling error-function shoulder appears to describe the transition between the diffuse rate of events in the fiducial volume and the higher natural event rate near the wall due to its intrinsic radioactivity as shown in Fig. 4.4. This functional form, $N(R) = Ae^{-(R-\mu)^2/(2\sigma^2)} + B \operatorname{erfc}[(R - R_{\text{wall}})/(\sqrt{2}\sigma_0)]$, encapsulates a selection of events within the $100 \text{ phd} \leq S1c \leq 500 \text{ phd}$ range that occur below the NR band mean. We quote the Gaussian mean μ as the wall position.

- $^{83\text{m}}\text{Kr}$ tail in S_2 .

The candidate events are first isolated in raw (uncorrected) $S_2 - S_1$ space, with a Landau fit in S_2 applied subsequently to the selection:

$$f(S_2) = \frac{1}{\pi c} \exp\left[-\frac{1}{2}(t + e^{-t})\right], \quad t = \frac{S_2 - M_p}{c}, \quad (4.2)$$

where M_p is the most-probable value; only events within a narrow window about M_p are projected into R and then fitted with the Gaussian + erf form above.

- Surface- α sample.

A single Gaussian in R is sufficient, because the α s are produced exactly on the PTFE surface (see below). The difficulty with this selection is lack of statistics due to the effectiveness of the materials screening campaign during

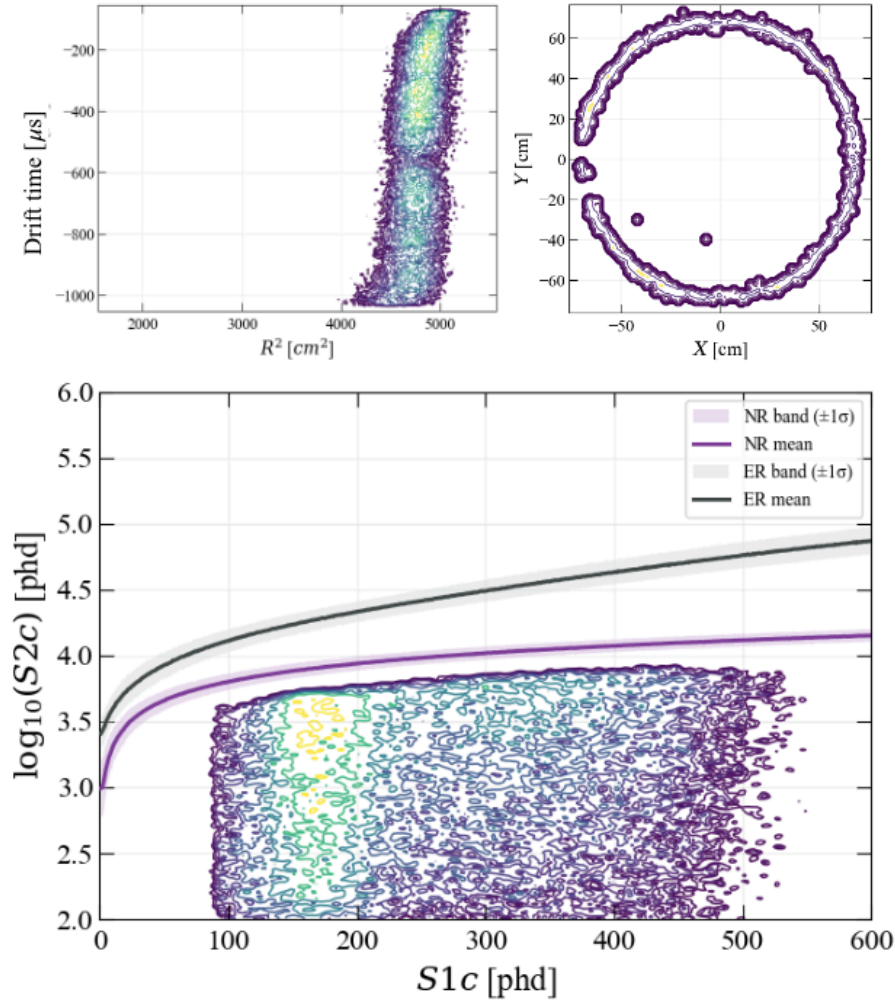


Figure 4.4: Event selections used to derive the charge-loss sideband wall definition. The top panels show the spatial and radial distributions of the selected population, while the lower panel displays the corresponding $S1$ – $\log_{10}(S2)$ space used to define the charge-loss region relative to the ER and NR bands.

and before commissioning, leading to a much cleaner detector. Mixing with other Rn daughters also poses problems in terms of achieving a clean sample as their signatures dilute and obscure the ^{210}Po peak we are looking for.

The close agreement of four of the curves can be traced to the way they depend on charge transport. The percentile/erf walls do exhibit the familiar S-shape caused by global field sagging, but they key off the point where essentially no electrons survive; this geometric boundary moves by only a few millimetres when the radial field strengthens in the “glow-spot” which marks the cathode ring-field cage interface. The NR charge-loss side-band, is also fitted with a Gaussian + error function model; here the Gaussian centroid remains stable because the selection criterion is tied also to an $S1$ (via the NR band) rather than to an absolute slice of $S2$. The surface αs (^{210}Po) originate from ^{210}Pb plate-out on the PTFE itself; the α particle and the accompanying ^{206}Pb recoil both deposit their charge inside the first few microns of PTFE, so practically no free electrons enter the liquid and no LXe drift occurs. What we reconstruct is therefore a purely geometric edge, almost impervious to local field variations.

The ^{83m}Kr charge-loss tail behaves differently for three reasons that are unique to that sample. First, each Kr cascade produces ≈ 5000 electrons, so even after losing several hundred in the enhanced radial field the event still lands inside the fixed acceptance window of $800 - 2000$ electrons. Second, because that window is absolute in S2, the population of accepted vertices is allowed to creep ever closer to (and even slightly beyond) the physical PTFE as the field steals more charge; this systematically pushes the fitted Gaussian mean outward. Third, the “uniform” Kr source guarantees thousands of events in every slice, so a $\mathcal{O}(1\text{ cm})$ translation of the peak is statistically significant. Low-energy NR and ER events, in contrast, start with only $20 - 100$ electrons; the same absolute deficit simply drops many of them below the faint-pulse detection threshold, leaving the Gaussian centroid a few millimeters inside the PTFE instead of outside it.

As the NR charge-loss side-band is matched in energy and topology to WIMP candidates and agrees with the geometry-anchored tracers to within 0.25 cm across 90% of the drift length, we adopt it as the baseline wall for WS 2024. The selection-specific bias of the Kr tail is retained only as a cross-check: we attach an extra uncertainty of 0.25 cm below $900\text{ }\mu\text{s}$ and 1.0 cm above that depth to the Kr curve alone, then combine that term in quadrature with the common $\pm 0.25\text{ cm}$ envelope. The resulting change in fiducial mass is $< 0.1\%$, comfortably smaller than the 1.2% systematic that arises from the intrinsic S2 position resolution.

Our approach builds directly on earlier xenon campaigns. XENON1T defined its 42 cm [118, 138, 139] fiducial cut with a Kr percentile wall; and LUX reported an outward kink of comparable size in its own Kr loss-tail near the cathode [140]. LZ extends that programme by adding the α -derived anchor, quantifying the cathode “glow-spot” systematic in situ, and, crucially, choosing the energy-matched NR side-band as the wall that governs the WIMP search exposures.

4.2.2 Recombination

A dual-phase xenon TPC records two anti-correlated observables: prompt scintillation photons (S1) and delayed electroluminescence (S2). Their partition is governed by the *recombination probability* $r(E)$, the fraction of the N_i electron–ion pairs in a track that reunite before the external electric field E extracts the electrons. Since $r(E)$ depends on both the field magnitude and the ionisation density of the track, any change in high-voltage settings or local field geometry displaces the ER and nuclear-recoil NR bands in $\log_{10}(S2/S1)$ space. Band migration therefore could become a powerful diagnostic of the field model. Below we outline the mechanisms by which E influences recombination, describe the expected signatures of field deviations, and compare analytical predictions, NEST, LZLAMA, and LZ calibration data.

Theory

A particle’s energy deposit produces N_{ex} excitons and N_i ion pairs ($N_{\text{ex}}/N_i \simeq 0.06$ in LXe [141–143]). In zero field nearly all N_i electrons recombine, boosting S1; in a finite field some are extracted, generating S2. Energy conservation is expressed by

$$N_\gamma = N_{\text{ex}} + rN_i, \quad N_e = (1 - r)N_i, \quad (4.3)$$

so an increase in E redistributes quanta from S1 to S2 without changing their sum. At $E = 0$ one finds $r \approx 0.9$ – 1.0 [144]; at very high field $r \rightarrow 0$. Beyond the extremes, two limiting formalisms bracket all data.

THOMAS–IMEL BOX MODEL (LOW-ENERGY LIMIT)

For compact deposits (tracks $\lesssim 5 \mu\text{m}$, ERs below 30 keV and essentially all low-energy NRs) electrons diffuse inside a uniform “box” of ions. Thomas & Imel derived [145]

$$r = \frac{\xi(E)N_i}{1 + \xi(E)N_i}, \quad (4.4)$$

where r denotes the electron-ion recombination probability, N_i is the number of ion pairs produced by the interaction, and $\xi(E)$ is the Thomas-Imel recombination parameter which encapsulates the competition between electron diffusion and drift within the ionisation “box”.

In the original Thomas-Imel derivation, the recombination parameter ξ was shown to scale approximately as E^{-1} under the assumption of a field-independent electron mobility [145]. At the electric fields relevant to this work the electron mobility exhibits only a weak field dependence. Consequently, in the low-energy regime in which the Thomas-Imel model is applied here, ξ is found to exhibit at most a very weak dependence on the electric field and is therefore treated effectively as constant⁴.

DOKE–BIRKS RECOMBINATION (HIGH- dE/dx TRACKS)

Long or high- dW/dx tracks (MeV ERs, α s, most NRs, W is used for energy here) are better described by a Birks-style saturation [69, 141, 142], where the LET (linear energy transfer) term is defined as the average energy deposited by a particle per unit distance travelled through a medium per unit density $\frac{1}{\rho} \frac{dW}{dx}$:

$$r(E) = r_g + (1 - r_g) \frac{LET}{1 + b(E)LET}, \quad b(E) = b_0(1 + \beta E)^{-1}, \quad (4.5)$$

with a “geminate” (electron rejoining its parent ion) floor $r_g \simeq (2-3) \times 10^{-2}$ [144].

Field suppression, track density and quenching

Higher field values suppress recombination, boosting S2 at the expense of S1 and driving $r \rightarrow r_g$ at large E . Perfect anti-correlation between S1 and S2 means their sum yields improved energy resolution. Dense tracks (NRs, α s) partially shield the external electric field, such that the field dependence of the number of recombining ions is small relative to N_i but not relative to the number of surviving electrons n_e . Consequently, while the relative change in S1 yield is modest, the corresponding relative change in S2 can be significant, and the treatment of field dependence must therefore be channel-dependent. In LUX, a 5 keV NR shows only $\sim 5\%$ change in light and charge yields across 50–600 V/cm, whereas for 5 keV ERs the average light yield falls by $\sim 15\%$ and the charge yield rises by a similar amount over the same span [129]. In LZ, the ER/NR band migration between WS 2022 (193 V/cm) and WS 2024 (97 V/cm) follows the same hierarchy (Fig. 4.5). The same appears in xenon X-ray cascades, which show higher recombination at lower field, with the denser double- K vacancy further suppressed at higher field [147].

⁴It is also noted that notation in the literature is not uniform: many references absorb the factor of N_i into the definition of the recombination parameter, for example defining $\zeta \equiv \xi N_i$, as in NEST and in [XENON2024TI]. In this work, ξ is defined such that the recombination probability is written explicitly in the form of Eq. (4.4)

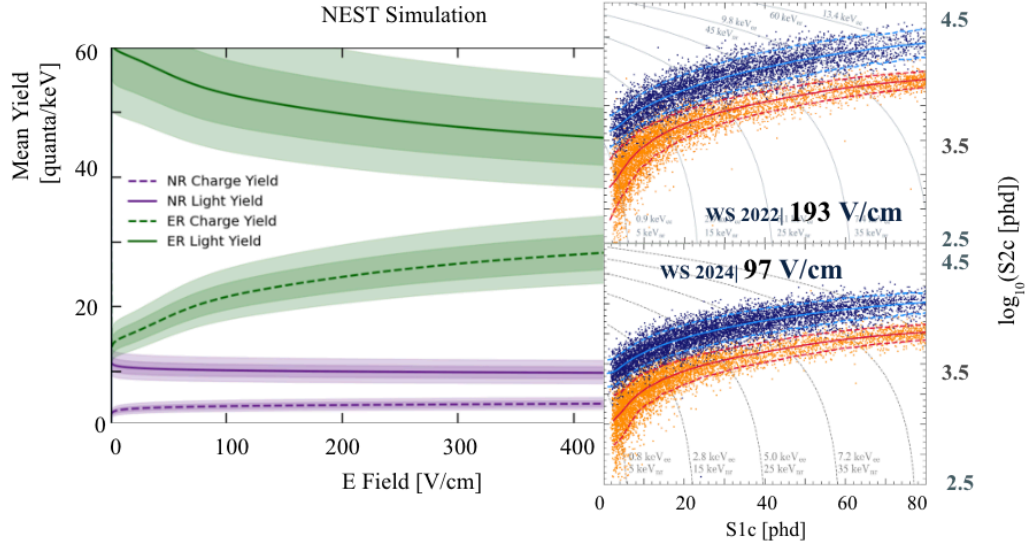


Figure 4.5: ER and NR bands in LZ for WS 2022 (193 V/cm) and WS 2024 (97 V/cm) [36, 49]. ER shifts to higher Q_y (lower L_y) at higher field, while NR changes modestly. The impact of field on charge and light yields are also visualised using NEST [146].

4.2.3 ^{83m}Kr

A precise in-situ measurement of the electric field within the detector would be ideal for understanding charge transport, calibrating position reconstruction, and quantifying systematics in light and charge yields. As discussed before, in a large dual-phase xenon TPC such as LZ, small spatial or temporal variations in the drift field can bias reconstructed event positions and energies, and in turn affect WIMP search sensitivity. Among the available calibration sources, the metastable isotope ^{83m}Kr offers an optimal probe for such *in situ* field measurements as traditionally used in previous experiments [126]. Its decay scheme, deployment method, and sensitivity to recombination physics enable high-precision, three-dimensional mapping of the field across the full active volume, with minimal operational impact on WIMP search data-taking [75].

^{83m}Kr is produced via electron capture from ^{83m}Rb and decays in two steps (Fig. 4.6), emitting mono-energetic internal conversion electrons of 32.1 keV ($T_{1/2} = 1.83\text{ h}$) and 9.4 keV ($T_{1/2} = 154\text{ ns}$). In LZ, both decays occur at the same spatial location, producing two temporally separated scintillation signals ($S1_a$ and $S1_b$) followed by a single ionization signal ($S2$). The short intermediate half-life ensures the $S1_a/S1_b$ separation is well resolved in time, while their identical origin means the relative light yield $S1_b/S1_a$ is independent of position-dependent LCE. This ratio depends almost exclusively on the local electric field strength through its effect on electron-ion recombination.

For electronic recoils above $\mathcal{O}(10\text{ keV})$, recombination suppression is significant and exhibits a monotonic dependence on drift field [146]. A weaker field results in more recombination, enhancing the $S1$ signal and suppressing the $S2$, while a stronger field has the opposite effect. Since both $S1_a$ and $S1_b$ originate from nearly identical microscopic interactions but at slightly different energies and recombination regimes, their ratio cancels most common mode

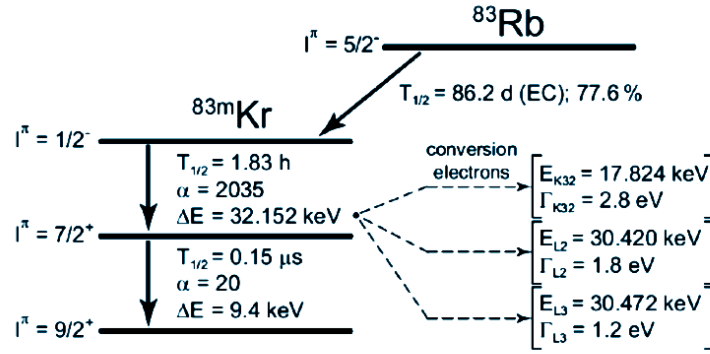


Figure 4.6: The ^{83m}Kr decay scheme [148].

detector effects, isolating the field-dependent component. As a result, variations in $S1_b/S1_a$ across the TPC can be robustly translated into fractional changes in the local drift field.

The statistical uncertainty in the vertical field variation for each run is obtained from the propagated error on the slope of the $S1_b/S1_a$ -drift-time fit, a study that was conducted by b. Schafer. These values are typically at the $\mathcal{O}(1 - 5\%)$ level in $\Delta E/E_{nom}$ for high-statistics injections, with larger uncertainties for early WS 2024 runs taken in isolated xenon states or for injections with incomplete fiducial coverage [149]⁵.

The choice of $S1_b/S1_a \rightarrow E$ conversion model introduces an additional systematic uncertainty on the absolute field scale. Comparing the empirical linear parametrisation and the NEST-based mapping, we find typical differences of $\lesssim 2\%$ in $\Delta E/E_{nom}$ for most runs, rising to $\mathcal{O}(5 - 10\%)$ [149] for cases where the slope is large or statistical errors are dominant. This systematic offset is common-mode across voxels and does not affect the relative mapping precision, which remains at the sub-percent level within a given injection.

Figure 4.7 illustrates the sequence from peak selection, through to a ^{83m}Kr -derived field map⁶; in later sections (§4.6.3) the agreement between ^{83m}Kr -derived volume-averaged fields and independent 131m calibrations will be discussed. The method thus provides both a high-precision snapshot of the instantaneous drift field and a robust validation point for field simulation tuning.

4.2.4 ^{131m}Xe

^{131m}Xe offers a rare combination of stability, uniformity, and strong field sensitivity in its photon yield, making it well-suited for mapping the electric field inside the TPC. Produced via the decay of ^{131}I (half-life 8.03 days, which is itself a product of neutron activation), ^{131m}Xe has a comparatively long half-life of 11.86 days (Fig. 4.8) [75], allowing it to remain in the active volume for weeks - long enough to outlast xenon mixing timescales in large detectors. Following

⁵This work is detailed in Bramwell Shafer's detailed work on field-mapping using ^{83m}Kr , which we refer to here as it provides a powerful method of validating the field maps.

⁶The figures here (unless specified) are produced independently from B. Schafer's work on the ^{83m}Kr maps but using very similar methodology. The full data-simulations comparisons refer directly to B. Schafer's extended analyses in later sections.

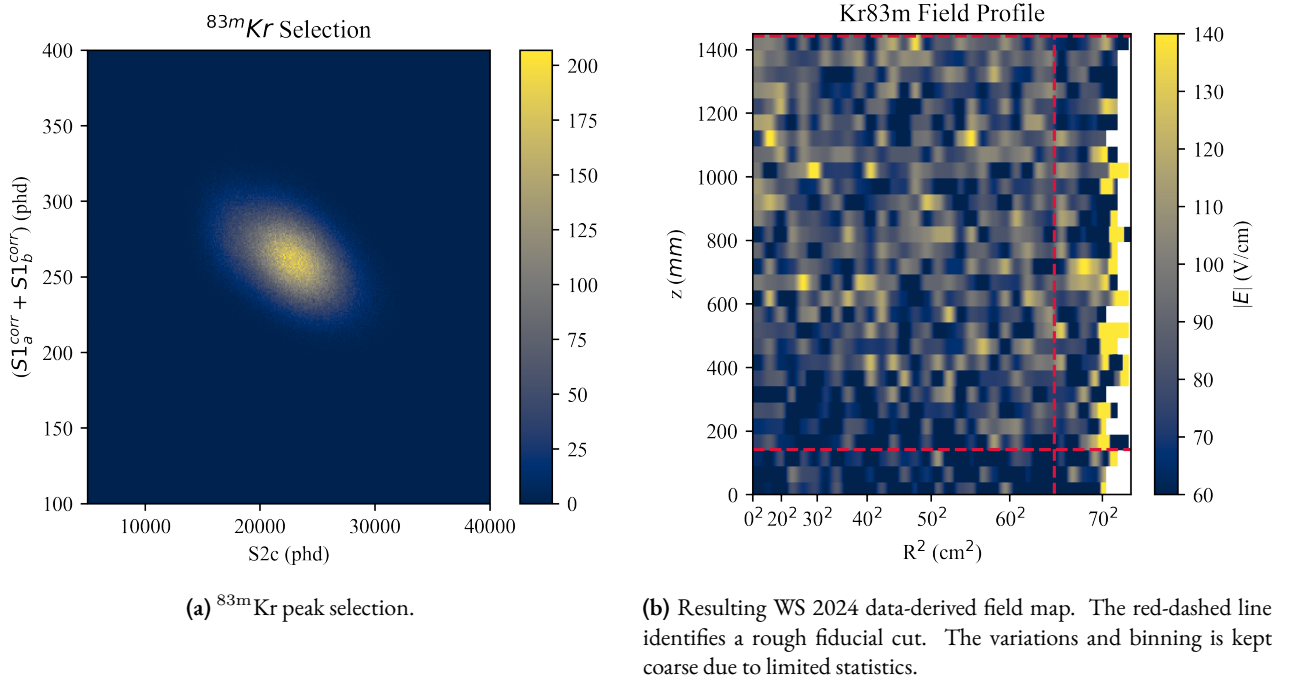


Figure 4.7: Illustrating some key components of the ^{83m}Kr -derived field maps.

decay from the parent, the daughter isotope is already well-mixed within the xenon, producing a clean, mono-energetic ($\sim 164 \text{ keV}$) electron-recoil population that is sensitive to field-dependent recombination effects. This uniform, ER-only calibration dataset enables spatial variations in photon yield to be mapped directly to variations in local electric field strength.

Compared to ^{83m}Kr , ^{131m}Xe can be deployed repeatedly over long campaigns, providing high-statistics, stable datasets with minimal spatial bias. As a precursor to field mapping, ^{222}Rn α -decays are first used to map the light-collection efficiency in (x, y, z) , under the common approximation that α S1 yields are field-independent. While NEST predicts a modest $\mathcal{O}(5 - 10\%)$ field dependence in α light yield between 50 and 500 V/cm (from NEST v2.1.0), this is far smaller than the ER dependence at the same energies and thus negligible at first order for LCE-correction purposes.

A more significant potential bias arises from the ^{131m}Xe decay scheme. The primary 164 keV γ is emitted in only $\sim 2\%$ of decays, with the remainder producing conversion electrons, Auger electrons, and X-rays (Fig. 4.8). These products are emitted near-simultaneously and are almost always reconstructed as a single scatter, but X-ray escape near detector boundaries can slightly reduce the detected energy and photon yield. After fiducial cuts, this effect impacts $\leq 1\%$ of events and is negligible for volume-averaged fields.

The calibration chain begins with α -based LCE maps (Fig. 4.9b) [151], used to correct raw S1 signals from ^{131m}Xe (Fig. 4.9a). The corrected photon distribution reveals clear spatial structure correlated with the underlying field map. Inversion of the photon-field relationship via the NEST 164 keV ER model yields the 3D ^{131m}Xe -derived field map (Fig. 4.9c). Fiducial-volume-averaged fields are then compared directly to ^{83m}Kr -derived values (Fig. 4.9d), providing a critical validation point for simulation-based tuning.

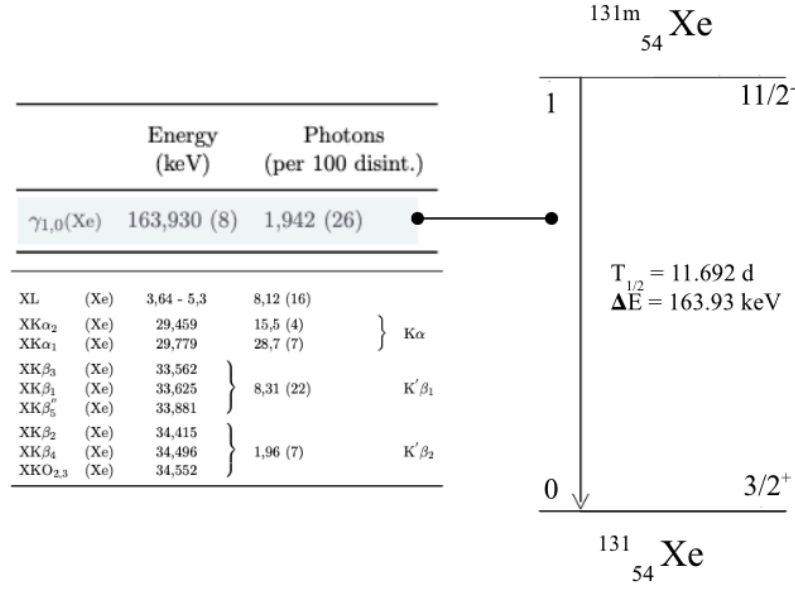


Figure 4.8: The ^{131m}Xe decay scheme, showing branching ratios for 164 keV γ emission ($\sim 2\%$) and the dominant conversion electron, Auger electron, and X-ray channels [150]. The X-ray escape probability is non-negligible only for events within a few mm of the TPC wall.

The dominant systematic in deriving electric fields from ^{131m}Xe is the model dependence of the ER photon-yield versus field at 164 keV, as parametrised in NEST. The inferred field in a given voxel is obtained by inverting the light-yield–field curve, so the fractional uncertainty on the yield propagates as

$$\delta E \approx \frac{\delta(\ln LY)}{|\partial \ln LY / \partial E|}, \quad (4.6)$$

with the slope $|\partial \ln LY / \partial E| \sim 4 \times 10^{-4} - 10^{-3} \text{ V}^{-1} \text{ cm}$ in the 80 – 200 V/cm range. Model uncertainties of 1 – 2% in LY therefore map to 7 – 12 V/cm (1σ) per voxel, larger near edges. Subdominant contributions arise from imperfect LCE correction using α sources ($\leq 2\%$, or a few V/cm) and from S1 peak-extraction biases in low-statistics voxels. X-ray-escape near detector walls affects only a small geometric fraction of events and is negligible after fiducial cuts. While voxel-level comparisons between simulation-derived and data-driven maps exhibit relative variations at the $\mathcal{O}(10\%)$ level, the fiducial-volume–averaged fields inferred from ^{131m}Xe differ from those obtained with ^{83m}Kr by $\sim 15 - 20\%$. This level of agreement is sufficient for a global cross-check but does not motivate the use of ^{131m}Xe as a primary tuning input. Instead, ^{131m}Xe –derived maps⁷ are employed here as an independent, data-driven validation of the simulation-based field models, providing confidence in the robustness of the tuning procedure without biasing it.

4.2.5 Electron Lifetime

LXe TPCs infer the drift-electron lifetime (τ_e) by fitting the depth-dependence of the S2 charge signal

$$S2(t_d) = S2(0)e^{-t_d/\tau_e^{eff}}, \quad (4.7)$$

⁷Courtesy of Mark Murdy.

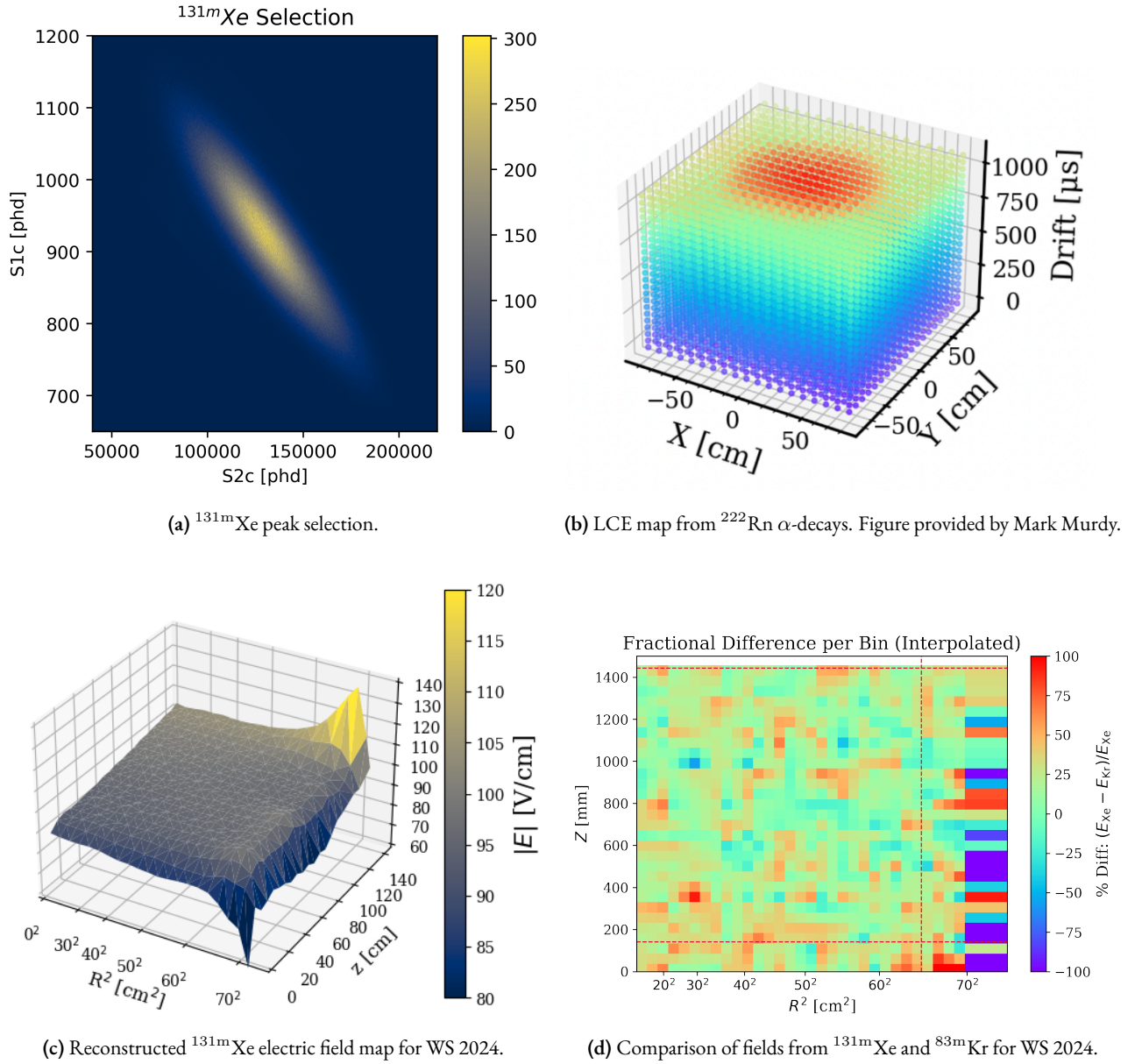


Figure 4.9: Summary of $^{131\text{m}}\text{Xe}$ field-reconstruction chain.

where t_d is the drift time. This fit assumes that the only process removing electrons is attachment on electronegative impurities. However, two additional field-related processes can bias this measurement. If the field-only signatures are distinct enough, electron lifetime calculation could function as an additional lever to tune our understanding of the fields in the TPC.

- **Spatial variation of E**

The drift field may vary by $\sim 10 - 30\%$ in the entire drift volume; the z -variation is a natural consequence of the field cage optimisation (§4.6), while grid deflection and edge-effects dominate the fluctuation evident at large radii. As the ion–electron recombination probability rises when E is weaker, the initial number of electrons N_0 depends on position. In the fit, this position-dependent pre-factor is absorbed into an “effective” lifetime τ_{e-}^{eff} , where

$$S2(t_d) = N_0(E)g_2e^{-t_d/\tau_{e-}} \Rightarrow \tau_{e-}^{\text{eff}} \neq \tau_{e-}. \quad (4.8)$$

In LZ's first WIMP search (WS 2022) this effect corresponded to an intrinsic lifetime of $\tau_{e-}^{field} = 289 \pm 72 \text{ ms}$ [152], far longer than the few- ms impurity-limited lifetime measured. This suggests that this effect is likely negligible.

- **Field-dependence of the electron-attachment rate**

The attachment cross-section of O_2 , H_2O and other impurities falls slowly with increasing E [112]. Changing the global drift voltage therefore changes the true lifetime itself. This effect led to an observable increase of more than double the lifetime between the first WIMP search and WIMP Search 2024 [153].

Despite the first case contributing negligibly to the lifetime according to the WS 2022 field map, the field-effect could in fact become relevant for comparisons between calibration sources, which probe different energy deposits and therefore different recombination regimes, as the XENON programme had observed. XENONnT noticed that the lifetime obtained with $^{83\text{m}}\text{Kr}$ (41 keV , low ionisation density) was systematically longer than that obtained with the mixed energy $^{222}\text{Rn}/^{218}\text{Po}$ alphas [154] as can be seen in Fig. 4.10. They were able to reproduce the effect and hence, trace it to

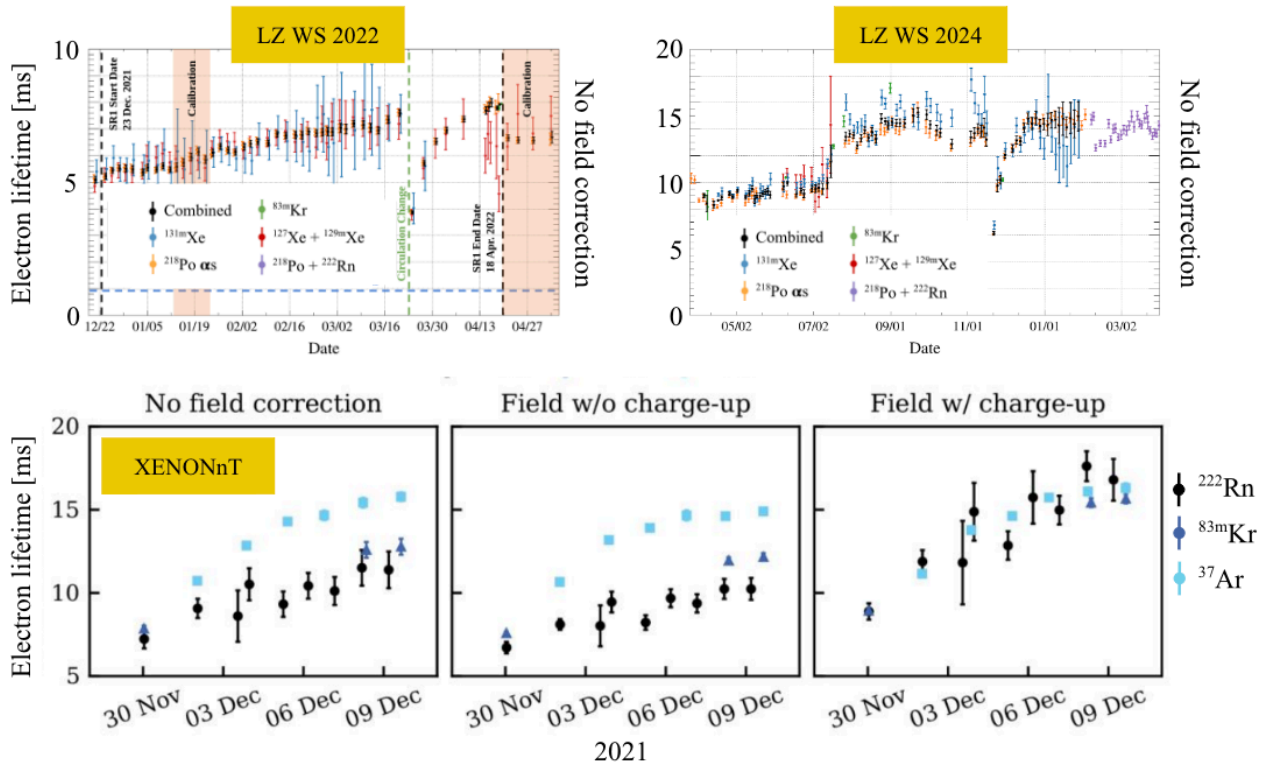


Figure 4.10: Electron lifetimes inferred from multiple calibration channels in LZ — ^{37}Ar , $^{83\text{m}}\text{Kr}$, and $^{222}\text{Rn}/^{218}\text{Po}$ —during WS 2022 (left) and WS 2024 (centre), alongside values reported by XENONnT (right; from [155]). For comparison, the maximum drift time within LZ across its field regimes is $\sim 1 \text{ ms}$, while for XENONnT, this is $\sim 2.2 \text{ ms}$. At XENONnT's low drift field ($\sim 25 \text{ V cm}^{-1}$), the charge yield—and thus the apparent lifetime - shows enhanced sensitivity to small field variations, requiring a field-dependence correction to place lifetimes from different energy deposits on a common scale. After applying this correction in LZ, all channels agree within uncertainties on a shared impurity-limited lifetime, demonstrating consistency across calibration methods. LZ Data credit: J. Genovesi.

the first mechanism above: a shallower electric field near the TPC top reduced the charge yield of alpha and low-energy beta tracks more than that of 41 keV ERs. The bias was then cured by dividing out the expected field-dependent yield:

$$S2_{corr}(t_d) = \frac{S2_{meas}(t_d)}{Q_y^{rel}(E(r, z))}, \quad Q_y^{rel}(E) = \frac{Q_y(E)}{Q_y(E_{ref})}, \quad (4.9)$$

Table 4.2: Field non-uniformity scales relevant to lifetime biasing within the defined fiducial volume of each experiment. The final column shows the order-of-magnitude S2 modulation when the fractional non-uniformity is folded with the field-slope of $Q_y(E)$ appropriate to each detector’s operating range (see text).

Experiment	E_{drift} [V/cm]	$\Delta E/E$	Drift length [m]	Est. $\Delta S2/S2$
XENONnT SR0	23	$\pm 13.2\%$	1.486	$(30\%) \times (13.2\%) \approx 4\%$
LZ WS 2022	193	$\leq 4.0\%$	1.456	$(5\%) \times (4.0\%) \lesssim 0.2\%$
LZ WS 2024	97	$\leq 6.2\%$	1.456	$(16\%) \times (6.2\%) \lesssim 1\%$

where $Q_y(E)$ is the charge yield from the NEST global fit and E_{ref} is the constant field assumed in calculations where a field-dependent Q_y is not incorporated (typically just the average field in the fiducial volume). This hence indicates the complete pipeline for determining the true electron lifetime, after de-convolving the field effects. After the correction the apparent lifetimes from ^{37}Ar , $^{83\text{m}}\text{Kr}$ and ^{222}Rn all converged to the same physical value ($\sim 38\text{ ms}$), demonstrating that the method isolates the impurity-driven attenuation.

The question still remains, however, of why is it that LZ did not see the same source dependent lifetime. The key lies in the operational drift fields of the two experiments. The magnitude of field-induced lifetime biases depends on two coupled factors: (i) the *absolute* drift field at which the detector operates, and (ii) the *fractional non-uniformity* of that field across the drift region. These in turn act through the field dependence of the charge yield, $Q_y(E)$, which is steep at low field and saturates (“plateaus”) at higher field. XENONnT operated in a low-field regime where modest spatial variations in E translated into large, position-dependent variations in Q_y for ER calibration lines, but not for dense α/NR tracks; the resulting curvature in $\log S2(t_d)$ biased lifetime fits in a source-dependent way. LZ, by contrast, has operated at substantially higher fields, on/near the plateau of $Q_y(E)$ ($E \gtrsim 80\text{ V cm}^{-1}$), where the same *absolute* voltage variation corresponds to a much smaller *fractional* change in Q_y , far below both statistical errors and impurity-driven slopes in the WS 2022 and WS 2024 data sets.

Direct comparison of electric-field configurations

XENONnT’s SR0 data were taken at a nominal drift field of $E_{\text{drift}} \simeq 23\text{ V cm}^{-1}$, set by a -2.75 kV cathode bias.⁸ Field-map reconstructions indicate a vertical field variation of $\Delta E \approx 5\text{--}8\text{ V cm}^{-1}$ across the 1.5 m liquid column, i.e. a fractional non-uniformity of $\Delta E/E \approx \pm 25\%$. LZ’s WIMP searches, by contrast, have been conducted at far higher absolute fields: $E_{\text{drift}} = 193\text{ V cm}^{-1}$ in WS 2022 and $E_{\text{drift}} = 97\text{ V cm}^{-1}$ in WS 2024. Electrostatic modelling (section 4.6) shows that the largest variation in the LZ drift region (within the fiducial volume), driven by the field cage resistors ladder, field cage-grid interfaces and PTFE charge, is typically no more than $\pm 10\text{ V cm}^{-1}$, corresponding to $\Delta E/E \leq 10\%$ even in the lower-field WS 2024 data set. The practical implication is immediate: a given *absolute* voltage deviation produces a fivefold smaller *fractional* perturbation in LZ than in XENONnT.

Charge-yield plateau renders LZ largely insensitive

The charge yield $Q_y(E)$ links field non-uniformity to lifetime bias because it controls the initial electron count N_0 that seeds the exponential attenuation. When $Q_y(E)$ changes rapidly with E , a modest field gradient along z imprints a strong depth dependence on N_0 ; the $\log(S2)$ curve acquires curvature that an exponential fit misinterprets as a finite

⁸Value quoted from the SR0 detector-operations summary; see also Ref. [154].

lifetime. When $Q_y(E)$ is flat, the same gradient has little effect.

NEST calculations show that the logarithmic derivative $|\partial \ln Q_y / \partial E|$ for 41 keV ERs takes the approximate values

$$\left| \frac{\partial \ln Q_y}{\partial E} \right| \simeq \begin{cases} 3.0 \times 10^{-3} \text{ V}^{-1} \text{ cm} & (E = 20 \text{ V cm}^{-1}), \\ 1.6 \times 10^{-3} \text{ V}^{-1} \text{ cm} & (E = 100 \text{ V cm}^{-1}), \\ 0.8 \times 10^{-3} \text{ V}^{-1} \text{ cm} & (E = 200 \text{ V cm}^{-1}), \end{cases} \quad (4.10)$$

while dense α /NR tracks flatten even sooner, with negligible slope already by $E \sim 50 \text{ V cm}^{-1}$. Thus, moving from XENONnT's low-field operating point into LZ's $97 - 193 \text{ V/cm}$ range reduces $|\partial \ln Q_y / \partial E|$ by roughly a factor of six for ERs, and even more for α /NR tracks; any given ΔE therefore induces a proportionally smaller fractional change in Q_y , and an even smaller bias in the lifetime fit.

From a field gradient to an effective ("pseudo") lifetime

To quantify the magnitude of the bias generated by mechanism 1 (section 4.2.5) we linearise the effect of a slowly varying field across the drift length. Let the local drift field be $E(z) = E_0 + \delta E(z)^2$ with $|\delta E| \ll E_0$, and let the charge yield scale locally as $Q_y(E) = Q_y(E_0) \exp[(\partial \ln Q_y / \partial E) \delta E]$. Inserting this into the usual lifetime expression with τ_{imp} defined as the pure impurity-dependent the electron lifetime, $S2(t_d) = N_0(E) g_2 e^{-t_d / \tau_{\text{imp}}}$, and expanding to first order in the field variation gives an "effective" exponential with lifetime

$$\tau_{\text{field}} \simeq \frac{t_{\text{max}}}{|\partial \ln Q_y / \partial E| \Delta E}, \quad (4.11)$$

where t_{max} is the full drift time and ΔE characterises the total field excursion across the drift region.¹⁰

Applying equation (4.11) to the two experiments:

- **XENONnT**

With $t_{\text{max}} = 2.08 \text{ ms}$, $|\partial \ln Q_y / \partial E| = 3.0 \times 10^{-3} \text{ V}^{-1} \text{ cm}$, and an approximate field variation $\Delta E = 3.07 \text{ V/cm}$ across the *fiducial volume* [155],

$$\tau_{\text{field}}^{\text{nT}} \approx \frac{2.08 \text{ ms}}{(3.0 \times 10^{-3})(3.0)} \approx 2.3 \times 10^2 \text{ ms}.$$

For an effective lifetime $\tau_{\text{eff}} = 15 \text{ ms}$ (taken as the maximum measured) [154],

$$\tau_{\text{imp}}^{\text{nT}} = (1/15 - 1/231)^{-1} \approx 16 \text{ ms}, \quad \Delta \tau_{\text{imp}} \equiv \tau_{\text{imp}} - \tau_{\text{eff}} \approx 1.0 \text{ ms} \quad (6.9\% \uparrow).$$

- **LZ (WS 2022)**

The 145.6 cm drift and $v_d = 1.53 \text{ mm } \mu \text{ s}^{-1}$ give $t_{\text{max}} = 950 \mu \text{ s}$. The field excursion is $\Delta E / E = 4.02\% \Rightarrow \Delta E = 7.8 \text{ V cm}^{-1}$. With the plateau slope $|\partial \ln Q_y / \partial E| = 0.8 \times 10^{-3} \text{ V}^{-1} \text{ cm}$,

$$\tau_{\text{field}}^{\text{LZ,193}} = \frac{0.950 \text{ ms}}{(0.8 \times 10^{-3})(7.8)} \approx 1.5 \times 10^2 \text{ ms}.$$

Taking $\tau_{\text{eff}} = 5 \text{ ms}$,

$$\tau_{\text{imp}}^{\text{LZ,193}} \approx 5.17 \text{ ms}, \quad \Delta \tau_{\text{imp}} \approx 0.17 \text{ ms} \quad (3.4\% \uparrow).$$

⁹This actually a very good approximation for the field behaviour as will be discussed in §4.6.3.

¹⁰Equation (4.11) follows by matching the curvature in $\ln S2(t_d)$ to the linear slope of a pure exponential.

- **LZ (WS 2024)**

With $v_d = 1.389 \text{ mm } \mu\text{s}^{-1}$ the 145.6 cm drift gives $t_{\max} = 1050 \text{ } \mu\text{s}$. The field excursion is $\Delta E/E = 6.18\% \Rightarrow \Delta E = 6.0 \text{ V cm}^{-1}$. For the intermediate-field slope $|\partial \ln Q_y / \partial E| = 1.6 \times 10^{-3} \text{ V}^{-1} \text{ cm}$,

$$\tau_{\text{field}}^{\text{LZ,97}} = \frac{1.050 \text{ ms}}{(1.6 \times 10^{-3})(6.0)} \approx 1.1 \times 10^2 \text{ ms}.$$

With $\tau_{\text{imp}} = 13.8 \text{ ms}$,

$$\tau_{\text{imp}}^{\text{LZ,97}} \approx 15.8 \text{ ms}, \quad \Delta\tau_{\text{imp}} \approx 2 \text{ ms} \quad (14.3\% \uparrow).$$

Vertical drift–field curvature (mechanism 1) introduces a “pseudo” increase in the fitted electron lifetime by modulating Q_y along z . Using the simulated wall–to–wall excursion ΔE from LZEF together with the field-dependent NEST slope [97, 144]

$$\left| \frac{\partial \ln Q_y}{\partial E} \right| (E) \simeq \frac{0.168}{E} - 8 \times 10^{-5} \text{ (V}^{-1} \text{ cm)},$$

we obtain the curvature bias $\Delta\tau_{\text{imp}} = t_{\max} / (|\partial \ln Q_y / \partial E| \Delta E)$ for the two field regimes; results are summarised in Table 4.3. In WS 2022 the bias is sub-dominant ($\sim 3\%$), while in WS 2024 it reaches $\sim 16\%$, requiring correction. Uncertainties combine (quadrature) $\sim 20\%$ on ΔE , $\sim 10\%$ on the slope interpolation, and fit statistics.

Table 4.3: Field–curvature pseudo-lifetime bias and corrected lifetimes.

Run	Nominal τ_{fit} (ms)	$\Delta\tau_{\text{imp}}$ (ms)	Corrected τ_{true} (ms)
WS 2022	5.0	+0.17 (3.4%)	5.17 ± 0.2
WS 2024	13.8	+2 (14.3%)	15.8 ± 0.4

The absence of a source-dependent divergence (^{83m}Kr , Rn/Po chain, ^{131m}Xe) reflects volumetric overlap and similar S2 (charge) response in the 10–100 keV ER-equivalent energy response range, producing a common-mode shift. The apparent multi-source discrepancy of XENONnT arose when combining $\mathcal{O}(\text{MeV})$ ^{218}Po alphas (weak $Q_y(E)$ / S2 field dependence due to strong recombination) with low-energy ER ^{83m}Kr (stronger $Q_y(E)$ / S2 field dependence) under a steeper low-field regime; applying field and $Q_y(E)$ corrections collapsed that spread. For future LZ purity ($\tau_e \gtrsim 30 \text{ ms}$), event-by-event $Q_y(E)$ correction will be needed to suppress residual $\mathcal{O}(10\%)$ bias.

Further validation: outer-edge lifetime excess in LZ

Although the global LZ lifetime is insensitive to mechanism 1 at WS 2022 purity, a *local* manifestation appears in the outermost radial slice of the January 2022 Kr dataset (Fig. 4.11). The annulus, centred at $R^2 \sim 5 \times 10^3 \text{ cm}^2$ ($R \approx 71 \text{ cm}$), returns a lifetime of $8200 \pm 1500 \text{ } \mu\text{s}$, whereas the interior slices cluster around $5269 \pm 270 \text{ } \mu\text{s}$. The observed excess is therefore

$$\Delta\tau_{\text{obs}} \approx (8200 - 5269) \text{ } \mu\text{s} \simeq 3.0 (\pm 1.5) \text{ ms}. \quad (4.12)$$

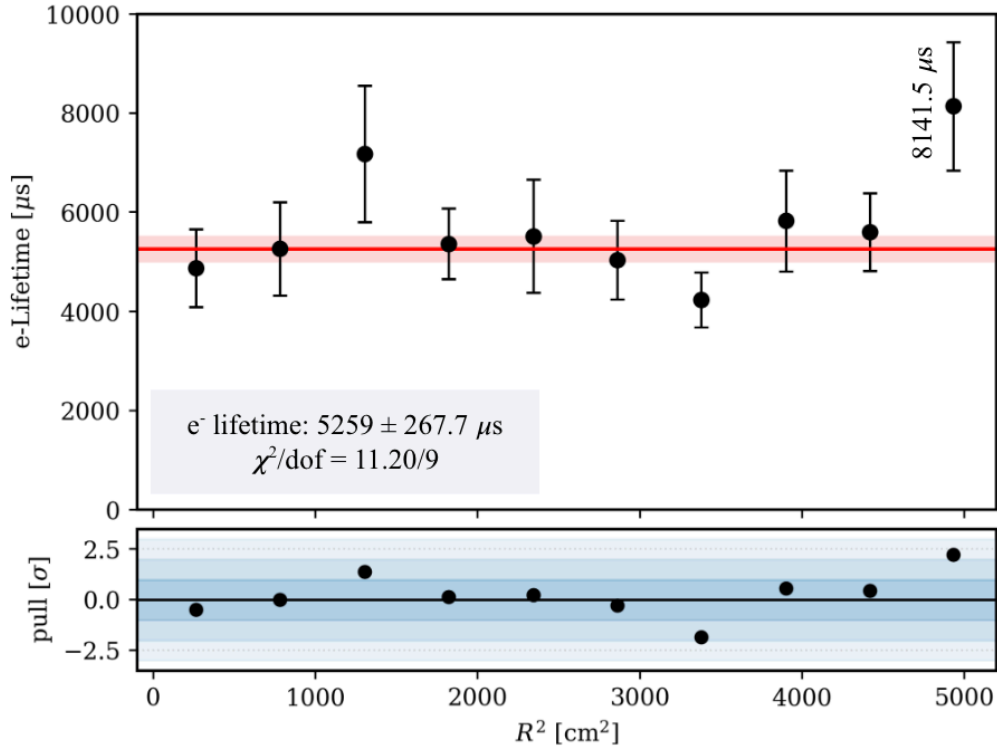


Figure 4.11: Electron lifetime τ_e vs. R^2 derived from ^{83m}Kr data for a period within WS 2022 with a weighted constant fit (red, $\pm 1\sigma$ band). Pulls are shown below with $\pm 1/2/3\sigma$ bands along with fit parameters.

Electrostatic modelling of the same configuration (shown explicitly in Fig. 4.11 as part of the full solution in section 4.6) reveals that the vertical drift field at the wall oscillates between 100 V cm^{-1} and 350 V cm^{-1} along z , a result reasonably well-approximated by a half-cosine (for L , the full cathode to gate length):

$$E(z) = E_0 + \frac{\Delta E}{2} \cos\left(\frac{\pi z}{L}\right), \quad E_0 \simeq 200, \quad \Delta E = 250 \text{ V cm}^{-1}. \quad (4.13)$$

Instead of assuming a constant charge-yield slope, the NEST-derived field dependence is integrated across the full profile. The slope is modelled as

$$\left| \frac{\partial \ln Q_y}{\partial E} \right| (E) \approx \frac{0.168}{E} - 8.0 \times 10^{-5} \quad (\text{V}^{-1}\text{cm}), \quad (4.14)$$

which smoothly interpolates between the known NEST values at 100 and 350 V/cm .

The average fractional change in charge yield is then computed analytically:

$$\Delta \ln Q_y = \left| \langle \ln \dot{Q}_y \rangle \right| t_{\max} \simeq 0.072 \quad \Rightarrow \quad \tau_{\text{field}} = \frac{950 \mu\text{s}}{0.072} \simeq 13 \text{ ms}, \quad (4.15)$$

and combined with the effective measured lifetime $\tau_{\text{imp}} = 5 \text{ ms}$ to yield the impurity-limited slope:

$$\tau_{\text{imp}} = \left(\frac{1}{\tau_{\text{eff}}} - \frac{1}{\tau_{\text{field}}} \right)^{-1} \simeq 8.1 \text{ ms}, \quad \Delta \tau_{\text{imp}} \approx 3.1 \text{ ms}. \quad (4.16)$$

This matches the observed outer-slice excess in equation (4.12) within statistical uncertainty. Any radial-field suppression would alter only the normalisation of S2, not the drift-dependent exponential slope, and thus serves only to

Table 4.4: Numerical ingredients for the LZ outer-wall back-of-the-envelope estimate shown previously.

Symbol	Value	Comment
E_0	193 V cm^{-1}	WS 2022 nominal drift field
ΔE	$\pm 125 \text{ V cm}^{-1}$	Wall field variation (LZEF)
L	145.6 cm	Active drift length
v_d	$1.53 \text{ mm}/\mu\text{s}$	Drift velocity at 193 V/cm , 174 K
t_{max}	$\sim 950 \mu\text{s}$	Full drift time (L/v_d)
$ \partial \ln Q_y / \partial E $	$0.8 \times 10^{-3} \text{ V}^{-1} \text{ cm}$	ER slope at $\sim 200 \text{ V/cm}$ (NEST)
τ_{imp}	5.0 ms	Representative WS 2022 impurity lifetime

broaden the uncertainty.

Hence, the apparent lifetime enhancement at the wall could be attributed entirely to mechanism 1 (vertical field curvature), once the correct $100 \rightarrow 350 \text{ V cm}^{-1}$ oscillatory variation and field-dependent Q_y slope are accounted for.

Implications

The comparisons above lead to four practical conclusions. First, XENONnT operated on the steep low-field flank of $Q_y(E)$ with a relatively large fractional field gradient; uncorrected lifetime fits were therefore unavoidably source dependent until the field- and source-specific $Q_y(E)$ corrections were applied. Second, during WS 2022 LZ operated on a flatter $Q_y(E)$ plateau with a modest fractional gradient, so the induced S2 modulation in the fiducial volume (sub- $\sim 3\%$ in lifetime, $\lesssim 1\%$ in instantaneous S2) lay below the statistical precision and no source separation was observable. Third, in WS 2024 the same mechanism produces a *larger common-mode* pseudo-lifetime bias ($\sim 16\%$ on the global fit) because of the lower nominal drift field and higher purity, but it still does not generate a source dependence: all routinely used internal calibrations ($^{83\text{m}}\text{Kr}$, radon/Po chain, $\text{Xe}^{131\text{m}}$) are volumetric and occupy the $10 - 100 \text{ keV}$ ER band where $|\partial \ln Q_y / \partial E|$ is smooth, so the curvature shifts all fitted lifetimes coherently. Fourth, a *local* amplification appears at large radius where the wall scallop drives a $100 \rightarrow 350 \text{ V cm}^{-1}$ vertical field oscillation; integrating the field-dependent NEST slope over this half-cosine profile predicts a mechanism-1 lifetime enhancement of $\sim 3.1 \text{ ms}$, matching the observed $\sim 3.0 \pm 1.5 \text{ ms}$ outer-slice excess. Looking forward, once LZ purity reaches $\tau_e \gtrsim 30 \text{ ms}$ an event-by-event $Q_y(E)$ correction (analogous to the XENONnT procedure [154]) will be required to suppress the residual $\mathcal{O}(10\%)$ curvature bias in high-precision lifetime measurements. Finally, while the absence of source-dependent lifetime measurements in LZ, unlike in XENONnT¹¹, is generally a positive indicator of detector uniformity, it also limits our ability to use such variation as an additional diagnostic handle for probing electric field structure. Nonetheless, this does not hinder our ability to interpret or correct field-related effects as will be shown in the following sections.

¹¹This statement is true up till the end of WS 2024, in the current data-taking period there have been evidence of such divergences, which will benefit from the full field-cognisant methodology proposed.

4.3 A 2D Axisymmetric Model of LZ

4.3.1 Far-Field Electrostatics Solution Concordance with the Concentric Wire Electrode Model

The LZ TPC employs four woven grids, whose diameters and pitches differ appreciably. The anode has the finest structure ($100\ \mu\text{m}$ wires with $2.5\ \text{mm}$ pitch), whereas the gate, cathode and bottom grids use either $75\ \mu\text{m}$ or $100\ \mu\text{m}$ wires on a $5\ \text{mm}$ pitch [67]. A fully resolved three-dimensional finite-element model of such a grid contains millions of elements; replacing the woven mesh by an axisymmetric model reduces this cost by approximately two orders of magnitude, sometimes more particularly for some adaptive meshing algorithms. The purpose of this section is to solidify the basis of this approximation quantitatively, first analytically, then numerically while spelling out the physical assumptions behind every step.

SQUARE MESHES AS A DOUBLE FOURIER SERIES

As a woven grid is periodic in x and y , the natural basis on the plane $z = 0$ can be written as [156]

$$\cos\left(\frac{2\pi mx}{p}\right) \cos\left(\frac{2\pi ny}{p}\right), \quad m, n \in \mathbb{Z}. \quad (4.17)$$

For a perfectly conducting mesh the potential is constant on the wires and, to leading order, free in the gaps. The boundary condition therefore admits the exact expansion:

$$V_{\text{mesh}}(x, y, 0) = V_{00} + \sum_{m, n \neq 0} A_{mn} \cos\frac{2\pi mx}{p} \cos\frac{2\pi ny}{p}, \quad (4.18)$$

with pitch p . Solving Laplace's equation for $z > 0$ multiplies every mode by

$$\exp\left[-2\pi z \sqrt{m^2 + n^2/p^2}\right], \quad (4.19)$$

such that mode $(m, n) = (1, 0)$ (or $(0, 1)$) is the slowest to fade. Taking the gradient of this single mode yields the envelope

$$\frac{|\Delta \mathbf{E}|}{E_0} \lesssim C_{\square} \frac{d}{p} e^{-2\pi z/p} \quad (\text{McDonald (2003) [156]}), \quad (4.20)$$

where d is the wire diameter and $C_{\square} \sim 1$.

RING SURROGATE AS A HANKEL SERIES

With axial symmetry the surface potential can be expanded in terms of bessel functions of the first kind, J_0 , with their corresponding cylindrical Fourier coefficients [157]

$$V_{\text{ring}}(r, 0) = V_0 + \sum_{n \geq 1} B_n J_0(k_n r), \quad k_n = n\pi/\Delta r. \quad (4.21)$$

We choose the radial spacing $\Delta r = p/2$. This equalises (i) the metal fraction, because the mesh covers $2d/p$ of each unit area while a ring covers $d/\Delta r$, and (ii) the slowest spatial frequency, because the first Hankel wave number becomes $k_1 = 2\pi/p$. Solving Laplace's equation adds an exponential factor $e^{-k_n z}$; with $\Delta r = p/2$ the leading term decays as $e^{-2\pi z/p}$. As $B_1 \propto d/p$, the error envelope is

$$|\mathbf{E}_{\text{mesh}} - \mathbf{E}_{\text{ring}}| \lesssim C_{\circ} \frac{d}{p} e^{-2\pi z/p} \quad (\text{Blum, Riegler \& Rolandi (2008) [157]}). \quad (4.22)$$

This equation, just like equation 4.20 only highlights the (dominant), z –relationship with amplitude (variation). Fig. 4.12 illustrates a different, more detailed view of the scalar potential; in the near vicinity of a wire held at a certain potential V , the appearance of the potential descriptions in the mesh and axisymmetric formalisms are explicitly shown, as are the rapidly diminishing amplitudes as a function of z in units of p . It is important to note that the shapes of the modes are indeed very different, and the inherent fingerprint of the two different wire geometries never disappear, but it is the magnitude of the deviation in the field values we care about and so it can be concluded that $\geq 1 - 2p$ away from the wire, the field equivalence achieved is more than satisfactory for calculations of bulk fields in TPCs.

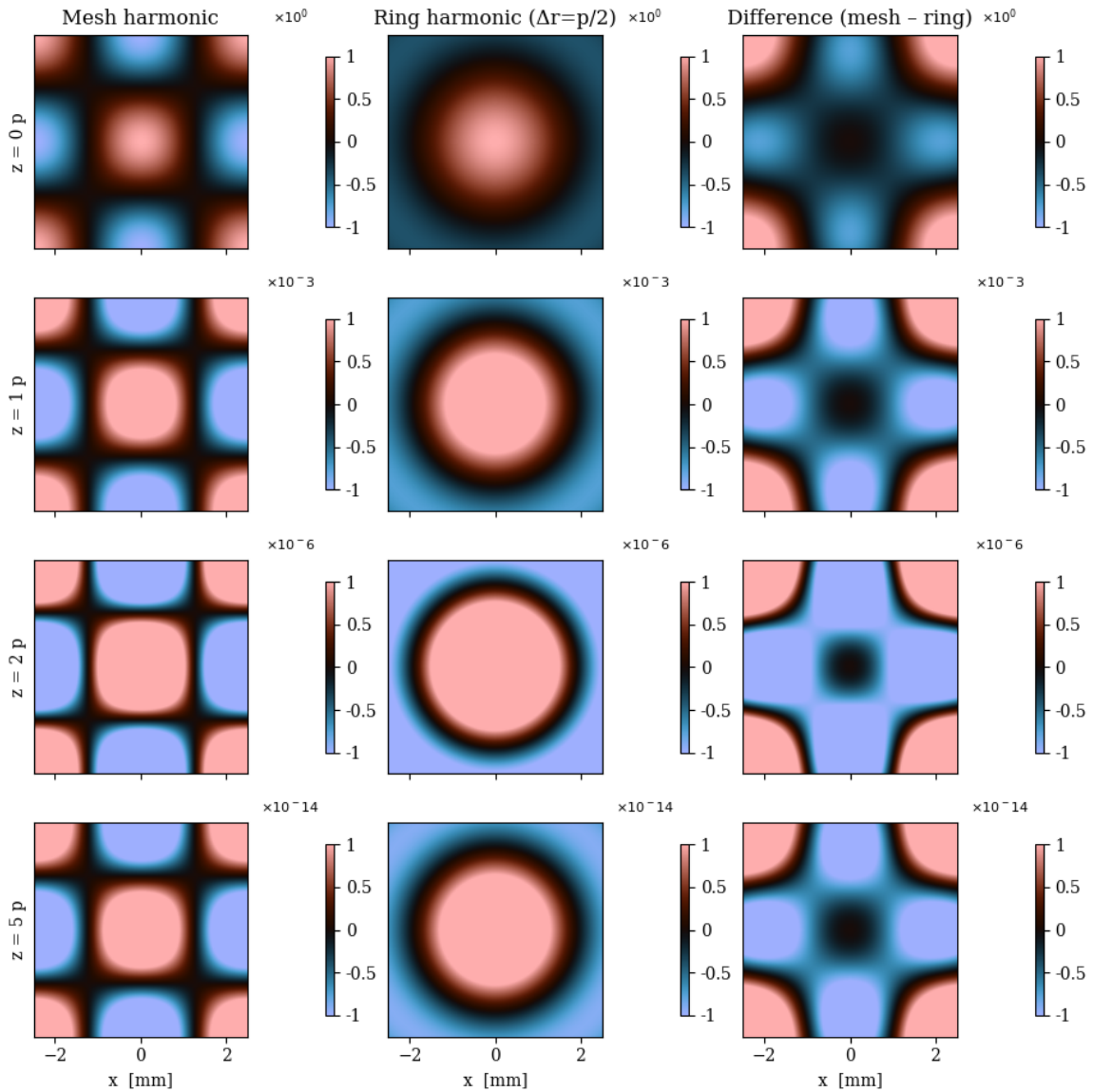


Figure 4.12: First non-constant harmonic of the electrode potential for a square mesh (left column), its concentric-ring surrogate with radial spacing $\Delta r = p/2$ (centre), and their signed difference (right). Rows correspond to heights $z = 0p, 1p, 2p, 5p$ above the grid (pitch $p = 5\text{ mm}$). Each colour bar spans the fixed interval $[-1, +1]$ in *reduced units*; the power-of-ten multiplier that converts those units back to physical potential is printed above every bar. The mesh and ring patterns differ sharply on the wire plane, but because both carry the common exponential factor $e^{-2\pi z/p}$ their amplitudes decline in lock-step. After one pitch the harmonic magnitudes have already fallen by a factor $\exp(-2\pi) \simeq 1.9 \times 10^{-3}$, and by five pitches both the harmonic and their difference lie below 10^{-14} of their surface values.

LINK TO FARADAY-CAGE HOMOGENISATION

Chapman, Hewett & Trefethen [158] replace a ring of n wires by an effective Robin boundary¹² and show that the interior field differs from the continuous-sheet solution by $\mathcal{O}(|\log r|/n)$. Setting $n = p/d$ reproduces the prefactor d/p in equations 4.20 and 4.22, tying the Fourier–Bessel picture to effective-medium theory.

ENVELOPE VALUES FOR THE FOUR LZ GRIDS

Table 4.5 converts equation 4.22 into numbers, using the pitches and diameters from Fig. 2.3. A conservative $C_{\square} = C_{\circ} = 3^{13}$ is applied. Even the finest grid (anode) produces a $\lesssim 0.25\%$ discrepancy one pitch above the wires; at

Table 4.5: Analytic envelope (equations 4.20, 4.22) for the four LZ grids.

Grid	p (mm)	d (μm)	d/p	$ \Delta E /E$ at $z = p$	at $z = 2p$
Anode	2.5	100	0.040	$\leq 0.24\%$	0.004%
Gate	5.0	75	0.015	$\leq 0.09\%$	0.002%
Cathode	5.0	100	0.020	$\leq 0.12\%$	0.003%
Bottom	5.0	75	0.015	$\leq 0.09\%$	0.002%

two pitches every plane is below 10^{-4} .

Numerical check with FENICS

Up to now, we have shown analytically that the full Fourier expansion of a perfectly conducting square mesh is dominated at all practical distances by its slowest decaying mode,

$$V_{11}(x, y, z) \propto \cos \frac{2\pi x}{p} \cos \frac{2\pi y}{p} e^{-2\pi z/p}, \quad (4.23)$$

and that all higher $(m, n) \neq (1, 1)$ modes are suppressed by at least a factor $e^{-2\pi z/p}$ for $z \gtrsim p$. While this motivates the use of a simpler axisymmetric surrogate, it is important to verify explicitly how close the woven and ring solutions remain under realistic conditions. To this end, we conduct finite-difference simulations of the two geometries and cross-check them against independent COMSOL studies.

The cathode plane was fixed at -50 kV for the purposes of these simulations, and the top electrode potential was adjusted so that the drift field above the cathode matched $E_{ave} = 303 \text{ V/cm}$ ¹⁴. Periodic boundary conditions were applied in the transverse x, y directions to emulate the infinite tiling of the mesh. To reduce computational cost, the domain height was truncated to $\sim 250 \text{ mm}$ above the cathode, with a Robin condition (where u denotes the perturbation about the uniform drift field due to the cathode wire structure),

$$\frac{\partial u}{\partial z} + \frac{2\pi}{p}u = 0, \quad (4.24)$$

¹²Finite wire spacing makes the boundary neither perfectly conducting nor perfectly insulating but something in between. In electrostatics a boundary condition of Robin type couples the potential V on a surface to its normal derivative: $\partial_n V + \lambda V = 0$, where λ encodes a boundary condition somewhere between a Dirichlet and Neumann condition. For $\lambda \rightarrow 0$ a perfect Neumann boundary is reproduced (as for an insulator), while for $\lambda \rightarrow \infty$ a perfect Dirichlet conductor is reproduced.

¹³These constants are dimensionless prefactors of order unity that arise because we kept only the leading harmonic when we truncated the series in equations 4.22 and 4.20. Higher order terms could result in diminishing deviations from a pre-factor of 1 so 3 is taken as a very conservative upper limit.

¹⁴This choice was deliberately to provide a direct comparison with earlier COMSOL studies.

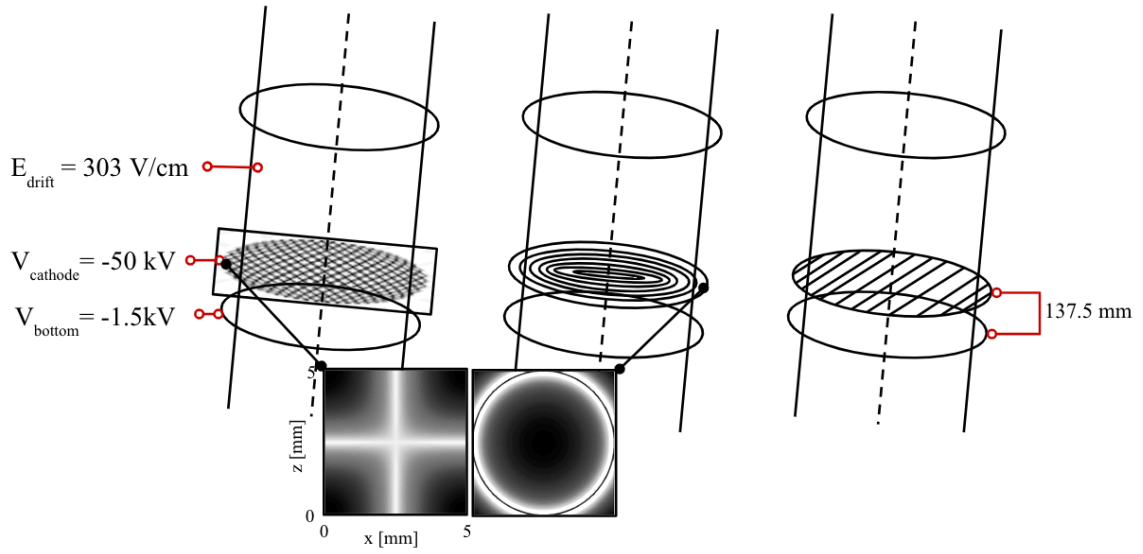


Figure 4.13: Simulation setup for comparing the woven cathode mesh with its axisymmetric ring surrogate. Dirichlet and Neumann boundary conditions used in the woven and axisymmetric models are indicated, with a parallel-wire configuration also shown for completeness (see COMSOL discussion). Insets illustrate the transverse field patterns immediately above the cathode: the woven cross (left) and its radially averaged ring representation (right).

imposed at the top boundary to enforce the expected $\exp(2\pi z/p)$ damping of higher harmonics. This ensures that the solver reproduces both the near-wire distortions and the correct asymptotic field. A schematic of the setup is shown in Fig. 4.13.

Fig. 4.14 shows the absolute difference in the longitudinal field between the woven and ring models, plotted as $\Delta E / E_{ave}^{woven}$. Both the color scale and contours are normalised to this fixed drift field (averaged for $z > 15 \text{ cm}$ away from the cathode), not to the local mesh field. As a result, the residuals appear more extended in z than in the analytic envelope plots, which are relative to the local background. The behaviour is nevertheless consistent: the difference falls exponentially with scale $\sim p/2\pi$ and by 10 – 15 pitches (within $\sim 10 \text{ cm}$) the discrepancy is already at or below the percent level. The magnitude of this near-field discrepancy also depends on the potential applied to the grid and the relative field strengths on either side. For the cathode, held at -50 kV , the fractional deviations reach the few-percent level but fall below 1% within 10 pitches. For the gate, however, the absolute potential is much lower (-4 kV), with a strong extraction field of order kV/cm on one side and the drift field of $\sim 300 \text{ V/cm}$ on the other. In this case the effect of higher-order modes is less pronounced in relative terms: the larger absolute field near the liquid–gas interface suppresses the impact of the residual oscillations, and the residual in the bulk drift region falls below the 1 – 2% level within roughly two pitches. Thus, while care is needed in the immediate vicinity of the grids, especially for high-voltage electrodes, the axisymmetric surrogate remains adequate for modelling the drift field throughout the active region of the detector.

Independent COMSOL calculations also support these conclusions (Fig. 6.14). In those studies the parallel-wire grid was used as a baseline, against which the woven mesh and ring surrogate were compared. The mesh–parallel and ring–parallel differences are each at the few-percent level directly above the wires, falling below 1% within ~ 10 pitches.

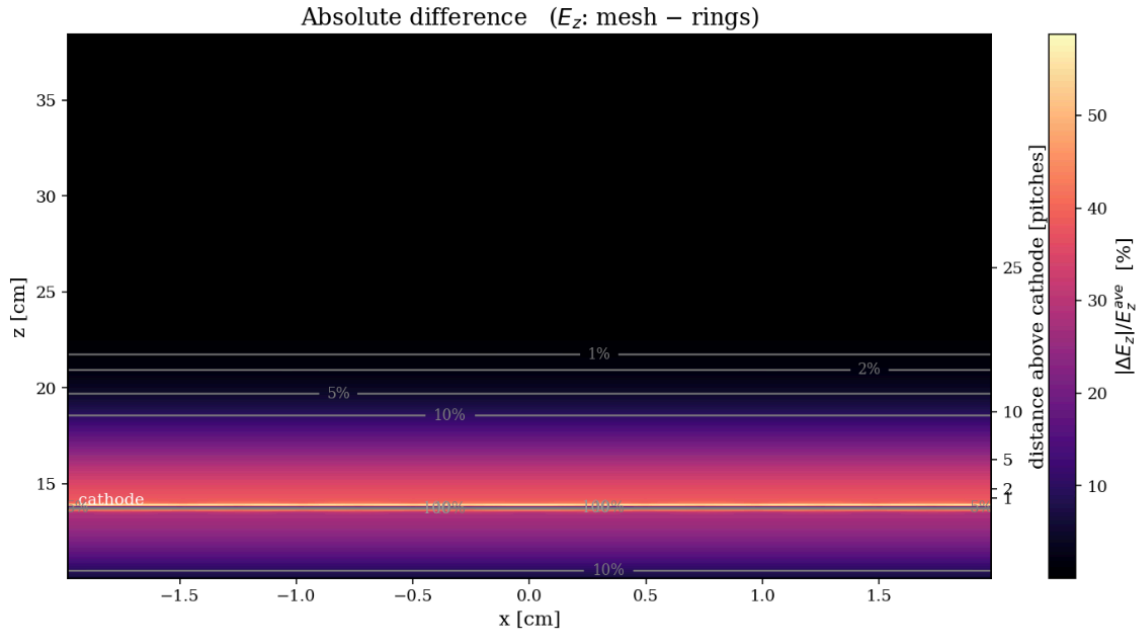


Figure 4.14: Absolute difference in the longitudinal drift field between the woven cathode mesh and its axisymmetric ring surrogate. The color scale and contours show $|\Delta E|/E_z^{ave}$ in %, with $E_z^{ave} = 303 \text{ V/cm}$ the average drift field far from the grid. Differences are largest immediately above the cathode wires but fall exponentially with distance, dropping below the 1 – 2% level after ~ 10 pitches ($\mathcal{O}(2 - 3 \text{ cm})$). Beneath this distance, typically event rates are dominated by high cathode/ near-grid rates from radiogenic populations so this threshold does not limit us in current physics searches.

Taken together, this implies that the direct mesh–ring difference is of the same order as in Fig. 4.14. Both approaches therefore broadly demonstrate that the axisymmetric ring approximation reproduces the bulk drift field to the required accuracy.

Finally, it is still worth noting that the numerical results clearly exhibit a somewhat slower suppression of residual structure than the analytic estimates of equations (5.22–5.24). This arises because the analytic envelope retains only the slowest decaying Fourier mode, while in practice higher-order harmonics contribute within the first several pitches. These higher modes are rapidly damped but do not vanish instantly, so the simulated mesh–ring discrepancy remains visible slightly further from the grid than the simple envelope would suggest. Nevertheless, both treatments agree on the essential point: the error falls exponentially with z/p , and beyond $\sim 10 - 15$ pitches the residual difference is comfortably below the percent level.

4.3.2 Implications of a Thin-Plate Approximation

To reduce computation time, the cathode and anode grids are rather approximated as planar electrodes with deflections of 0.32 mm and 1.0 mm , respectively; these values are derived from studying the size of S2s as a function of radius [115]. The approximation can be applied as the far-field regime (greater than a few pitches), encompassing regions exceeding a distance of some multiple wire pitches from the grids ($\mathcal{O}(mm)$), is more pertinent for characterizing the bulk electric fields within the extraction region. Deviations in the electron trajectory in the immediate vicinity of the wires due to more circular equipotentials in a localised, radial electric field regime, rarely have a significant influence on the overall reconstructed energy or position of the event of interest. The approximation then entails the application

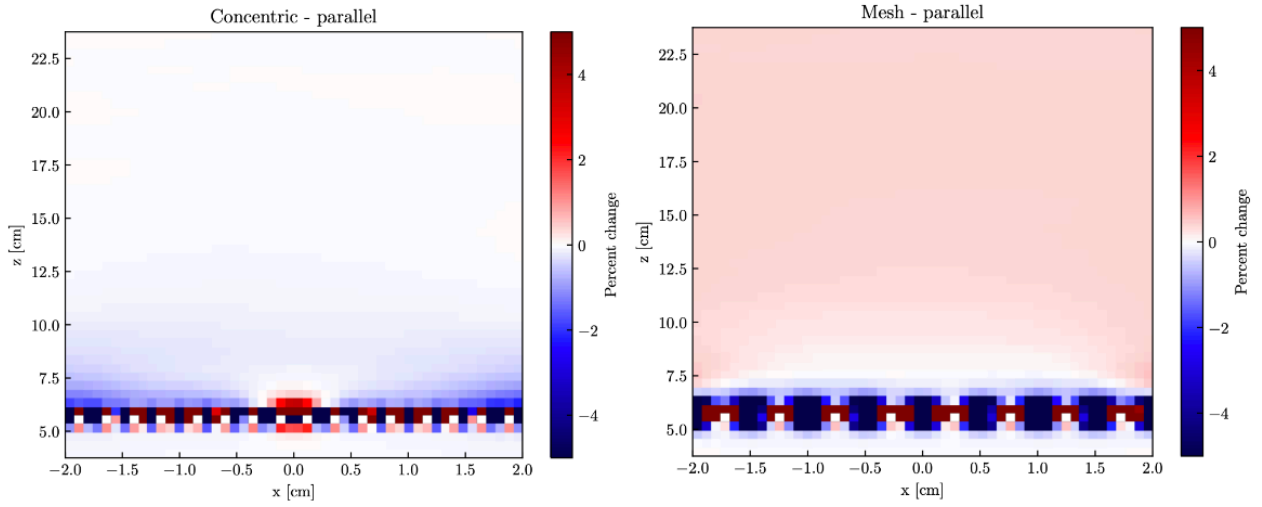


Figure 4.15: Percent change in the longitudinal field relative to a parallel-wire baseline using COMSOL. The concentric-ring surrogate (left) and woven mesh (right) are each compared against the parallel-wire grid. Going from parallel to concentric wires, the discrepancies are already below 2% within ~ 5 cm (~ 10 pitches), and continue to fall further with depth into the drift region. Though the difference map from a parallel to a woven mesh shows higher variation, it is still clear that the direct mesh-ring difference is of the same order, consistent with Fig. 4.14. Plots produced by L. Tvrznikova [81].

of a correction factor ΔE to *shift* the *true* anode voltage, V_0 , slightly in order to replicate the far-field potentials in the more uniform field volume of the extraction region. This factor can be derived by reducing the problem to a capacitor with two dielectric materials (the plate approximation) and comparing this to the electrostatics problem of a unit cell with a wire in the middle (the gate), bound by Neumann (continuity) and Dirichlet conditions (defined voltages at the electrodes). The derivation is modified from [159].

For a **wire** electrode,

$$E_1 = \frac{(V_0 - V_1)}{b_1} - \Delta E, \quad (4.25)$$

and for a **plate** electrode,

$$E_1 = \frac{(V_0^P - V_1)}{b_1}, \quad (4.26)$$

where b_1, b_2 are the distances of the anode from the gate and the PMTs respectively, and E_1, E_2 are the corresponding fields in the same volumes, defined by V_0 , the true wire anode potential, and V_1 , the gate potential. V_0^P is then the equivalent plate potential required to reproduce the correct far-field profile in the extraction/electroluminescence region, by applying a correction $\Delta E b_1$ to the wire case. A diagrammatic representation is provided in Fig. 4.16 and

$$V_0^P = V_0 - \Delta E b_1 \quad (4.27)$$

, where the potential difference correction is derived to be,

$$\Delta E = \frac{b_2}{b} \left(\frac{(V_0 - V_2)}{b_2} - \frac{(V_1 - V_0)}{b_1} \right) \left(\frac{K}{1 + K} \right), \quad (4.28)$$

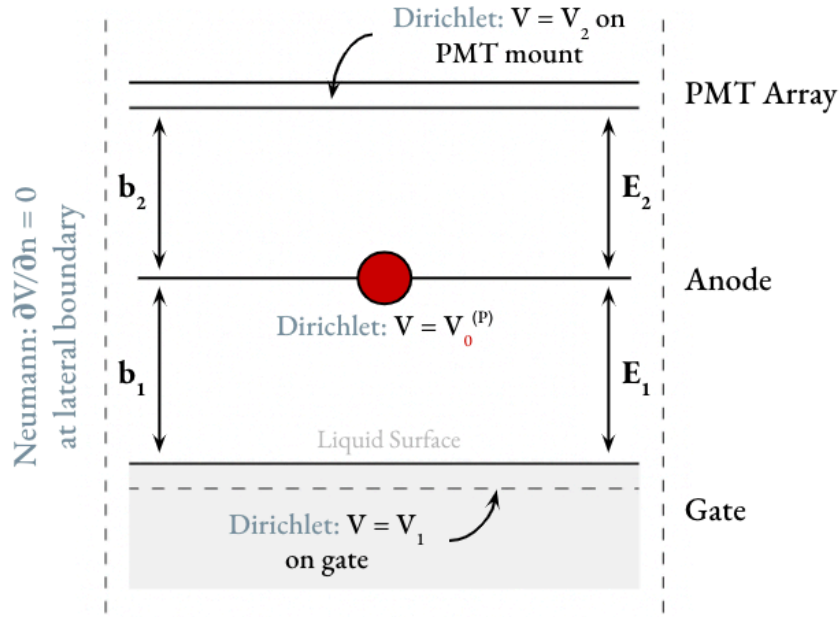


Figure 4.16: Schematic cross-section of the extraction region showing the wire-to-plate approximation. The top PMT plate at $z = 1538$ mm is held at potential V_2 , the anode wire mesh—approximated by an effective plate at potential V_0^P —lies at $z = 1469$ mm, and the gate plate (liquid surface) at potential V_1 bounds the liquid region below. Dirichlet boundary conditions ($V = V_2$, $V = V_0^P$, $V = V_1$) are applied on each electrode surface, while Neumann ($\partial V/\partial n = 0$) conditions enforce field symmetry at the lateral dashed boundaries. The electric fields E_2 (PMT–anode, over distance b_2) and E_1 (anode–gate, over distance b_1) are indicated by the vertical arrows, and the shaded region denotes the liquid phase.

for $K \equiv \frac{ab}{2\pi b_1 b_2} \ln\left(\frac{a}{2\pi r}\right)$, the ratio of the per-unit-length capacitance of a single wire cell to that of the equivalent parallel-plate capacitor¹⁵, and a is the wire anode pitch (with the axisymmetric model, modified to half of the real woven mesh anode pitch ($a/2$) as discussed in 4.3.1), $b = b_1 + b_2$, V_2 is the PMT voltage and r is the radius of the wire. The resulting simulation input anode voltages to replicate the correct gas and liquid extraction fields for WS 2022 & WS 2024 were found to be 3569 V, 1112 V & 3097 V.

4.3.3 The Final Model

The final electrostatic model is built by tessellating the detector in GMSH 4.11 and solving Laplace’s equation with FENICS 2019.2. Dropping sub-millimetre hardware—screws, ribs, cable glands keeps the unstructured mesh below ≈ 3 million elements, so a single solve finishes in under a minute; any residual bias is absorbed later when the map is tuned to calibration data. The materials actually retained are collected in table 4.6. Electrode geometries are simplified only as far as field accuracy allows (table 4.7): the anode is treated as a solid plate and corrected according to § 4.3.2 ($< 0.3\%$ error), whereas the gate, cathode and bottom grids are represented by concentric rings spaced at half-pitch; § 4.3.1 shows this “ring surrogate” reproduces $|E|$ to better than 0.25% one pitch above the wires and to $< 0.05\%$ RMS throughout the 1.45 m drift. Field-shaping rings are modelled exactly, and all field values are stored on a 2D rz mesh that is later revolved, reducing file size by a factor ≈ 50 while matching the cylindrical symmetry used in event reconstruction. Grid deflections measured during installation [67], 0.81 mm (gate), 0.79 mm (anode) and 1.00 mm (cathode), are

¹⁵See [159]

Table 4.6: Dielectric constants retained in the electrostatic model.

Material	ϵ_r	Comment
Liquid xenon (179 K)	1.85	Latest measurements used in [84]
Gaseous xenon	1.00	Ideal gas; influence $< 0.1\%$
PTFE reflector panels	2.10	Literature band 2.04 – 2.13
PEEK stand-offs	3.20	Between anode-gate rings only
Stainless steel (electrodes)	∞	Treated as Dirichlet conductors

Table 4.7: Geometric representations used inside the solver.

Component	Model in FEniCS	Adequacy / proof
Anode grid	Solid plate + plate-correction	$< 0.3\%$ local error (§4.3.2, [152])
Gate, cathode, bottom grids	Rings at $\Delta r = p/2$	$< 0.25\%$ at $z = p$, RMS $< 0.05\%$ (§4.3)
Field-shaping rings	Exact 2D line segments	Fully axis-symmetric geometry
PTFE surfaces	Smoothed solids	Omitting ribs shifts $ E $ by $< 0.05\%$ [152]
Field-evaluation grid	2D r - z mesh, revolved	Cuts file size $\sim 50\times$; matches reconstruction symmetry

imposed as parabolic offsets [152]; they alter the drift field by at most 0.05% , confirming that small planarity errors are negligible at the present 0.5% accuracy target. Finite transparency is handled after the solve with the “grid-funnelling” parametrisation ($\Delta t/t_0 = -0.0312(1 - \cosh(x/1.246))$, $C = 0.294 + 0.774 \mathcal{R}^{-0.707}$, $\mathcal{R} = |E_{bulk}|/|E_{gate}|$); this captures the observed S2 compression without perturbing the primary PDE solution. The resistor chain is the real LZ $58 \times 1 \text{ G}\Omega$ (two in parallel per section) design, giving a $\sim 200 - 500 \text{ V cm}^{-1}$ gradient (across different science runs), so no voltage scaling is required. With these ingredients the axisymmetric solve is $25 - 30$ times faster than a fully resolved wire model while still meeting the field-uniformity specification.

Finally, future iterations will require an updated skin model (the current geometry remains as a placeholder from early iterations of skin design). As the minimum skin thickness and potentials are not affected at all, the upgrades are not expected to change drift-region fields by any more than a few $10^{-2}\%$ according to separate COMSOL simulations by the author¹⁶, so they do not impact the conclusions drawn in this thesis. This model is being worked on currently and should be available in the near future within a new release.

4.4 The LZ Electric Field Simulations Package

The LZ Electric Fields simulations package, LZEF [160], was developed¹⁷ in order to produce field and drift maps to more accurately capture inhomogeneities occurring within the fields of the TPC or skin. These maps can affect our understanding of pulse shapes, particularly S2 shape, which in turn can affect our intuition of backgrounds and their rates (isolated S1s and S2s and their sources), directly impacting analyses of data. However, the observed fields could also be induced by various other physics effects, such as charge transport properties on different metal or dielectric surfaces, field leakage due to the high transparency of the gate ($\sim 97\%$) and cathode ($\sim 92\%$) grids, the potential

¹⁶This formed the basis of the new XLZD skin/ cryostat design (chapter 6) and therefore was checked very carefully.

¹⁷The LZEF package was developed by former graduate student, R. Watson. This work builds on the previous framework and extends its application by tuning it to fields beyond the criteria used for LZ’s first science run.

repercussions of shorted resistors, among other considerations. In reality, it is reasonable to assume that the observed fields represent a convolution of several effects, which are difficult to disentangle and quantify. The final simulated field and drift maps are therefore sensitive to a variety of parameters and relationships, which are not trivially extracted from literature. This section aims to explore methods towards achieving the ultimate goal of the package: to really enhance our sensitivity to the implications of the design of the LZ TPC (in terms of fields, this would translate to S2 size and shape, for example) and try to make sense of the contribution of other effects, like charge transport models, diffusion, grid deflection (as discussed in chapter 3), field leakage, and others, which would not be possible through back-of-the-envelope calculations.

A critical part of the tuning and development process of the simulation package is then the justification and thorough evaluation of the model parameters and assumptions on which the framework of the full simulation is built. This constitutes an iterative process, which is intimately interlinked with our choice of meshing and interpolation algorithms and numerical methods employed to solve the different equations describing the problem. It is also dependent on the interplay with experimental data where possible, be it from LZ or other similar experiments. The ultimate aim of the simulation package is to be able to investigate and characterise the contributions of these effects and by doing so, provide a means by which to explore and reach a generalised picture of the dominant physics mechanisms which may result in the changing behaviour of fields in various regions of the LZ TPC (or TPCs in general) explored further in Section 4.6.

4.4.1 Finite Element Simulations

The geometric complexity of the TPC motivates a finite element analysis (FEA) approach to tackling the associated electrostatics problem. This method allows greater sensitivity to localised changes within the volume by defining subdomains in the form of mesh cells, each with their own boundary conditions, leading to solutions which can be recombined into a higher granularity global solution. In this case, FEM seeks a field solution $u_i = u(x_i)$, associated with each node of the mesh in a vector space V . This forms the global definition of the vector space: a system of equations $A\mathbf{u} = \mathbf{f}$, where A is the finite element matrix and $\mathbf{f}$ is the source term, equivalent to a free charge density in this case [161]. To tackle situations where boundaries or material interfaces have disparate dielectric permittivities, the weak formulation is also applied. Numerical computations can encounter difficulties at these locations, particularly when dealing with higher-order derivative terms due to discontinuities in adjacent cell parameters. The weak formulation addresses this challenge by transforming the governing differential equation into an equivalent integral form. This transformation simplifies the evaluation of derivatives, enhancing the numerical stability of the algorithm without compromising the convergence towards the exact solution. In the context of LZ, the electric field map is derived by solving Poisson's equation. A derivation of this formulation is outlined in the following.

Starting with Gauss' law using the electric displacement field $\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}$, where ϵ_0 is the permittivity of free space, $\mathbf{P}$ is the polarisation density contributing to a bound charge density, and $\mathbf{E} = -\nabla\phi$, where ϕ is the scalar electric potential:

$$\nabla \cdot \mathbf{D} = \rho_f \quad (4.29)$$

$$-\nabla \cdot (\epsilon \nabla \phi) = \rho_f. \quad (4.30)$$

Now consider solutions $\mathbf{v}$ of the weak formulation, equivalent to the solutions of the strong formulation $\mathbf{u}$, satisfying:

$$\vec{v}^T A \vec{u} = \vec{v}^T f. \quad (4.31)$$

In integral form, Equation 4.29 becomes:

$$-\int v \nabla \cdot (\epsilon \nabla \phi) d^3x = \int \rho_f v d^3x. \quad (4.32)$$

Applying Green's formula, for $\vec{n}$, the outward-pointing normal vector to the surface S defining the boundary of the vector space V ,

$$\int_V \xi \nabla^2 \zeta dV = - \int_V \nabla \xi \cdot \nabla \zeta dV + \int_S \xi \frac{\partial \zeta}{\partial n} dS,$$

Equation 4.32 can be written as:

$$\int (\nabla v) \cdot (\nabla \phi) d^3x - \int v \frac{\partial \phi}{\partial n} d^2x = \int \rho_f v d^3x. \quad (4.33)$$

Note that for simplicity we set $\epsilon = 1$, which will not be the case for liquid xenon or PTFE. Finally, choosing to exploit the largely axisymmetric geometry of LZ, it makes sense to transform from a Cartesian to a cylindrical coordinate system. This is discussed further in Section 4.3.

$$\int (\delta_r v \delta_r \phi + \delta_z v \delta_z \phi) r dr dz + \int \sigma_f r dr dz - \int \rho_f v r dr dz = 0. \quad (4.34)$$

This formulation is applied by the open-source software FENICS [162] in order to compute the full electric field profile in the detector.

4.4.2 Drift Simulations & Drift Map Production

Following the generation of these “field maps”, we can now assess their impact on charge transport and drift in the forward field region of the TPC: a crucial factor in determining the S2 signal's size and shape. Below, we summarise the architecture of LZEF and the key numerical methods at the heart of its drift-simulation framework. For further details and validation plots, see Smith (2023) [152].

Physical Assumptions & Included Effects

Before deconstructing the details of how drift maps are built, it is useful to summarise the core assumptions of LZEF's drift simulation and the physical processes we track. Table 4.8 lists the geometry, field solution, boundary handling, and the five key observables that are recorded for each electron trajectory.

Drift Map Generation Algorithm

Drift maps are built by sampling individual electron trajectories (essentially “stream lines” from field solutions) throughout the TPC, recording information at each integration step, the drift time, S2-reconstructed radius, incremental transverse and longitudinal diffusion, and whether the path strikes a boundary.

Seed points are first initialised both below the gate grids ($\sim 3 \text{ mm}$), sampled uniformly in R^2 and “snapped” to the gaps between the grid wires, and along the PTFE wall at fixed intervals such that $\Delta z \approx 500 \mu\text{m}$. Further corrections must

Table 4.8: Summary of the core assumptions, boundary treatments, and tracked observables in LZEF’s drift simulations.

Aspect	Implementation
Geometry & field	2D axisymmetric (r, z) LXe volume, including woven gate and cathode meshes plus PTFE walls. Static electric field solved via FEM (FENICS [162]), with manual mesh-density control: ~ 1 mm near electrodes/walls, several cm in the bulk.
Boundary treatment	Electrons hitting PTFE are “captured” (no S2). Near-wall seed points duplicated and nudged ε inward to avoid interpolation gaps. Electrons reaching the gate are assigned an S2 emission position obtained by averaging over all possible azimuthal phases relative to the wire pattern, compensating for the loss of ϕ information in the axisymmetric model.
Drift time	Time for an electron to reach the liquid–gas interface at $z = 1461$ mm.
S2 radius	Radial coordinate of the electron cloud upon exiting into the gas layer, reconstructed via PMT hits of S2 light.
Wall-attachment probability	Fraction of trajectories intercepted by the PTFE at $R = 728$ mm.
Transverse diffusion	Analytical Gaussian $\sigma_T = \sqrt{2D_T t}$ with $D_T \approx 55$ cm ² /s in bulk; Monte Carlo Gaussian steps within 2 cm of PTFE.
Longitudinal diffusion	Analytical $\sigma_L = \sqrt{\frac{2D_L t^3}{L^2}}$ with $D_L \approx 25$ cm ² /s over drift length L .

be applied to ensure that the funnelling effect of field lines, especially near the gate grid, does not skew the calculated S2-reconstructed radius too far from the experimental values. This effect typically leads to additional deflections in the charge drift trajectories that are essentially an artifact of the simulations modelling the woven mesh structure as axisymmetric, but can be solved by setting a standoff distance (2.5 mm) at which the trajectory’s crossing point is logged corresponding to an experimentally-validated match in the S2-reconstructed position [152] of an event. From each seed, electron trajectories are integrated in both the forward (toward the liquid–gas interface) and reverse (toward the cathode) directions using the classical fourth-order Runge–Kutta method (RK4). RK4’s $\mathcal{O}(\Delta t^5)$ local truncation error permits time-step sizes large enough for good computational efficiency, yet small enough to resolve the steep field gradients in the vicinity of mesh elements without appreciable phase-space drift. At each sub-step we log the elapsed time, local field vector $\mathbf{E}$, and incremental contributions to the mean-squared transverse and longitudinal displacements (via the known diffusion coefficients D_T , D_L); any trajectory not reaching the liquid surface, for example, intersecting the PTFE wall instead, is flagged as “captured” and removed from subsequent S2 statistics.

Once continuous field-line solutions are obtained, we apply a “stride” down-sampling: only one point per cell, or within a fixed radius of its parent seed, is retained, ensuring sub-millimeter interpolation error while capping the total number of vertices. Within the 2 cm boundary shell adjacent to PTFE, a Monte Carlo diffusion module augments each RK4 step with random Gaussian displacements of width

$$\sigma_T = \sqrt{2D_T \Delta t}, \quad \sigma_L = \sqrt{2D_L \Delta t}$$

, after which any wall-captured paths are excluded from the diffusion statistics. This feature is not a default and can be switched on or off by the user.

To guarantee seamless coverage of the entire (r, z) domain, seed points at $r = 0$ and along all physical boundaries are duplicated and nudged radially by a small offset ε , and any interpolation query outside the main hull falling back to a nearest-neighbour. Finally, the down-sampled endpoints serve as vertices for a Delaunay triangulation (via QHULL) or Voronoi-based mesh refinement (particular near the wall & grids), and each drift quantity $f(r', z')$ is computed by barycentric interpolation within the enclosing simplex. The result is a continuous, reliable drift map with uniform sub-millimeter accuracy robust against most physical but arbitrary electrode configurations.

Robust interpolation: ensuring reliable field maps

In the final “drift-map product”, we must query quantities, drift time, S2-reconstructed radius, diffusion widths, and wall-attachment probability, at arbitrary points (r', z') throughout the TPC volume. In LZEF, the popular open-source software QHULL [163] is used to do this. A natural first thought is to resample onto a uniform (r, z) grid and use bilinear interpolation, but our samples lie on an irregular, field-shaped mesh: seeds funnel through grid gaps, cluster near PTFE walls, and avoid the detector center. Bilinear interpolation would either (a) blur fine features by resampling millions of endpoints onto a coarse lattice, or (b) produce “cut-across” shortcuts in unsampled regions, creating blind spots.

Instead, we use Delaunay triangulation, which subdivides every point cloud into triangles (also called a *simplex* or facet) so that no point lies inside any triangle’s circumcircle, and interpolate within each enclosing triangle using barycentric weights¹⁸. In our first LZEF runs, however, this produced pathological “sliver” triangles, non-uniform simplex shapes, and even gaps, especially in regions of rapid field variation (near walls) or extreme uniformity (center), leading to artificial over-/under-densities in reconstructed S2 maps. In the latest releases of LZEF, we therefore introduced three targeted refinements:

- Localised Voronoi refinement in high-variation regions.

Challenge: In the 2 cm shell adjacent to the PTFE, the field gradients and seed clustering produce tiny, needle-thin Delaunay triangles with large circumradii, which spike local interpolation error.

Solution: Compute a constrained Voronoi diagram in this band whose cells naturally adapt to local point density and guarantee coverage, and convert each cell back into well-shaped triangles. Although Voronoi and Delaunay are dual structures, Voronoi explicitly enforces locality by construction of nearest-neighbor regions, preventing the extreme aspect ratios that can slip through a pure Delaunay quickhull method.

- Global vertex jitter in uniform-field central regions.

Challenge: Far from electrodes, trajectories run nearly parallel in a uniform field, giving regularly spaced, grid-like points. This uniformity paradoxically induces large, elongated triangles spanning many centimeters due to the degeneracy in the minimal convex hull constructable, degrading interpolation accuracy.

Solution: Apply a small random perturbation ($0 - 100 \mu\text{m}$) to each seed’s (r, z) before triangulation. This breaks exact alignments without altering the physical geometry, yielding a more isotropic simplex size distribution and bounding maximum edge lengths across the mesh.

¹⁸These ratios of sub-triangle areas opposite each vertex that naturally extend linear interpolation to arbitrary meshes. A more visual description is provided in [152] in Chapter 4, page 102 – 3.

- Higher seed density in mesh-gap channels.

Challenge: Under-sampling around the woven gate grid lets interpolation “shortcut” across unsampled voids, mis-assigning S2 radii by several millimeters.

Solution: Impose a finer radial seeding ($\Delta r \approx 1 \text{ mm}$) in the vicinity of each grid wire and ring gap, explicitly resolving vertical drift channels so that simplices cannot span unsampled gaps.

These refinements transform our interpolation pipeline into a more robust drift simulation tool: the mesh covers the full active volume without gaps, all simplices meet strict aspect-ratio and size constraints, and spatial interpolation errors stay uniformly below our sub-millimeter requirement.

4.5 A Pure-Geometry Field Solution

The field in the $\mathcal{O}(\sim \text{mm})$ -wide annulus adjacent to the PTFE wall is highly non-uniform as discussed in §4.2.1 and Fig. 4.2. Here we return briefly to this discussion, in specifically the context of LZ’s two WIMP search campaigns. As each $\sim 2.45 \text{ cm}$ -tall field shaping ring is separated by a small mm -scale gap (speculated residual due to the imperfect “locking” of the panels going from room-temperature assembly to the cryogenic operation temperatures), the equipotentials resemble a stack of shallow cusps rather than smooth cylinders. Field lines therefore “scallop”; electrons released in this region are repeatedly guided toward the wall at each concave segment (Fig. 4.17).

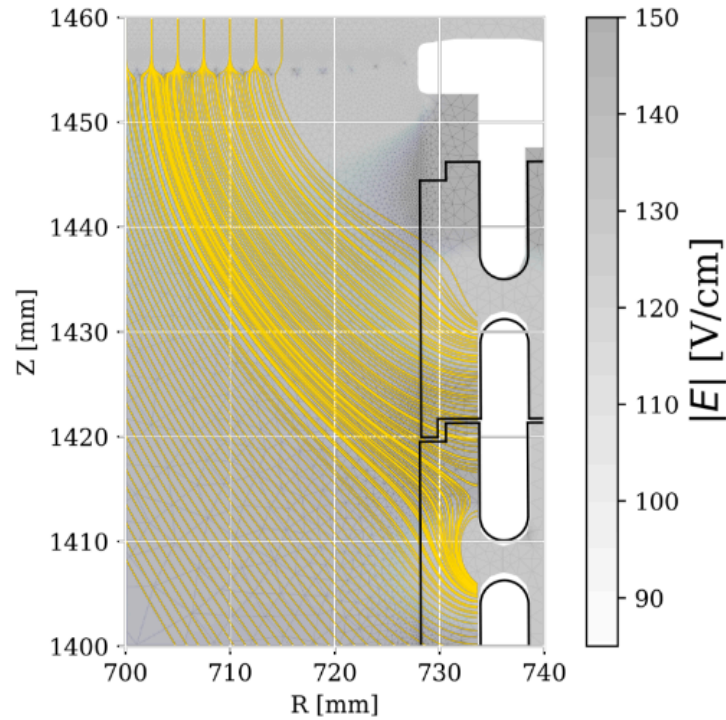


Figure 4.17: Pure-geometry field solution in the PTFE annulus, showing selected field lines (yellow) traced from the liquid bulk towards the gate region and the corresponding field-strength contour map (gray-scale). The scalloping of equipotentials at each field-shaping ring gap induces local inward deflections of field lines in the mm -scale annulus adjacent to the wall, producing the characteristic “cusp” segments that underpin the geometry-only wall contour (red dashed curve in subsequent figures).

Between intersections, inward diffusion could also be speculated to potentially widen the probability envelope describing this effect but due to the expected magnitude of the diffusion coefficients discussed in chapter 3 as a function of field, this effect is assumed to be negligible compared to the observed near-wall effects. More specifically, using the EXO-200 parametrisation $D_T(E) \approx 35 \text{ cm}^2 \text{ s}^{-1} (250 \text{ V cm}^{-1}/E)^{1.3}$ [125], the transverse diffusion constant in the central drift field for the two WIMP searches can then be approximated as

$$\begin{aligned} \text{WS 2022: } E_0 &= 193 \text{ V cm}^{-1} \rightarrow D_T \simeq 49 \text{ cm}^2 \text{ s}^{-1}, \\ \text{WS 2024: } E_0 &= 97 \text{ V cm}^{-1} \rightarrow D_T \simeq 120 \text{ cm}^2 \text{ s}^{-1}. \end{aligned} \quad (4.35)$$

Propagating each value over the full drift time ($t_d \approx 950 \mu\text{s}$ for WS 2022 and $t_d \approx 1100 \mu\text{s}$ for WS 2024) gives

$$\sigma_{\text{diff}} = \sqrt{2D_T t_d} = \begin{cases} 3.0 \text{ mm} & (\text{WS 2022, bulk}) \\ 5.4 \text{ mm} & (\text{WS 2024, bulk}). \end{cases} \quad (4.36)$$

Even if the local field were to drop by a further 20 % in the last centimetre ($E \rightarrow 0.8E_0$), the corresponding RMS spreads, $\sigma_{\text{diff}} = 3.4 \text{ mm}$ (WS 2022) and 6.2 mm (WS 2024) - would still be $\lesssim 1 \text{ mm}$ larger than the bulk values. By contrast, the observed wall-edge broadening exceeds this 3–6 mm scale and exhibits an exponential radial dependence characteristic of field scalloping and charge loss rather than the $\sqrt{t}$ -scaling of diffusion. We therefore treat diffusion as sub-dominant in the near-wall position-resolution budget.

Monte-Carlo tracking (LZEF-intrinsic) using the geometry-only field map then shows that electrons born within a few millimetres of the wall have a substantial probability of intersecting the PTFE before reaching the liquid surface. The extent of this finite wall-attachment probability is also in fact a field-dependent phenomenon. Different electrode potential configurations correspond to different voltage steps between adjacent rings in an optimised field cage, leaving these charge-loss zones susceptible to changes in drift field (Fig. 4.18).

Further, when an electron attaches to the wall it either recombines locally or drifts slowly along the PTFE surface before being re-emitted as delayed single-electron noise. In both cases the prompt S2 is attenuated. The resulting charge-loss (QL) events appear in calibration data as a band with suppressed S2 and, consequently, a biased reconstructed radius. These are both shown in Fig. 4.4.

That degradation is not uniform with radius. Fig. 4.19 also plots the statistic

$$\sigma_R^M \sqrt{S2(R)}$$

and shows the result for the WS 2024-like configuration. Inside $R \lesssim 65 \text{ cm}$ the curve is almost flat, indicating that the resolution is governed by photon statistics alone. Within the final $\sim 3\text{--}5 \text{ cm}$, however, the profile departs sharply from the plateau (P_1) and follows an exponential rise

$$\sigma_R^M \sqrt{S2(R)} \propto P_0 \exp\left[\frac{r - r_{\text{wall}}}{r_0}\right] + P_1, \quad (4.37)$$

with a characteristic length $r_0 \simeq 2.4 \text{ cm}$. The exponential behaviour — together with the fact that the rise is larger in the lower-field WS 2024 configuration — implies the presence of an additional, wall-related mechanism that dominates

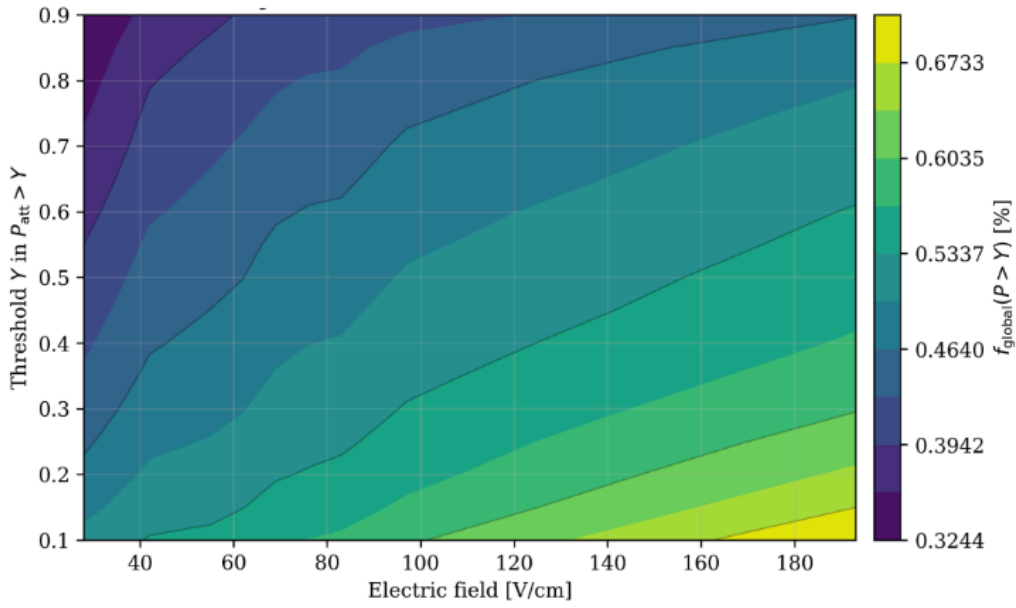


Figure 4.18: Global fraction with $P_{\text{att}} > Y$ versus drift field E and threshold Y . The affected volume increases smoothly with E and decreases with stricter Y ; even at 193 V/cm it remains $\lesssim 0.6\%$ for $Y = 0.5$. This parametric scan summarises the full range of fields LZ has operated at; for each a map similar to Fig. 4.2 was generated. We note here that the maps generated to create this sweep do not incorporate wall-charge effects.

over diffusion or photon statistics in the outermost annulus. Charge tracking shows that a combination of field-line scalloping and stochastic charge loss inside those pockets cannot reproduce both the length-scale (P_1) and the field dependence of the tail, diffusion alone would add only a gentle $\sqrt{t}$ -like broadening (cf. table 4.9). In short, the region within a few millimetres of the PTFE wall exhibits the highest spread in reconstructed radius, and the exponential departure from the central plateau is direct evidence for an additional, wall-driven effect that must be modelled beyond the pure-geometry field solution.

Table 4.9 (geometry-only uncertainties) lists the geometric and statistical contributions; combining them yields

$$R_{\min}(z) = R_{\text{geom}}(z) - 4 \text{ mm}, \quad R_{\max}(z) = \begin{cases} R_{\text{geom}}(z) + 2.3 \text{ mm} & (\text{WS 2022}), \\ R_{\text{geom}}(z) + 2.4 \text{ mm} & (\text{WS 2024}). \end{cases} \quad (4.38)$$

Any data points lying outside these bounds cannot be reconciled with a charge-free field map. Finally, Fig. 4.20 overlays the wall position derived from the QL edge in $^{83\text{m}}\text{Kr}$ data with the prediction of the geometry-only field map for WS 2022 and WS 2024. In WS 2022 the discrepancy is at the sub-millimetre level over most of the drift length and rises modestly near the cathode. In WS 2024 the inward curvature of the data edge is noticeably larger, reaching several millimetres at the longest drift times.

Standard nuisance variations - global alignment, dielectric constant, grid potential fluctuations - translate the simulated curve but do not reproduce its depth-dependent curvature. The trend therefore indicates an unmodelled radial field component that grows with running time. Possible physical origins will be explored qualitatively in the next section

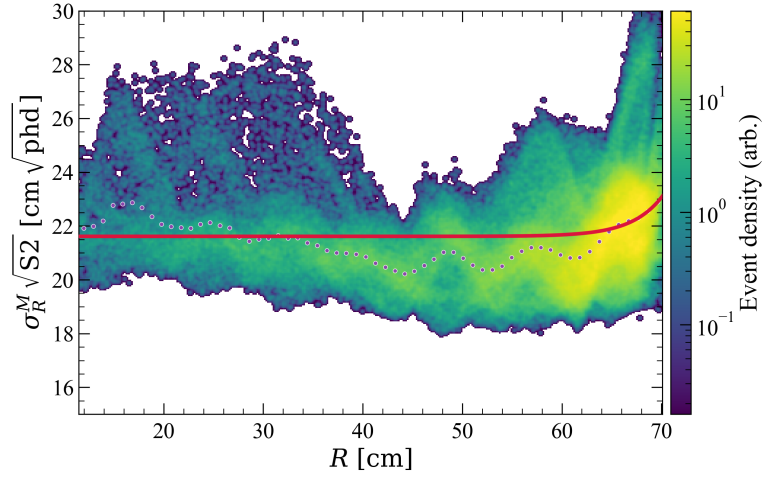


Figure 4.19: Position resolution as a function of the radius R (cm) using ^{83m}Kr data in WS 2024-like operation configuration. The near-wall exponential can be seen clearly but the data does not necessarily plateau at $R = 0$ cm. The dotted line traces ΔR bin centres while the red line shows the fit to equation 4.37.

Table 4.9: Incremental inward bias and statistical broadening at the PTFE wall (in mm) that are *not* included in the pure-geometry FENICS field map for WS 2022 and WS 2024 field configurations.

Effect	WS 2022	WS 2024	Reference scale / notes
Field-line scalloping	-2.73	-2.67	This work, FENICS map (Fig. 4.2); systematic inward shift
Extra transverse diffusion [†]	+0.4	+0.8	EXO-200 $D_T(E)$ fit [125]; assumes 20% field drop near wall
Optical / tiling broadening	+1.0	+1.0	LUX position-resolution study, Fig. 15 [164] (drift-time independent)
Charge-loss (QL) variance	+2.0	+2.0	^{83m}Kr edge behaviour; only within a few mm of PTFE
σ_{stat} (quadrature)	+2.3	+2.4	$\sqrt{\Delta\sigma_{\text{diff}}^2 + \sigma_{\text{opt}}^2 + \sigma_{\text{QL}}^2}$ (1 σ outward blur)
Envelope bounds	$R_{\text{min}} = R_{\text{geom}} - (\approx)2.7$ mm, $R_{\text{max}} = R_{\text{geom}} + 2.3$ mm (WS 2022) / +2.4 mm (WS 2024)		

[†] Incremental diffusion term is the *difference* between wall and bulk RMS spreads; bulk diffusion is already included in the simulation.

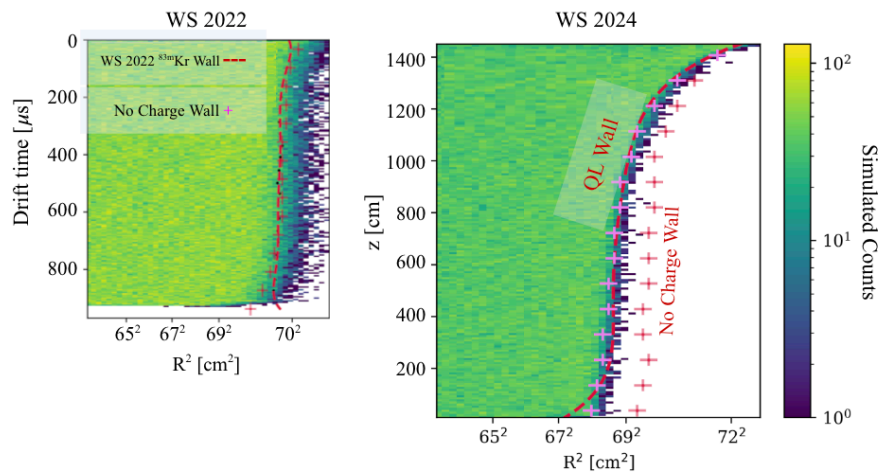


Figure 4.20: The QL wall as derived in WS 2022 (left) and WS 2024 (right) shown as red dotted lines. The largest deviation occurs near the cathode for both datasets but for WS 2024, the difference between the pure-geometry simulation wall and the data-derived wall is very evident throughout z (dt).

(§4.6); here we simply note that the effect is large enough to influence fiducial-volume determination and charge-loss corrections.

4.5.1 Wall Shape Field Dependence

Building on the insights from WS 2022 and WS 2024, we now explore how a pure-field distortion of the TPC boundaries evolves across a broad span of drift fields, leveraging both measurement and simulation.

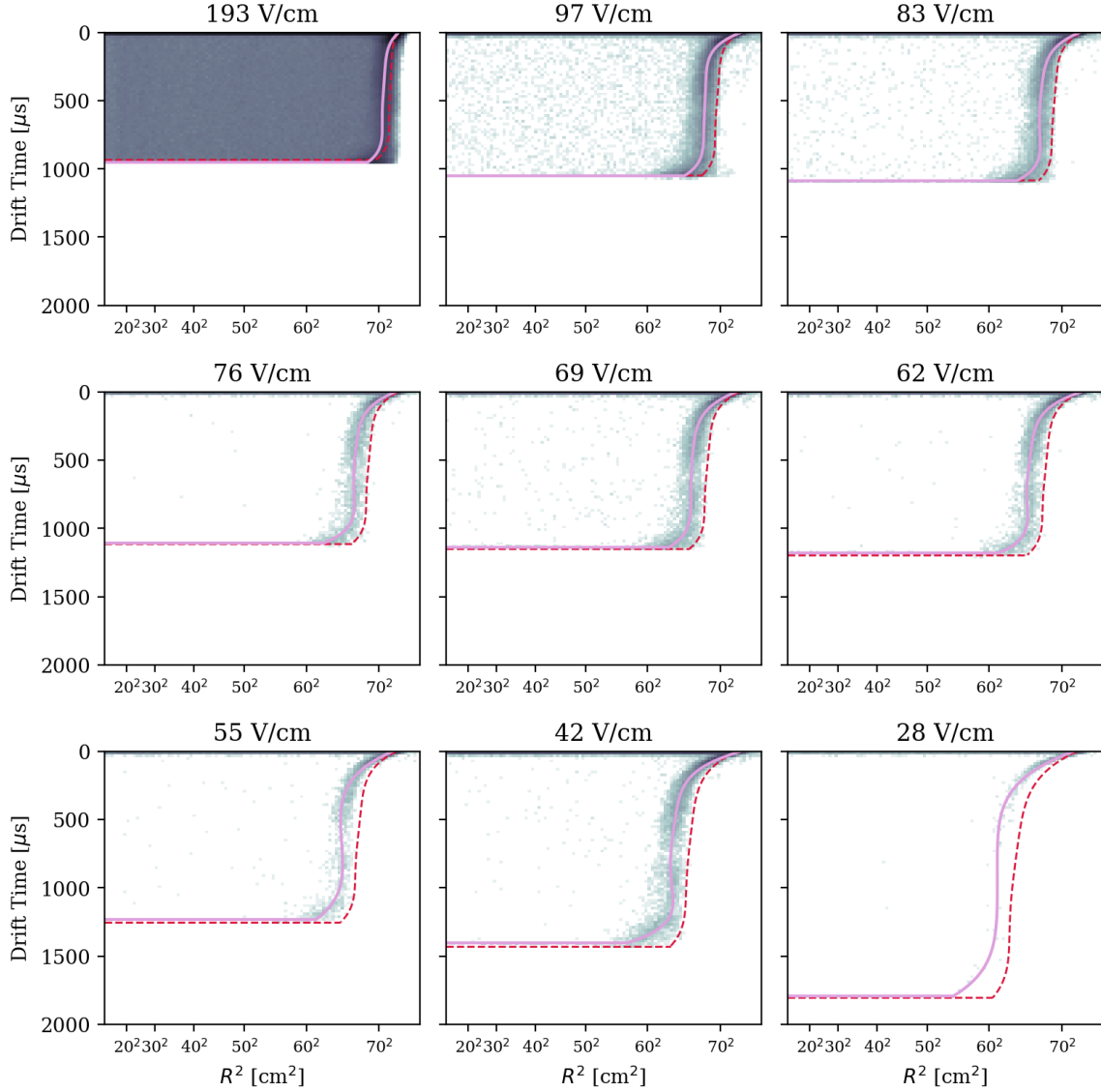


Figure 4.21: Drift time versus R^2 for ^{131m}Xe calibrations and simulations taken at nine drift-field settings. The colour scale is logarithmic in counts, common to all panels. The red curve is the geometry-only FEniCS wall (and maximum drift) contour; the plum line marks the corresponding data-derived wall.

To that end, we use our extensive ^{131m}Xe calibration data, collected at nine distinct drift-field settings, which delivers high statistical precision and, as shown in §4.2.1, consistent wall-profile fits across multiple methods. With this agreement established, we adopt the ^{131m}Xe -derived wall contour as our data benchmark and overlay the FEM-based “geometry-only” simulation contours for each field. The comparison is presented in Fig. 4.21.

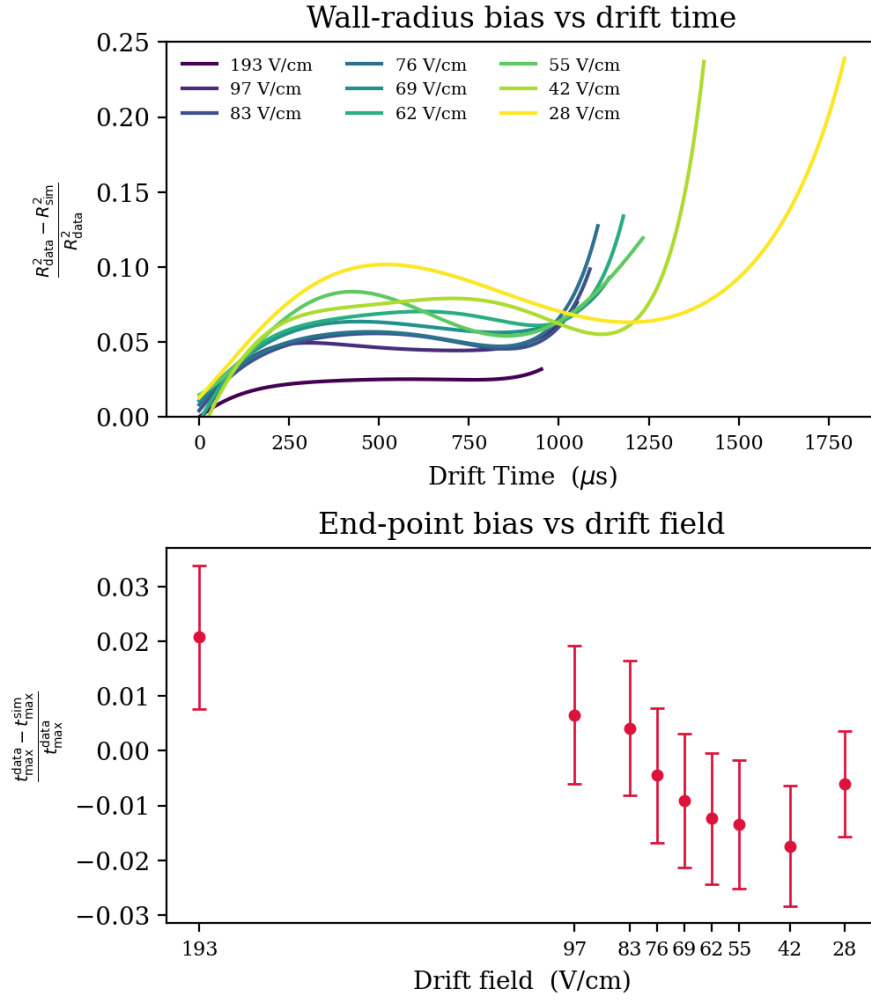


Figure 4.22: Fractional wall-radius bias and endpoint agreement for LZ’s ^{131m}Xe wall profiles. **(Top)** Relative deviation $\frac{R_{data}^2 - R_{sim}^2}{R_{data}^2}$ plotted versus drift time for nine drift-field settings; curves are coloured from 193 V/cm (dark purple) down to 28 V/cm (yellow). Error envelopes on the fractional bias are omitted for clarity. **(Bottom)** Fractional endpoint bias $\frac{t_{max}^{data} - t_{max}^{sim}}{t_{max}^{data}}$ versus nominal drift field, with 1σ statistical uncertainties on the endpoint shown as vertical error bars.

Building on our WS 2022/WS 2024 envelope (table 4.9), we now compare the fully data-derived wall to the pure-geometry contour across nine drift fields (Fig. 4.21) and quantify the residual bias (Fig. 4.22). In table 4.9 we showed that non-field effects, field-line scalloping ($\approx -2.7\text{ mm}$), extra diffusion ($\approx +0.4\text{ mm}$), optical broadening ($\approx +1.0\text{ mm}$) and S2-variance blur ($\approx +2.0\text{ mm}$), together produce at most a $\pm 2.4\text{ mm}$ uncertainty in the apparent wall position. Yet at low fields (28 – 55 V/cm) we measure an inward shift of 6 – 8 mm ($\Delta R/R \gtrsim 10\%$), far exceeding that budget. This demonstrates that neither cold-electron diffusion nor any geometry-only effect can explain the strong field dependence of the wall curvature.

By contrast, in the hot-electron regime ($E \gtrsim 100\text{ V/cm}$) the endpoint bias

$$\frac{t_{max}^{data} - t_{max}^{sim}}{t_{max}^{data}} \quad (4.39)$$

remains below 1%, corresponding to $\lesssim 1 \text{ mm}$ of z -reconstruction error. Such tight agreement (Fig. 4.22 bottom) validates our Chapter 3 drift-velocity model and confirms that, once collective-mode scattering sets in, our simulations faithfully reproduce the true drift time-to- z mapping in LZ.

Together, these results paint a clear picture: the geometry-only field map and known “static” blurs suffice at high drift field, but below $\sim 100 \text{ V/cm}$ an additional inward distortion appears. In the next section we will show how a modest PTFE surface charge can account for this extra bias, providing a unified explanation of both the hot and cold regimes.

4.6 Evidence of Triboelectric Charging on PTFE

Polytetrafluoroethylene (PTFE) is the canonical reflector and electrical insulator inside modern tonne-scale Xe TPCs. At 295 K its volume resistivity exceeds $10^{17} - 10^{18} \Omega \text{ cm}$ (surface resistivity $\gtrsim 10^{16} \Omega \text{ sq}$) and the relative permittivity is $2.0 - 2.1$ [165]. The Maxwell relaxation time $\tau = \epsilon_0 \epsilon \rho$ is therefore $\geq 3 \text{ Myr}$ at room temperature and grows by roughly three additional orders of magnitude on cooling to 175 K , so bulk conduction is frozen for the lifetime of any dark-matter run. In this context, the term triboelectric charging is used to denote the accumulation of static surface charge on PTFE arising from contact and separation with surrounding detector materials during assembly and thermal cycling.

Electret¹⁹ studies reveal three trap ensembles in PTFE. Isothermal surface-potential decay (ISPD) on corona-charged films locates shallow surface traps at $0.8 - 1.0 \text{ eV}$ with densities $\sim 10^{18} \text{ m}^{-3}$ [166]; their half-lives for positive (hole) charge are $\sim 10 \text{ min}$ at 295 K . Equivalent negative surfaces persist for $2 - 3 \text{ h}$, indicating deeper electron binding. Photostimulated-discharge spectroscopy then uncovers a sparser band of deep traps at $4 - 6 \text{ eV}$ that release charge only under far-UV light or above $\sim 150^\circ \text{C}$ [167]. Ultraviolet photo-electron spectroscopy fixes the PTFE photo-emission threshold at 10.6 eV , while VUV absorption peaks at 7.7 eV [168], placing xenon scintillation photons ($8.4 - 10.6 \text{ eV}$) in an energy range capable of addressing both the shallow ($0.8 - 1.0 \text{ eV}$) surface traps and the deep ($4 - 6 \text{ eV}$) bulk trap states.

As the de-trapping probability scales as $\exp(-E/kT)$, cooling from 295 K ($kT \approx 0.026 \text{ eV}$) to 175 K ($kT \approx 0.015 \text{ eV}$) lengthens half-lives by $10^2 - 10^3$. Extrapolating the ISPD data gives weeks for hole migration but years to geological epochs for electron release at LXe temperature [169, 170]. Thus bulk charge remains immobilised, whereas holes confined to the upper micron can still hop laterally on experiment-time scales.

Surface charge on the PTFE walls originates from three complementary processes: direct photo-injection by xenon VUV light ($8.4 - 10.6 \text{ eV}$), triboelectric or micro-discharge events that can deposit surface densities up to $\mathcal{O}(10^2) \mu\text{C m}^{-2}$ [171, 172], and the continual neutralisation of trapped electrons by drifting Xe^+ ions, which then redistributes laterally through the shallow ($\approx 0.9 \text{ eV}$) trap manifold on week-long time-scales. These mechanisms are directly visible in current detectors: LUX observed delayed electron populations and low-S2 wall events [173], a small fraction of which could potentially be attributable to photo-liberation of electrons previously stored on PTFE; LZ sees a slow inward creep (§4.6.4) of the reconstructed wall that is reproduced by finite-element models when a surface charge is applied; and XENONnT, which machined 2 mm copper wires into every PTFE panel to provide a bleed path, reports a stable

¹⁹Defined as a permanently polarised piece of dielectric material, analogous to a permanent magnet.

$\sigma \leq 0.5 \mu\text{C m}^{-2}$ and correspondingly smaller radial “bite” [155]. Together these observations demonstrate that although bulk charge remains immobile at $\sim 175 \text{ K}$, shallow-trap hopping and engineered grounding paths govern the time-dependent field distortions that must be modelled for accurate fiducialisation.

To quantify the impact of such surface charge, consider a cylindrical sheet density σ , which produces a radial field

$$E_r(r) = \frac{\sigma}{2\epsilon_0\epsilon_r} \frac{r}{R_{\text{wall}}}.$$

For $\sigma \approx -5 \mu\text{C m}^{-2}$ (near LUX’s maximum reported charge density) and $\epsilon_r = 2.1$, $E_r \approx 1 \text{ kV cm}^{-1}$ half-way across the LZ drift radius, sufficient to bend electron trajectories by centimetres and bias reconstructed positions by a comparable amount. Radial compression can pull high-radius γ events into the nominal WIMP search box, or even cause real low-energy single scatter events to lose their S2s, while electrons that later detach from PTFE generate solitary S2s liable to pair accidentally with isolated scintillation flashes. Accurate modelling of PTFE wall charge is therefore essential both for defining the fiducial volume and for understanding low-energy accidental-coincidence backgrounds.

Table 4.10: Key PTFE parameters used in the wall-charging simulations.

Quantity	Representative value	Source
Bulk resistivity ρ (295 K)	$(1-3) \times 10^{18} \Omega \text{ cm}$	[165, 174, 175]
Dielectric constant ϵ_r	2.0–2.1	[165, 174, 175]
Shallow trap depth	0.8–1.0 eV (e^- , h^+)	[166]
Deep trap depth	4–6 eV (e^-)	[167]
Photo-emission threshold	10.6 eV	[168]
Typical triboelectric σ (air)	$\lesssim \mu\text{C m}^{-2}$	[172]
σ reproducing LZ field	$< 1 \mu\text{C m}^{-2}$	this work

Taken together, these considerations justify treating PTFE as a quasi-permanent electret at liquid-xenon temperature: electrons injected into the polymer occupy multi-eV traps and remain immobilised, while holes in shallower states can still hop laterally over week-long time-scales, continuously reshaping the wall-field profile. The remainder of this section quantifies that evolution in LZ and, in doing so, extends the limited literature on PTFE charging under cryogenic conditions, work that will help establish a more robust baseline both for small-scale R&D studies and for the design of next-generation xenon detectors.

4.6.1 Alternative Explanations for Field Distortion

Open or shorted shaping-ring resistor

The field cage acts as a static voltage divider: each ring sits at $V_i = V_{\text{cathode}} + i\Delta V$. If one resistor breaks the chain, a single potential step ΔV appears. Gauss’s law then introduces a radial component $E_r \simeq \Delta V/r$ that is confined to roughly one ring spacing ($\approx 2 \text{ cm}$) above and below the fault and remains perfectly static in time²⁰). Due to the nature of the distortions observed, and their time-varying behaviour, resistor-faults are ruled out.

²⁰See Fig. 3.10 (page 97) of [81].

Positive-ion (“hole”) accumulation in PTFE

A positive surface sheet charge ($\sigma > 0$) imposes $\mathbf{E}_{LXe} \cdot \hat{\mathbf{n}} = \sigma/\epsilon_0$, forcing field lines outward and expanding the reconstructed radius: the opposite to observations. Hole traps also empty more rapidly than electron traps at 173 K (§4.6), so a hole-driven distortion should relax much faster than any electron-driven effect. This has not been observed in previous experiments and though it was speculated in LZ (see §4.6.4), it was later shown that a pure negative charge density was in fact responsible for the wall behaviour observed.

Electron space-charge in the LXe “skin”

Taking WS 2022 as an example, with an approximate production rate of electrons at 77 kHz [152] and a generous residence time $\tau = 0.1$ s in the fraction of m^3 skin volume, the density is

$$n \lesssim \frac{7.7 \times 10^4 \text{ s}^{-1} \times 0.1 \text{ s}}{0.15 \text{ m}^3} \approx 5 \times 10^4 \text{ e m}^{-3}.$$

Gauss’s law then gives

$$E_r \lesssim \frac{ne\delta}{2\epsilon_0} \approx 4 \times 10^8 \text{ V cm}^{-1}, \quad (4.40)$$

six orders below the $\geq 10 \text{ V cm}^{-1}$ radial field needed to displace the wall by centimetres: particularly telling given that this is an absolute upper bound estimate using the full SE production rate rather than even a dominant background. XENON100’s SE study [176] places an upper bound of $Y_\gamma^{tot} \leq 2 \times 10^{-5} \text{ e}^- \text{ photon}^{-1}$ for all 175 nm photo-processes, reinforcing that the effect of skin charge, is very unlikely to be able to bridge the gap in near-surface charge production required to achieve the wall displacement observed within the TPC.

Bulk mechanical or thermal motion

Uniform PTFE thermal contraction would shift S1 and S2 positions identically and halt once cryogenic equilibrium is reached; associated grid sag also chiefly alters $E_z(r)$ not $E_r(r)$. No such effect, other than that attributable to electrode voltage configuration changes, have been observed, and along with the time-dependent shifts in the wall position and temperature stability means this is not so viable as a source for the field behaviour observed.

Photo-electric charging by xenon scintillation

LXe scintillation photons carry $h\nu \approx 7.1 \text{ eV}$, barely above PTFE’s work function. XENON100 constrains the combined quantum yield of all photon-driven processes to $Y_\gamma^{tot} \leq 2 \times 10^{-5} \text{ e photon}^{-1}$ [176]. Even if every liberated electron stuck to the reflector, the annual surface-charge growth would be²¹

$$\Delta\sigma \leq 10^{15} \gamma \text{ m}^{-2} \text{ d}^{-1} \times 2 \times 10^{-5} \text{ e phot}^{-1} \times 365 \text{ d} \times e \approx 0.07 \mu\text{C m}^{-2} \text{ yr}^{-1},$$

which could be a plausible contributor to the charge density on the PTFE surface, though given that this is a very conservative upper limit, might still be much too weak to be the primary source.

²¹ Even if every interaction produced 10^5 VUV photons at a constant 1 kHz rate and all of them struck 1 m² of PTFE ($\approx 10^{14} \text{ m}^{-2} \text{ d}^{-1}$), the XENON100 yield limit of $2 \times 10^{-5} \text{ e } \gamma^{-1}$ implies $\Delta\sigma \leq 0.07 \mu\text{C m}^{-2} \text{ yr}^{-1}$: over $100\times$ below the surface-charge density required by field fits. Realistic photon fluences are orders of magnitude smaller.

Cathode glow and micro-sparks

Micro-discharges could release bursts of electrons near the cathode (“hotspots”) and even μC -scale deposits change reconstructed radii by millimetres. However, no obvious trend has been found correlating flare-ups with near cathode wall migration, though this could be plausible in principle, as long as injected charge reaches the PTFE and does not neutralise too quickly.

4.6.2 Simulated Surface Charge on PTFE

From this point, we assume an axially varying surface-charge density on the PTFE reflector is responsible for field distortions, such that, when combined with the nominal high-voltage configuration, the measured wall radius as a function of drift time $r_{data}(t)$ should be reproducible. The unknown charge distribution is represented in a low-dimensional basis and estimated by minimising the misfit between simulated and measured walls. This methodology is explained in more detail in the following

Field representation and basis construction

Let $\mathbf{E}_0(\mathbf{x})$ denote the electrostatic field in the absence of PTFE charge (the “nominal” HV solution), computed with the full detector geometry and electrode potentials. To capture charge-induced distortions we pre-compute a set of N charge-only basis fields $\{\mathbf{E}_i(\mathbf{x})\}_{i=1}^N$ (Fig. 4.23). Each basis field is generated by imposing a uniform surface charge density σ_0 on one axially delimited PTFE patch while keeping all electrodes at their nominal potentials; the resulting field with *HV and charge* is solved once and the nominal field is subtracted point-by-point to yield the charge-only response:

$$\mathbf{E}_i(\mathbf{x}) \equiv [\mathbf{E}_{HV+patch\,i}(\mathbf{x}) - \mathbf{E}_0(\mathbf{x})] \quad (4.41)$$

In this work the PTFE is partitioned into $N = 9$ contiguous axial patches that span the full drift height. A single patch field therefore represents the unit response to a uniform σ_0 on that axial segment²². All maps are stored on the same (r, z) mesh; coordinates are in millimetres, field components in $V\,cm^{-1}$. With these definitions, the model field for a vector of patch amplitudes $\mathbf{a} = (a_1, \dots, a_N)$ is the linear superposition

$$\mathbf{E}(\mathbf{x}; \mathbf{a}) = \mathbf{E}_0(\mathbf{x}) + \sum_{i=1}^N a_i \mathbf{E}_i(\mathbf{x}). \quad (4.42)$$

The a_i are proportional to the physical surface charge on patch i ; in absolute units one has $\sigma_i = a_i \sigma_0$.

From field map to a wall boundary curve

Given $\mathbf{E}(\mathbf{x}; \mathbf{a})$, we then predict the wall by integrating electron trajectories forward in time from a line of seed points just below the liquid surface. Particle kinematics follow the empirical drift velocity $v_d(E)$ law (as derived and measured in §3.1.4) evaluated at the local field magnitude $|\mathbf{E}|$ ($V\,cm^{-1}$). The electron velocity is taken parallel to the field, $\dot{\mathbf{x}} = v_d(|\mathbf{E}|)\hat{\mathbf{E}}$, which is integrated with a fixed-step fourth-order Runge–Kutta scheme. For each seed we record the cylindrical radius r when the trajectory first intersects a plane $z = z_{surf}$ near the liquid surface and the corresponding drift time t ; the step size is chosen so that reducing Δt by a factor of two changes the wall RMS by $\ll 1\,mm$. This defines the simulated wall $r_{model}(t; \mathbf{a})$. The data wall $r_{data}(t)$ is then provided either as a polynomial parametrisation

²²Any other choice of segmentation or smooth basis functions can be accommodated with the same machinery.

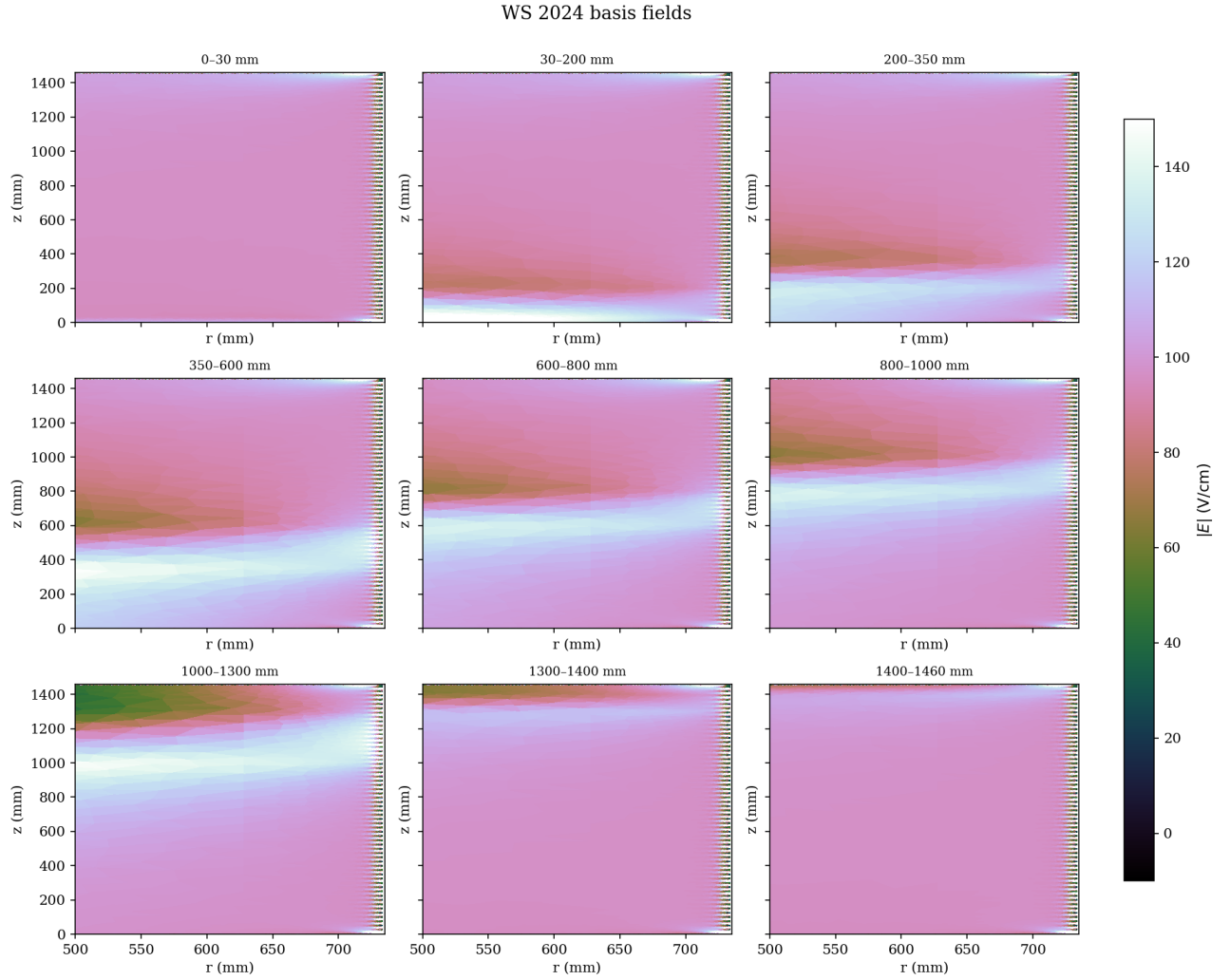


Figure 4.23: Field maps used to construct the charge-basis fields for the WS 2024 tuning. For each axial patch (later to be referred to as P0-P8), a uniform surface charge (exaggerated here for demonstration purposes) is applied on that segment while keeping all electrodes at nominal potentials; the charge-only response $\mathbf{E}_i(\mathbf{x})$ is then calculated according to equation 4.41. These nine panels constitute the basis fields used in the WS 2024 tuning, over which patch coefficients are fitted by superposition.

or as a set of (t_k, r_k) samples²³. For fitting we evaluate both model and data on a common grid of drift times $\{t_k\}$ spanning the fiducial window, using linear interpolation of $r_{model}(t; \mathbf{a})$ where necessary. Optionally, points near the cathode where loss effects dominate can be down-weighted or excluded.

Optimisation strategy and challenges

The misfit is non-convex and non-differentiable in places (because the drift time binning and the “first-intersection” operation introduce mild kinks). We therefore use Powell’s direction-set method, a derivative-free optimiser that performs sequential 1-D line searches along an evolving set of directions and periodically updates the direction set to accelerate towards a minimum. Powell is robust to moderate noise in χ^2 and requires only function evaluations, which is advantageous when each evaluation entails a full field superposition and many trajectory integrations. We initialise at $\mathbf{a}=\mathbf{0}$ (uncharged), optionally with small seed values motivated by previous runs. Convergence is declared

²³In this case the same polynomial fit is performed intrinsically within the code before input into the optimisation block.

when the fractional improvement of χ^2 along every direction falls below a tolerance or when the step sizes become smaller than a prescribed threshold²⁴.

Physical constraints may also be applied where appropriate. Consistent with the conclusions of earlier discussions, a net negative surface charge provides the most physically plausible explanation for the observed wall movement; accordingly, we impose $a_i < 0$ as a constraint in these studies. The present model is not without limitations, notably the assumption of axial symmetry: any genuine azimuthal structure is imperfectly represented within the axial basis and may manifest as coherent residuals. This could be addressed by extending the basis to include limited ϕ segmentation (tackled in §4.7), or by adopting a fully three-dimensional solver with sectorised charge patches, as implemented in LUX [126]. However, both approaches substantially increase the number of fit parameters and the computational cost, particularly in the current LZEF workflow, where the bridge between custom triangular mesh generation and a stable tetrahedral equivalent is a difficult one to cross. An alternative would be to employ COMSOL or comparable software, which incorporates advanced meshing algorithms directly into the solver setup, thereby eliminating the need for manual adaptive meshing and requiring only the specification of an overall mesh density.

4.6.3 The WIMP Search 2024 Field Solution & Conclusions

Using the described methodology, the WS 2024 results are presented in this section. Since the present methods were originally developed in preparation for WS 2024, this solution is discussed in full, followed by a comparison²⁵ to previous analyses of WS 2022.

WS 2024 Average Best-Fit Solution

The tuned field solution obtained by constraining the PTFE surface to carry negative-charge-only reproduces the observed drift-time–dependent wall radius with sub-millimetre accuracy (Fig. 4.24). The final fit yields $\chi^2/dof = 0.68$, with an RMS deviation of 0.82 mm , demonstrating that the data wall can be described to better than 0.2% across the full drift range. The solution is dominated by a large negative charge density at the cathode-side PTFE (patch P0), at the level $\mathcal{O}(\mu\text{C}/\text{m}^2)$. Additional contributions appear in the uppermost patches (P7–P8), while the mid-wall patches are consistent with zero within uncertainties. This pattern is physically plausible; strong negative charge accumulation near the cathode may at first seem unintuitive but can be readily explained due to the occurrence of large local field variations near the cathode ring-wall boundary producing potential wells “deep” enough to trap negative charge densities of larger magnitudes. This strong localised charge trapping, along with weaker deposition near the gate, and negligible charging elsewhere along the wall is then sufficient to reproduce the observable wall profile without demanding unphysically high, area-averaged charge densities.

In order to reduce residuals below the millimetre level, an *affine correction* was introduced to the modelled wall shape before comparison with data. In practice this means rescaling the simulated wall radius as $r \rightarrow a \cdot r + b$ ²⁶. This correction addresses two systematic effects:

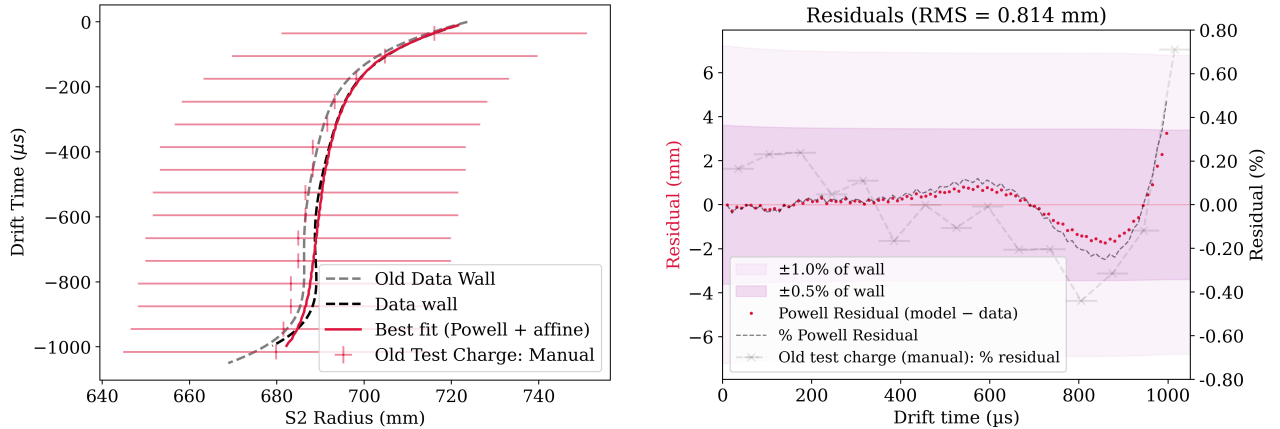
²⁴For more information on Powell’s algorithm and an overview of how it works, please refer to appendix B.

²⁵Following the work by R. Watson (2022) [152], who presented the first tuned WS 2022 field maps using different but complementary methods.

²⁶We do not modify the wall shape; we apply a bounded radial affine correction $r \rightarrow ar + b$ (with $a \approx 1$, $|b| < 1 \text{ mm}$) to reconcile the physical PTFE edge in simulation with the data’s diffusion-smeared drop-off, ensuring a like-for-like comparison

- A small global bias in the drift-time–radius mapping, caused by imperfections in the empirical polynomial used to parametrise the observed wall.
- A weak linear stretch mismatch between simulated trajectories and reconstructed positions, reflecting residual systematics in the field map or in position reconstruction.

Mathematically, the affine term introduces two nuisance parameters (a, b) that absorb global offset and stretch, while leaving the z -dependent curvature determined solely by the surface-charge distribution. Without this step, the optimiser compensates for global mismatches by spreading unphysical charge across multiple patches; with it, the charge solution reflects genuine distortions of the wall curvature. The improvement in fit quality (RMS reduced from $\sim 2.5 \text{ mm}$ to 0.8 mm) demonstrates that this correction is both necessary and physically well-motivated. Fig. 4.24 shows the tuned wall solution compared to data, along with the residuals expressed as a percentage of the wall radius. For comparison, a manually tuned, earlier, more “pushed-in” wall definition (hence, expected to correspond to a higher required charge density) is also shown to demonstrate both fits and their corresponding charge density profiles. The difference is large and will form an important aspect of the uncertainties and degeneracies discussion to follow.



(a) Reconstructed wall position as a function of drift time. The WS 2024 data wall is shown in black (dashed), the Powell + affine best-fit solution in red, and an older wall definition in grey (dashed). Manual charge tuning results are overlaid as pink markers with uncertainties.

(b) Residuals between the Powell + affine fit and the data. Red points show deviations in mm , with shaded bands indicating $\pm 0.5\%$ and $\pm 1.0\%$ of the wall radius. The corresponding fractional residuals are shown on the right axis in grey. Manual charge-tuned % residuals are also plotted for comparison.

Figure 4.24: Comparison of WS 2024 wall reconstruction and residuals. Both manual and the Powell + affine-tuned field solution achieved residuals to within $\sim 1\%$ of their respective definitions, the latter achieving residuals to within $\lesssim 0.5\%$.

For comparison and completeness, a parallel fit was also performed without the sign constraint, permitting both positive and negative patch charges. This solution achieves an artificially improved statistical agreement by exploiting compensating positive and negative patch charges. This yields an impressive $\chi^2/\text{dof} = 0.016$ and an RMS deviation of 0.118 mm (Fig. 4.25) but at the cost of large compensating positive and negative charges across multiple patches, inconsistent with the expected charging mechanism. While this solution demonstrates the degree of degeneracy available to the fit, the negative-only result is the physically meaningful description of the detector.

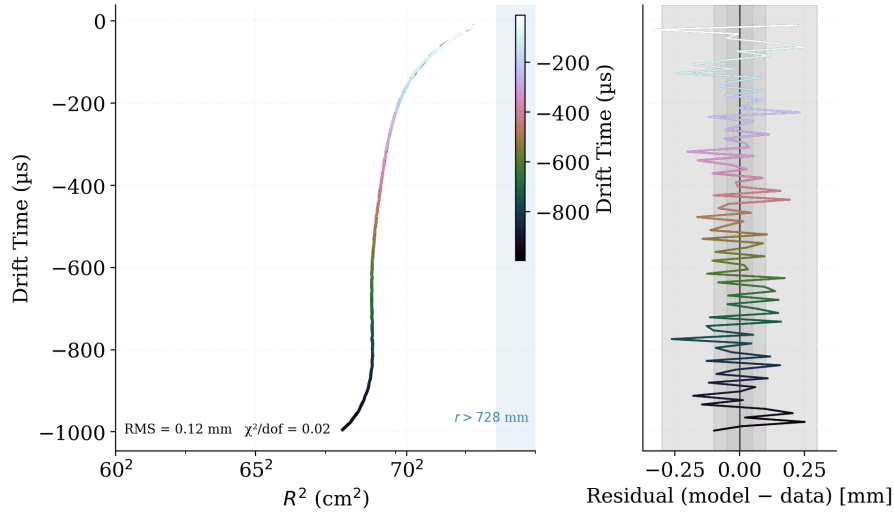


Figure 4.25: Data wall and best-fit wall in R^2 vs drift-time. The coloured curve shows the $\pm$ charge fit (nine patch-charge amplitudes, both signs allowed) with an affine (a, b) refit; the shaded band marks the excluded region $r > 728$ mm. The absolute residuals ($model - data$) in mm are coloured by the same drift time.

Table 4.11: Per-patch PTFE surface charge densities for WS 2024. Patch z -ranges follow the nine segments used in the fit. The “fitted” column shows the Powell + affine, negative-only solution with 1σ uncertainties for the fit coefficients associated with each basis field (in units of ϵ per patch area). The “manual” column shows the piecewise profile used in cross-checks (non-zero in P0, P6–P8), converted to the same units. Note that the manual solution refers to an older (early 2024) definition of the wall with a greater observed “push-in” effect than the most recent wall definition, for which a Powell-based fit has been used.

Patch	z range (mm)	Δz (mm)	σ_{fitted}	σ_{manual}
P0	0–30	30	229.68 ± 22.90	60.27
P1	30–200	170	0.196 ± 1.025	0
P2	200–350	150	0.00023 ± 0.964	0
P3	350–600	250	0.00027 ± 0.380	0
P4	600–800	200	0.00027 ± 0.428	0
P5	800–1000	200	0.00018 ± 0.410	0
P6	1000–1300	300	0.000015 ± 0.331	1.0245
P7	1300–1400	100	26.01 ± 1.45	1.2053
P8	1400–1456	60	17.66 ± 5.79	18.080
Area-averaged density, fitted			$\bar{\sigma}_{\text{fitted}} = -1.41 \pm 0.31(stat) \mu\text{C}/\text{m}^2$	
Area-averaged density, manual			$\bar{\sigma}_{\text{manual}} = -2.27 \mu\text{C}/\text{m}^2$	

Uncertainties and Degeneracies

Uncertainties on the fitted charges were first estimated from the Powell covariance and validated using bootstrap resampling of the wall data. Both approaches yielded consistent results: the cathode patch (P0) is determined at $\sim 10\%$ precision, the uppermost patches (P7–P8) at the 10–30% level, while the mid-wall patches are effectively unconstrained. Crucially, every bootstrap realisation confirms the requirement for a strongly negative charge localised near the cathode. The per-patch results are listed in Table 4.11 with statistical errors only.

To probe the structure of degeneracies, the full covariance matrix was analysed. The patch-to-patch correlation matrix (Fig. 4.26) shows strong positive correlations between neighbouring segments and significant anti-correlations

between distant ones, indicating that multiple charge configurations can yield nearly identical wall shapes.

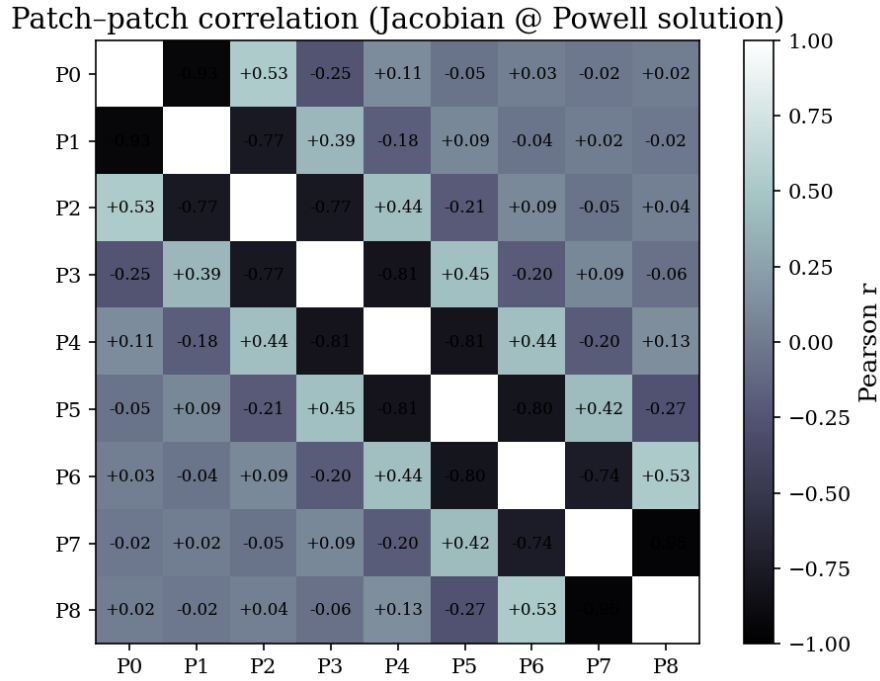


Figure 4.26: Patch-patch correlation matrix for the Powell-affine fit solution in WS 2024. Each entry shows the Pearson correlation coefficient between fitted surface charge densities in the nine z -segments. Strong anti-correlations are seen between the cathode (P0) and both mid-wall and upper patches, while neighbouring segments show positive correlations. This structure reflects the degeneracies of the inverse problem and motivates the modal decomposition analysis.

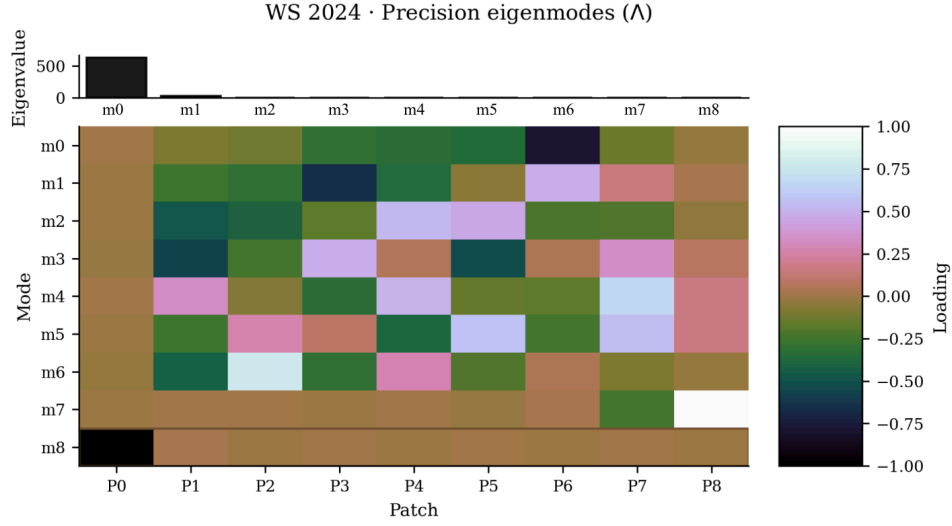
A more quantitative understanding requires transforming to an orthogonal modal basis. Three complementary decompositions were employed:

1. Fisher precision modes

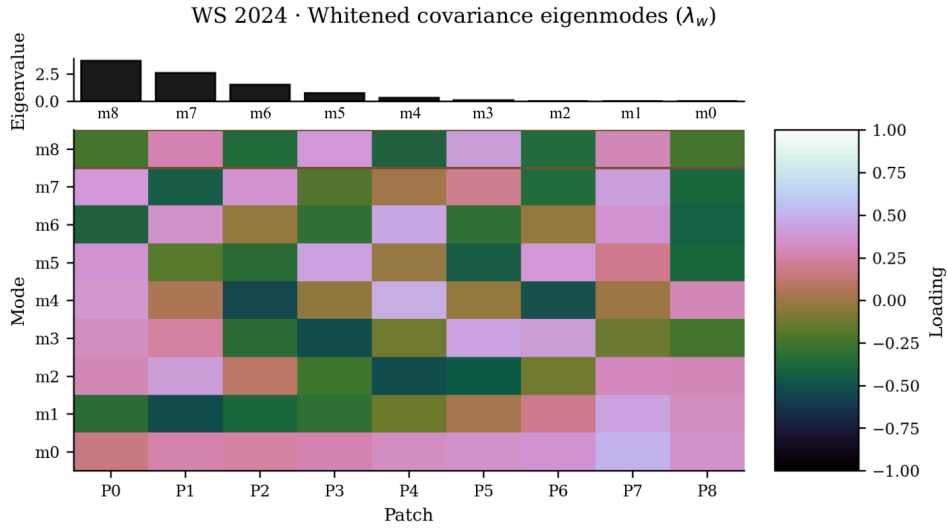
Diagonalising the inverse covariance (the Fisher information matrix) yields modes ranked from most-constrained to least-constrained in absolute precision. The eigenvalue spectrum (Fig. 4.27) spans nearly seven orders of magnitude, demonstrating the extreme hierarchy between well-measured and effectively null directions. Importantly, the cathode-dominated mode appears at the *low-precision end* of this spectrum: its large variance reflects the fact that the global amplitude of the cathode charge trades off against a small affine calibration and anti-correlated leakage across other patches. Thus, although it is technically a “weak” precision mode, this does not undermine its physical significance.

2. Whitened covariance modes

By normalising each mode to its 1σ spread, the “whitened” basis (Fig. 4.27) avoids the misleading bias where a single large patch charge inflates the variance. This representation cleanly separates directions with tight fractional uncertainties from those that are weakly constrained, and makes clear that the cathode mode corresponds to a coherent global structure rather than numerical noise.



(a) Eigenmodes of the Fisher matrix $J = \Sigma^{-1}$; the eigenvalue Λ sets the mode's 1σ as $1/\sqrt{\Lambda}$ such that small Λ corresponds to more degenerate directions.



(b) Eigenmodes of the whitened covariance $\Sigma_w = D^{1/2}\Sigma D^{-1/2}$; the eigenvalue λ_w is the fractional variance of the mode (smaller λ_w corresponds to tighter constrained modes).

Figure 4.27: WS 2024 patch-charge eigen-decomposition. Bars show the eigenvalue spectra; heatmaps show modal loadings across patches P0–P8. The precision spectrum is highly ill-conditioned ($\Lambda_{max}/\Lambda_{min} \sim 1.3 \times 10^7$) revealing strong inter-patch degeneracies. The physically dominant pattern is $m8$, dominated by the cathode-adjacent patch: it appears weakly constrained (small Λ) because charge trades off with neighbouring patches and most of the total charge resides on that patch, inflating its absolute variance.

3. Composition SNR

The best-fit solution $\mathbf{u}_\star$ was projected into the modal basis, and each projection compared to its 1σ spread. The resulting signal-to-noise ratios (SNR)(Fig. 4.28) show that the fitted solution lies many σ away from zero along the cathode-dominated mode, despite its large variance in absolute terms. This demonstrates that the cathode patch contribution is required at *very high significance*. The remaining modes are either weak dipolar adjustments or near-null directions with little effect on the wall shape, fully consistent with the degeneracies observed in the patch-to-patch correlations.

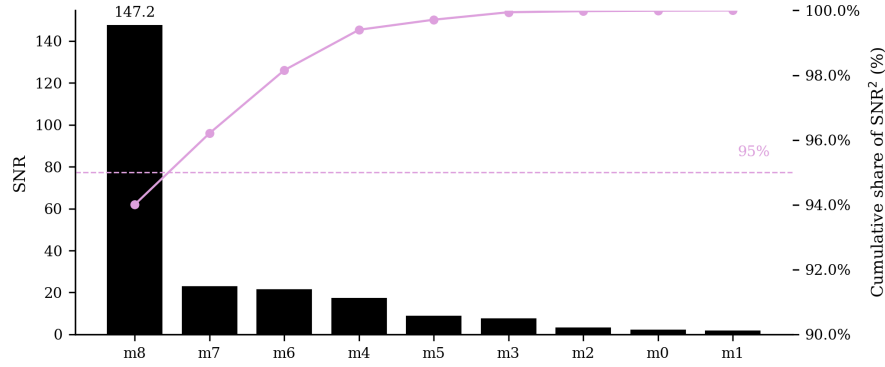


Figure 4.28: Projection of the best-fit WS 2024 solution onto the covariance eigenbasis. For each mode the amplitude $|\alpha|$ is compared to its 1σ spread, yielding a modal signal-to-noise ratio (SNR). The cathode-dominated mode ($m8$) is required at $> 100\sigma$ significance despite its large variance in absolute terms, demonstrating that the data decisively demand a cathode patch contribution. All other modes contribute at far lower significance, corresponding to subdominant dipolar structures or nearly null degrees of freedom.

Finally, the comparison in Fig. 4.24 between the Powell–affine tuned solution and an earlier “manual” charge profile highlights the systematic component of the cathode amplitude uncertainty. Both solutions reproduce the wall shape to within experimental resolution, yet imply area-averaged charge densities that differ by a factor ~ 1.6 ($|\bar{\sigma}_{\text{fitted}}| = 1.41 \pm 0.31_{\text{stat}} \mu\text{C}/\text{m}^2$ vs. $|\bar{\sigma}_{\text{manual}}| = 2.27 \mu\text{C}/\text{m}^2$). This is the expected manifestation of the low-precision cathode mode identified in the eigen-analysis: the wall observable constrains its shape but not its absolute scale. We therefore assign a systematic envelope on the integrated charge corresponding to this degeneracy and also to solutions associated with slight changes in the Powell initialisation condition. In practice this can be expressed as:

$$\bar{\sigma} = -(1.41 \pm 0.31_{\text{stat}} \pm 0.2_{\text{sys}}) \mu\text{C}/\text{m}^2. \quad (4.43)$$

This systematic is not an additional free degree of freedom but precisely the amplitude degeneracy of the cathode mode, already identified as the weakest precision direction in the Fisher basis.

Taken together, these complementary views provide a cohesive interpretation:

- The wall observable tightly constrains the *shape* of the radius–time curve, which decisively requires a cathode-dominated charge pattern.
- The apparent weakness of this mode in the precision spectrum is simply the manifestation of its amplitude degeneracy with affine calibration and anti-correlated leakage.

- The projection of the best-fit solution onto this mode has $\text{SNR} \gg 1$, establishing the presence of cathode charge at very high significance, even though its absolute amplitude is uncertain at the factor-of-few level.

Hence we can rest assured that the eigenmode analysis confirms that the tuned WS 2024 solution is physically meaningful: the cathode patch is demanded by the data, while the remaining modes represent the expected degeneracies of this inverse problem rather than sources of genuine uncertainty. However, there does remain some uncertainty in the exact quantification of the charge required to replicate the wall profile, primarily arising from per-patch charge degeneracies rather than statistical uncertainties associated with one particular fit solution. The best way to mitigate this would be dedicated R&D efforts to understand the physical mechanism via which PTFE charges (and discharges) without which, constraining the fits remains highly subject to very data-driven optimisation algorithms.

Stability of ER and NR bands

The stability of ER and NR bands was tested against positional and field variations within WS 2024. Across fiducial-volume slices (centre, top, bottom, wall), the ER band mean varied by only 0.06% and its width by 0.39%, while the NR band mean and width varied by 0.03% and 0.23%, respectively. Comparison of the tuned WS 2024 field map with a uniform 96.5 V/cm field (the $^{83\text{m}}\text{Kr}$ derived average; 97.1 V/cm in simulation) showed differences of $< 0.3\%$ in band means and $< 6.5\%$ in widths. Additional uniform-field simulations spanning 70–140 V/cm confirm the weak field dependence: NR bands shift by $< 0.5\%$ and ER bands by $\lesssim 1\%$ relative to the WS 2024 nominal. Through these simulations, the WS 2024 field map yields $ER \rightarrow NR$ (lower-half) leakages broadly consistent with NEST expectations²⁷ at the level of $(1\text{--}1.5) \times 10^{-3}$ for $g_1 \simeq 0.116$.²⁸ Fig. 4.29 shows the CH3T (calibration data) ER

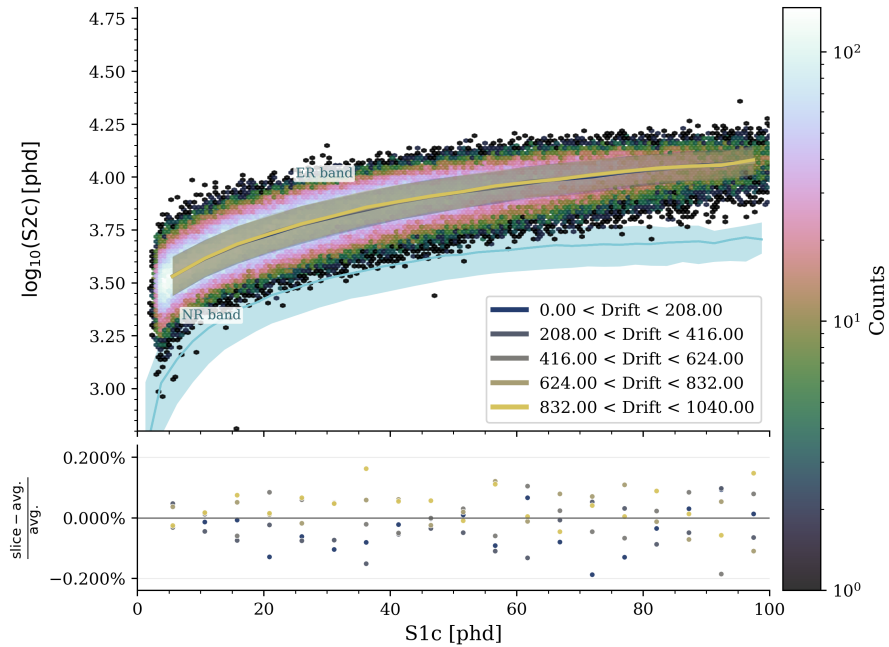


Figure 4.29: CH_3T calibration data in corrected ($S1c$, $\log_{10}(S2c)$) space with simulation-derived ER/NR bands. Coloured bands show drift-time slices; the lower panel shows the residuals of the band positions derived from different drift slices compared to the full-volume average, consistent with percent-level band stability.

²⁷See v3, Fig. 14 of [97].

²⁸Calculation of g_1 presented in an internal presentation by A. Chawla (2024).

leakage into the *lower half* of the NR band. Integrated over the full S1 range, WS 2024 exhibits a systematically higher leakage than WS 2022 by $\mathcal{O}(10\text{--}30\%)$, qualitatively in line with the NEST field-dependence at similar g_1 .

The significance of these results is twofold. First, LZ operated in a regime where $ER \rightarrow NR$ leakage should only be weakly dependent on drift field (consistent with NEST), yet this “stable” region is not perfectly flat: within the same g_1 regime the leakage fraction can vary at the $\mathcal{O}(1 - 2)\times$ level across the nominally “flat” field range. Our preliminary, lower-statistics cross-check (with leakage defined as the fraction of simulated CH_3T ER events below the NR median and integrated over $3 \leq S1 \leq 80$ phd) shows WS 2024 higher than WS 2022 by $\sim 10\text{--}30\%$, which sits comfortably within the NEST spread at similar g_1 . Operating between 80–390 V/cm (see §6.2.1 and [97]), with exceptions such as XENON100 [177] and LUX Run 4 [178], thus provides a practical tolerance to HV configuration changes and helps ensure that discrimination performance does not vary dramatically with field, an important “safety margin” to preserve in XLZD. Second, because the ER/NR band positions are only percent-level sensitive to typical field-map variations, the principal reconstruction impacts of the electric field arise instead through charge transport, drift times, and S2 morphology. These detector-response aspects merit closer attention for future experiments, while background discrimination remains robust against moderate field variations,²⁹ provided the leakage is consistently defined (e.g., lower half vs full band) and statistics are sufficient.

Validations & Comparisons to WS 2022

Using a streamlined reimplementation of the WS 2022 wall fit, we reproduce the expected trend as per our discussions in (§4.6): the PTFE wall is initially consistent with zero surface charge during the first science run, with an average charge density calculated to be $\bar{\sigma} = (-0.105 \pm 0.150) \mu\text{C m}^{-2}$, which “increases” (in magnitude) to $(-0.345 \pm 0.030) \mu\text{C m}^{-2}$ over ~ 4 months (including post-WS calibrations). This rise has been hypothesised to be associated with the high-rate, changing-configuration calibration period after the first WIMP search, and although a robust causal connection remains unproven [152] it is in fact in line with observations from LUX [126] and other previous experiments and it would make sense that the relatively short (4 months) timescale over which this “wall charging” was observed was due to the changing detector conditions (§4.5.1). By WS 2024, the required surface charge was larger by about a factor of four, reaching a representative $\bar{\sigma} \simeq -1.41 \mu\text{C m}^{-2}$ after $\sim 1\text{--}2$ years. Taken together, these observations support progressive PTFE bulk charge-up across campaigns as expected and corroborated in previous experiments ([126, 155, 176]).

Fig. 4.30 presents the tuned electric-field maps for WS 2022 and WS 2024. Table 4.12 summarises, for each configuration (within $z : \{3, 140\} \text{ cm}$, $r : \{0, 72\} \text{ cm}$) averages of the drift field, together with independent cross-checks from $^{83\text{m}}\text{Kr}$ - and $^{131\text{m}}\text{Xe}$ -derived fields (§4.2.3, §4.2.4). For WS 2024 these determinations are consistent at the percent level, thereby validating both the wall-based tuning procedure and the NEST conversions from $^{83\text{m}}\text{Kr}$ S1b/S1a and Rn-corrected $^{131\text{m}}\text{Xe}$ photon yields to field.

The maps also provide a calibrated mapping between drift time and depth. Within a chosen volume selection ($r \lesssim 65 \text{ cm}$, $100 < z < 1450 \text{ mm}$), events near $r \simeq 68 \text{ cm}$ exhibit an approximately linear $dt \leftrightarrow z$ relation, whereas

²⁹Assuming operation within the “right” field window; see §6.2.1.

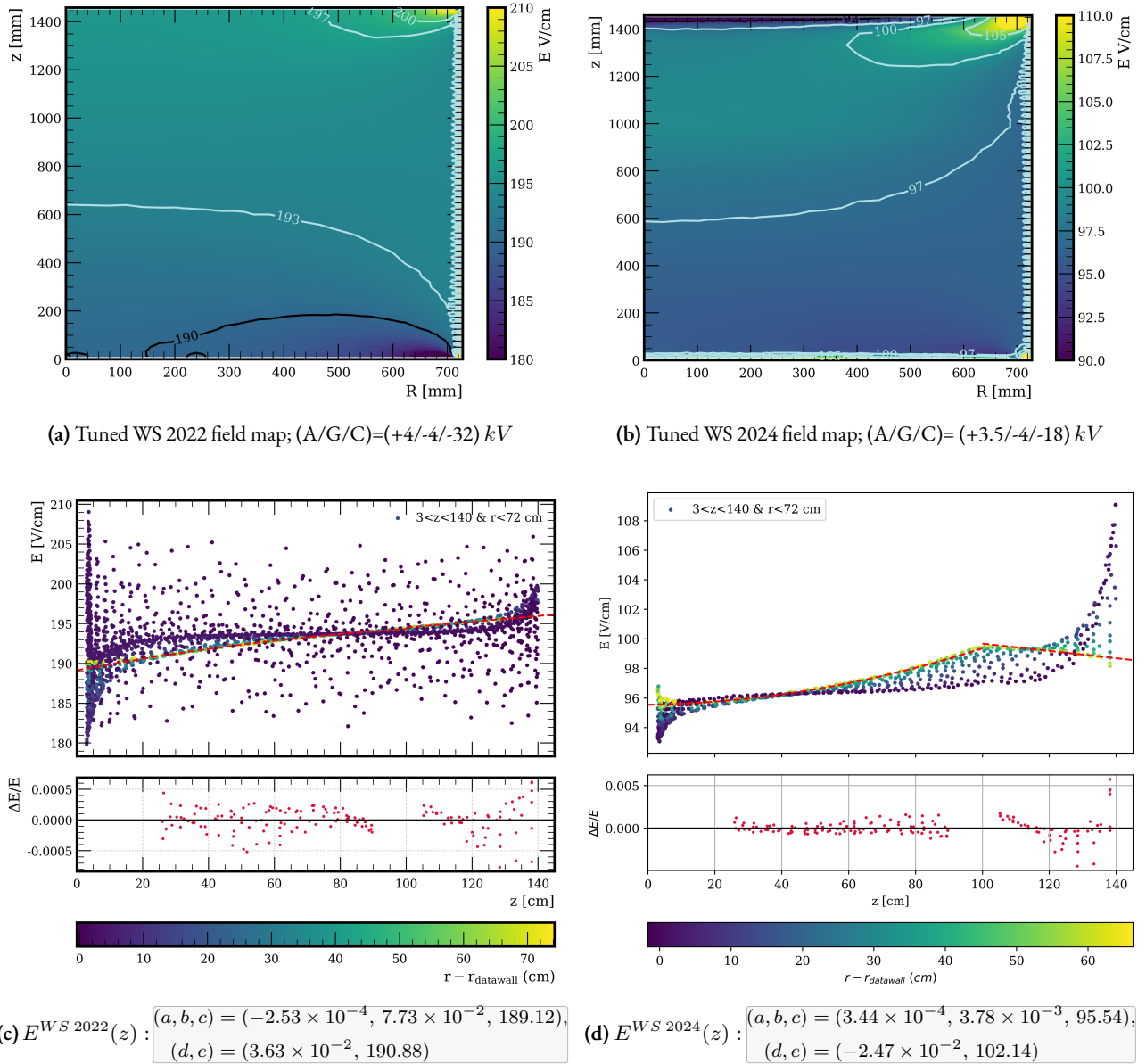


Figure 4.30: Tuned electric-field maps (V/cm) and depth projections ($z(dt)$) for the two science runs. The fits in panels (c) and (d) establish a mapping between $z(cm)$ and $E(\mu s)$ in the two field configurations. A piecewise fit is performed to capture slightly different field behaviour near cathode at $z > 105 cm$ (corresponding to the high charge-density patch of charge observed in data and applied in simulations). The fit functions are as follows:

$$E(z) = \begin{cases} az^2 + bz + c, & z \leq 100 cm, \\ dz + e, & z > 100 cm. \end{cases} \quad (4.45)$$

The fit coefficients are given for each as a proxy of the average field corresponding to a given z -value.

Table 4.12: FV-averaged drift field by campaign and method (RMS uncertainties).

Method	SR1 (WS 2022) [V/cm]	SR3 (WS 2024) [V/cm]
Kr 83m	193.00 ± 0.72	96.50 ± 0.39
Xe 131m	—	97.8 ± 0.4
Simulation (ϕ -avg.)	192.9 ± 2.1	97.3 ± 2.2

tracks within $\sim 10\text{--}15\text{ cm}$ of the wall display the expected curvature that mirrors the wall geometry, consistent with peripheral distortions induced by surface charge. The modest overall gradient in both regimes indicates that, over the FV (closer to $r < 68\text{ cm}$), average electron trajectories are well approximated as straight lines toward the extraction region, supporting the reconstruction assumptions used elsewhere. These relationships for the fiducial volume are given as follows:

$$\begin{aligned} z_{WS\ 2022}\ (mm) &= -1.57351573\ dt\ (\mu s) + 1459.4844826 \\ z_{WS\ 2024}\ (mm) &= -1.39877509\ dt\ (\mu s) + 1456.58820 \end{aligned} \tag{4.46}$$

Despite clear indications of a net accumulation of negative surface charge from WS 2022 to WS 2024, the mechanism cannot be isolated from these data alone: hardware interventions, calibration campaigns, and changes in the nominal field configuration alter both the wall field and charge-transport conditions. To approach a³⁰ purely temporal assessment, we therefore restrict our studies to a period of steady operation in WS 2024 and follow the evolution of the ^{131m}Xe -derived wall position and the corresponding surface-charge requirement. In the discussion that follows, we analyse the observed “pushing-out” of the wall, an effect that superficially resembles discharge, and show that it arises from slow temporal redistribution of surface charge on PTFE within the TPC, constituting the first such measurement.

4.6.4 Temporal Behaviour

While the fundamental properties of PTFE establish it as a quasi-permanent electret under LXe conditions (§4.6), the apparent charge evolution in data often shows additional structure beyond static bulk immobilisation. Several processes can contribute to such behaviour. External stimuli—including high-rate calibrations, micro-discharges near the cathode, and spurious electron emission—can intermittently deposit or redistribute charge. Changes in field regime may impact wall movement even more. Even in the absence of identifiable events, shallow-trap hopping and lateral transport across the upper micron of the PTFE surface can produce week-to-month scale variations in the effective wall field, in contrast to the geological retention times of deep-trapped electrons. These subtle processes complicate attempts to isolate a purely temporal signal.

Evidence for temporal dependence is best sought in data where confounding variables are minimised. In WS 2024, repeated ^{131m}Xe injections provided a clean calibration source with stable drift fields, no evidence of grid light leaks, and no reason to suspect changes in PTFE roughness. Under these conditions, the reconstructed wall position can be used as a proxy for charge evolution with time. Fig. 4.31 shows the measured trend: over a period of ~ 10 months the wall appears to recede, suggesting an apparent “discharge” of the wall. However, the observed timescale is inconsistent with the expected immobilisation of PTFE bulk charge and is not accompanied by enhanced wall-event rates that would signal active emission.

This motivates a more quantitative approach. Rather than interpreting the wall shift as direct discharge, we calculate the PTFE surface charge densities required to reproduce the observed temporal variation. In doing so, the analysis distinguishes between genuine charge loss and effective redistributions within shallow traps, thereby probing the

³⁰At least “as close to a” pure temporal assessment as can be managed.

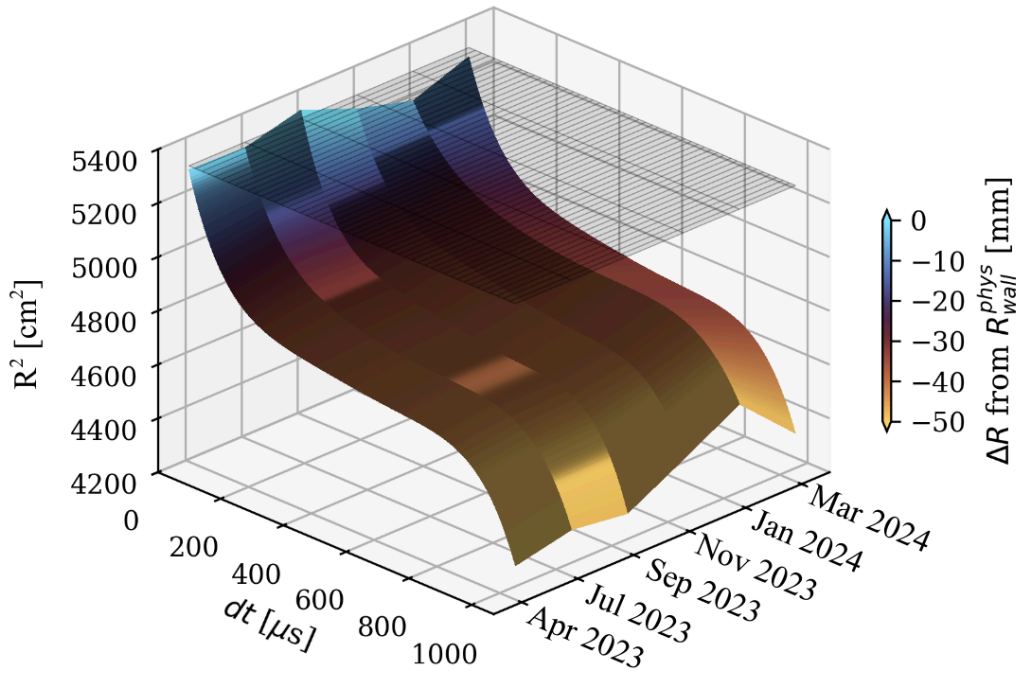


Figure 4.31: Temporal evolution of the reconstructed TPC wall in WS 2024, expressed in terms of displacement from the physical PTFE wall at 72.8 cm as a function of drift time and calendar date. The apparent and unexpected inward motion from $\sim$ April 2023 to Jan/Feb 2024 suggests effective charge evolution despite stable operating conditions.

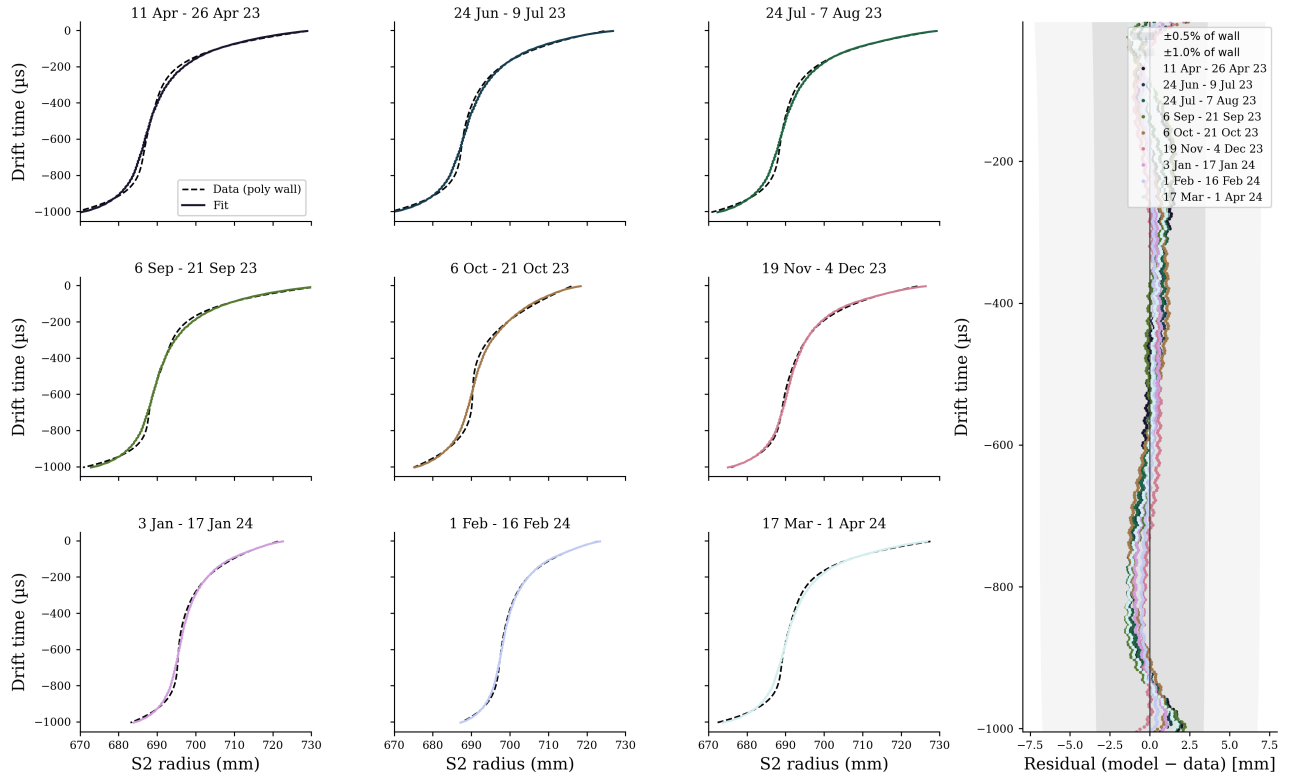


Figure 4.32: Temporal stability of the wall model. For each chosen month: data (black dashed) and best fit (coloured), with residuals for each as a function of drift time (right). Gray bands mark $\pm 0.5\%$ and $\pm 1\%$; residuals remain small across all slices.

mechanisms responsible for long-term wall evolution.

For the months studied, the wall model reproduces the data well: all residuals are sub- mm to $\sim mm$ level and $\chi^2/dof \lesssim 1$. Fig. 4.32 shows the residuals of select months, demonstrating that they stay within the $\pm 1\%$ bands almost everywhere, with the largest deviation ($1.36 mm$) in one of the earliest time slices (also with a correspondingly higher χ^2/dof implying a harder shape to fit to the patch profile). Using an extended set of wall profiles from ^{131m}Xe

Table 4.13: Wall-fit quality and inferred area-averaged PTFE surface charge density for each time slice. The quoted uncertainty is the per-slice RMS spread of the patch contributions to $\bar{\sigma}$, computed from the best-fit patch parameters. We use this as a conservative proxy to capture patch degeneracies and intra-slice variation; it is not a covariance-propagated 1σ on $\bar{\sigma}$.

Time slice	$ \bar{\sigma} [\mu\text{C}/\text{m}^2]$	RMS dev. (mm)	χ^2/dof
11 Apr – 26 Apr 23	2.124 ± 0.463	0.92	0.885
25 May – 9 Jun 23	1.772 ± 0.443	1.36	1.910
9 Jun – 24 Jun 23	1.906 ± 0.404	0.91	0.867
24 Jun – 9 Jul 23	1.699 ± 0.449	0.76	0.595
9 Jul – 24 Jul 23	1.805 ± 0.398	0.77	0.623
24 Jul – 7 Aug 23	1.629 ± 0.402	0.80	0.669
7 Aug – 22 Aug 23	1.702 ± 0.453	0.72	0.541
22 Aug – 6 Sep 23	2.065 ± 0.457	1.00	1.042
6 Sep – 21 Sep 23	2.345 ± 0.498	0.87	0.795
21 Sep – 6 Oct 23	1.754 ± 0.449	0.67	0.467
6 Oct – 21 Oct 23	1.632 ± 0.449	0.81	0.679
21 Oct – 4 Nov 23	1.475 ± 0.353	1.11	1.282
4 Nov – 19 Nov 23	1.736 ± 0.438	0.32	0.109
19 Nov – 4 Dec 23	1.736 ± 0.438	0.47	0.232
4 Dec – 19 Dec 23	1.686 ± 0.443	0.82	0.700
19 Dec – 3 Jan 24	1.195 ± 0.297	0.35	0.129
3 Jan – 17 Jan 24	1.641 ± 0.453	0.55	0.313
17 Jan – 1 Feb 24	1.815 ± 0.416	0.45	0.214
1 Feb – 16 Feb 24	1.690 ± 0.454	0.28	0.083
16 Feb – 2 Mar 24	1.574 ± 0.451	0.35	0.129
2 Mar – 17 Mar 24	1.752 ± 0.448	0.42	0.183
17 Mar – 1 Apr 24	1.783 ± 0.449	0.80	0.658

calibrations, a constrained fit of the time evolution with

$$|\sigma(t)| = |\sigma_0| e^{-t/\tau} + |\sigma_\infty|. \quad (4.47)$$

yields a characteristic timescale of $\tau \simeq 74.7 \pm 70.5$ d, $|\sigma_0| \simeq -0.440 \pm 0.211 \mu\text{C m}^{-2}$ and a plateau at $|\sigma_\infty| \simeq -1.644 \pm 0.096 \mu\text{C m}^{-2}$ ³¹. As a baseline we also fit a constant to the series, obtaining $c = 1.710 \pm 0.053 \mu\text{C m}^{-2}$. Allowing a linear trend $a + bt$ (weighted by the per-slice RMS) yields $b = (-1.04 \pm 0.52) \times 10^{-3} \mu\text{C m}^{-2} \text{ day}^{-1}$ ($\approx -0.031 \mu\text{C m}^{-2}/\text{month}$). The slope differs from zero at $\sim 2\sigma$ (two-sided $p = 0.046$; one-sided $P[b < 0] = 0.977$), but model comparison shows only weak preference for the trend over a flat line: F-test $p = 0.060$ and $\Delta\text{AIC} = -2.0$ in favour of the linear model. Over the WS 2024 window the implied change is $\sim 0.34 \mu\text{C m}^{-2}$,

³¹Uncertainties on σ_0 and σ_∞ are from the fit covariance; the large fractional uncertainty on τ reflects the sparse time sampling and limited leverage.

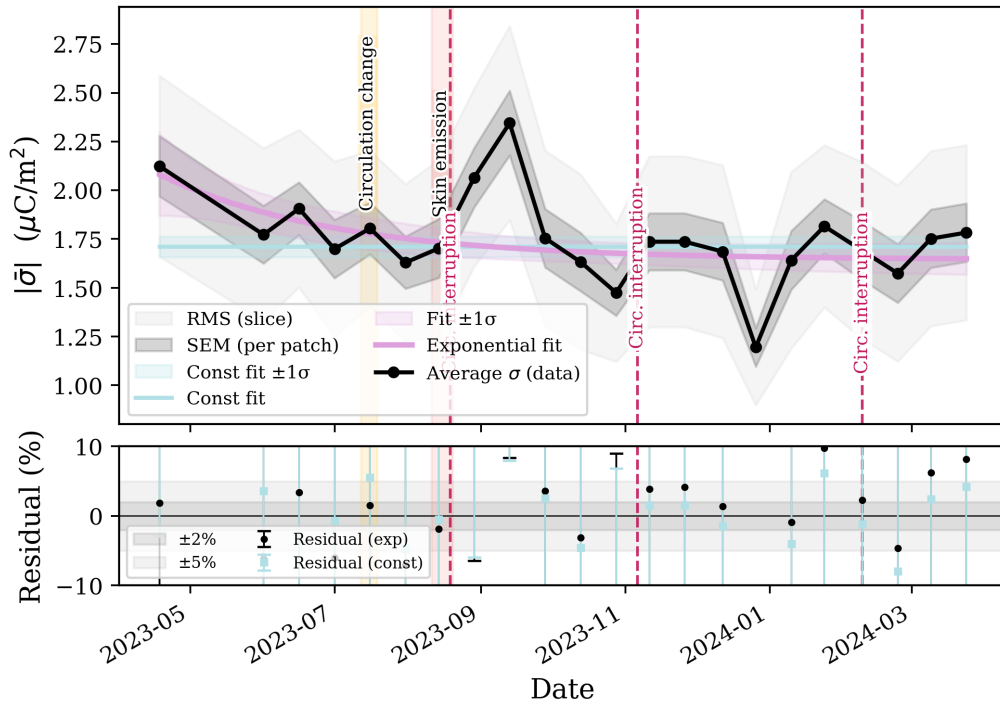


Figure 4.33: Temporal evolution of the area-averaged PTFE surface charge density (negative) $|\bar{\sigma}|$ during WS 2024. Points show per-slice means with dark-gray SEM and light-gray RMS envelopes. The magenta curve is the robust exponential fit with its $\pm 1\sigma$ band; the cyan line/band is a constant- σ fit. Shaded annotations mark the circulation change (yellow) and skin-emission period (rose); dashed lines indicate brief circulation interruptions. Lower panel: residuals (percent) to the exponential (black) and constant (blue) fits with $\pm 2\%$ and $\pm 5\%$ guides.

comparable to the SEM/RMS envelope (Fig. 4.33), so a strictly stationary level cannot be excluded at the 5% level. Together with the exponential fit, the data is suggestive of a gentle relaxation toward a plateau. This favours slow *redistribution* within shallow traps (changing the effective surface field) rather than net loss of deep-trapped charge.

By contrast, LUX saw monotonic charging (from ~ -2.5 to $-5.6 \mu\text{C m}^{-2}$ with $\tau \approx 181$ d [81]). This is not inconsistent with our WS 2024 behaviour: both follow the same first-order kinetics $d\sigma/dt = -(\sigma - \sigma_\infty)/\tau$, with the sign set by the initial offset from the asymptote. Here the slices begin more charged (in magnitude) than the long-term level and relax downward; LUX started less charged and moved toward a more negative plateau. Over year-scale baselines in LZ (WS 2022 $\rightarrow$ WS 2024) the wall still migrates inward, indicating a slower cumulative build-up on top of the short-timescale re-equilibration seen here. A longer time series with systematic error propagation (per-slice SEM³²/RMS³³ and fit covariance) will be needed to sharpen τ and test for multi-component behaviour under stable operating conditions.

³²**SEM (standard error of the mean):** computed per slice from the patch contributions x_i to $\bar{\sigma}$, with sample variance $s^2 = \frac{1}{N-1} \sum_i (x_i - \bar{x})^2$ and $\text{SEM} = s/\sqrt{N}$ ($N = 9$ patches here). It estimates the statistical uncertainty on the slice mean under the (approximate) assumption that patch fluctuations are independent.

³³**RMS (spread across patches):** the sample standard deviation s of the same x_i . It reflects the intra slice dispersion (including patch degeneracies/model imperfections) and is shown as a conservative envelope; it is *not* an uncertainty on the mean and therefore does not shrink with N .

4.7 Evidence and Implications of Azimuthal Asymmetry

Thus far it was introduced that the LZEF framework was built under the assumption that a 2D field and drift map formulation would be sufficient to describe the charge dynamics within the LZ TPC, motivated by the geometric symmetry of the LZ detector and the assumed (to first-order) homogeneity of any mechanisms which may induce field distortions. These assumptions were proven to be justified in the first WIMP search, where an accurate field model,

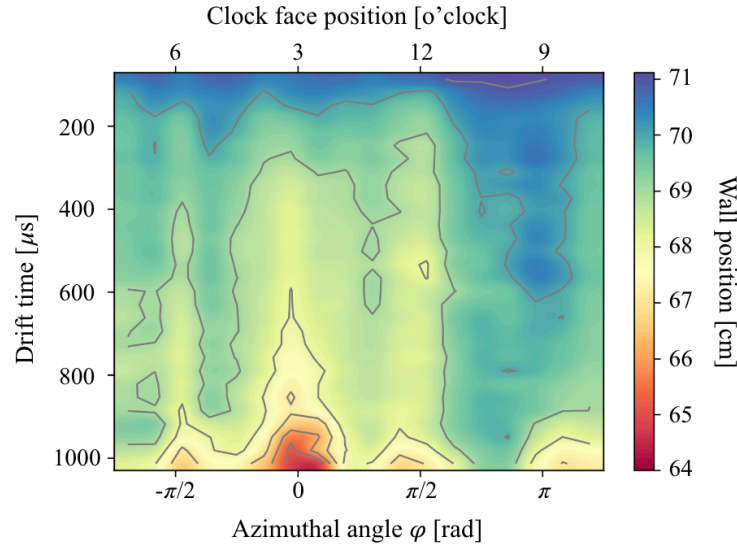


Figure 4.34: Drift-time–dependent wall position as a function of azimuthal angle, reconstructed from WS 2024 data. The colour scale indicates the wall radius in centimetres. Clear azimuthal variations are visible, with deviations of several centimetres near the cathode (large drift times), demonstrating that the detector wall is not azimuthally symmetric and motivating a slice-by-slice field tuning procedure. Figure reproduced using code by A. Musalhi.

capable of reproducing the wall and calibration source distributions observed in data, was produced [152]. Unfortunately, as seen in earlier experiments like LUX, the field behaviour showed a non-trivial evolution with time (§4.6.4) such that by WS 2024, azimuthally asymmetric wall movement implied a more complete 3D field description may be required. We next consider employing LZEF to understand the implications of the observed behaviour particularly in the context of reconstruction, tackling the challenge of the pursuit towards a quasi-3D field model, currently achieved by stitching together field solutions tuned to ϕ –sliced observations of the TPC.

Evidence for the azimuthally varying wall position is shown in Fig. 4.34. It presents the reconstructed wall radius as a function of drift time and azimuthal angle, where clear scalloping of the boundary is observed at up to the few-*cm* level, particularly towards the cathode. This behaviour demonstrates that the wall cannot be described by a single azimuthally averaged contour. The relationship can be made explicit by comparing wall reconstructions extracted in twelve ϕ –slices to the average wall definition (black lines in Fig. 4.35): while agreement is good in the upper half of the TPC, significant divergences emerge at long drift times, with some slices displaced outward by more than a centimetre. Together, this establishes that the assumption of azimuthal symmetry is not valid in WS 2024 data.

The corrected Powell fit reproduces each ϕ -slice wall to sub-*mm*–few-*mm* precision across the full drift range. In the

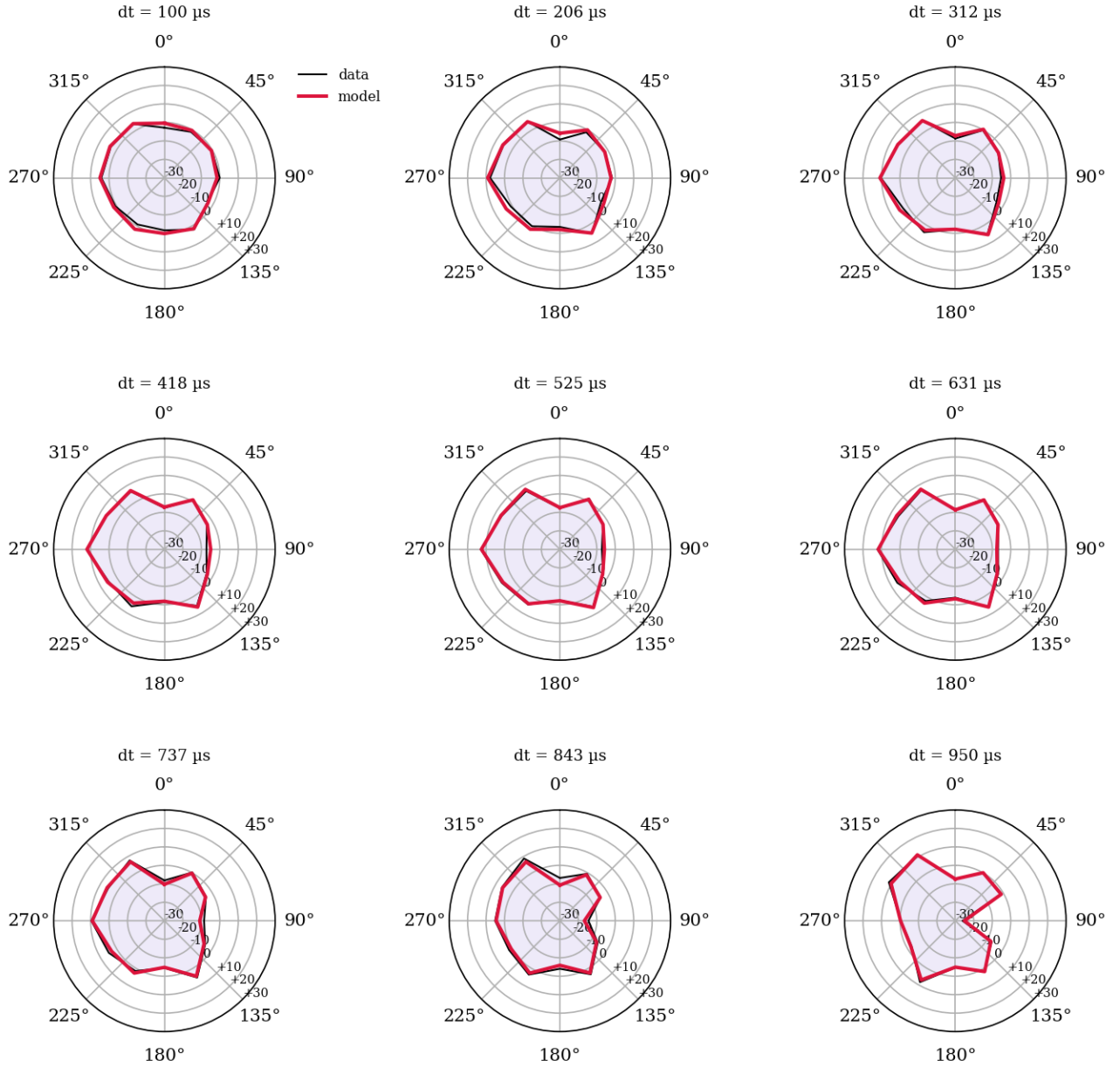


Figure 4.35: Polar “scallop” comparison of the wall-radius deviations $\Delta r(\phi)$ at fixed drift times from $dt = 100$ to $1000 \mu s$. The lilac fill (black outline) shows the data wall per ϕ -slice; the red curve is the model evaluated on the same times. Here $\Delta r(\phi) = r_\phi(t) - \bar{r}(t)$ is referenced to the ϕ -averaged wall at that t . Radial tick labels are in millimetres. The model tracks the observed azimuthal structure at all depths, with the largest mismatches appearing at late drift times near the cathode.

Table 4.14: Per- ϕ wall-fit residuals (RMS of model – data) for the Powell + affine solution, sorted from smallest to largest RMS.

Slice	RMS [mm]
2 o'clock	0.25
5 o'clock	0.62
10 o'clock	0.68
9 o'clock	0.81
1 o'clock	0.85
4 o'clock	1.06
11 o'clock	1.11
6 o'clock	1.42
3 o'clock	1.69
8 o'clock	1.75
7 o'clock	1.86
12 o'clock	2.69

10 time-slice polar panels shown in Fig. 4.35, the model (red) tracks the measured scalloping (plum) at all depths, with small systematic structure appearing mainly at long drift times (near the cathode). Table 4.14 summarises the typical RMS residuals per slice, where $0.6 - 1.1$ mm envelopes most of the slices with goodness-of-fit captured by respectable $\chi^2/dof \sim 0.4 - 1.3$; the best slices reach ~ 0.25 mm, while the most challenging (12 o'clock) attains 2.69 mm.

Beyond reproducing the wall contours, the slice-by-slice fits allow an estimate of the *effective* PTFE surface charge density required to support the observed distortions. The result is shown in Fig. 4.36: typical slices require $|\sigma| \sim (1 - 2) \mu C/m^2$ with slice-to-slice variations at the factor-of-two level for the most different wall shapes. The crimson ring marks the azimuthally averaged reference ($\bar{\sigma} \approx 1.41 \mu C/m^2$; a correlated systematic floor of $\pm 0.20 \mu C/m^2$ is carried from the average-wall robustness tests and folded in quadrature with the fit statistical error to form the pale band. Most slices remain within $\sim 1\sigma$ within this reference. Two cases particularly deserve comment.

- At 1 o'clock the central value is close to the average, but the systematic is asymmetric ($-1.01, +0.36 \mu C/m^2$): alternative Powell initialisations converge to a second, lower- σ family of acceptable solutions, producing a negative tail in the uncertainty (we visualise this through the widened total band in the panel).
- At 3 o'clock the inferred charge can be substantially larger: fits that emphasise the pronounced cathode push-in admit solutions with mean σ up to $\mathcal{O}(-10) \mu C/m^2$. As this is far outside the dynamic range of the other slices, we cap the drawn wedge at the outer tick and indicate the off-scale extent with an arrow in Fig. 4.36. Physically, this reflects that a very localised cathode-patch charge can reproduce the sharp inward excursion of the wall at $dt \sim 1$ ms without requiring large charge elsewhere along z . Consistent with this picture, WS 2024 data show a localised excess of events in the same sector after standard quality and fiducial selections (Fig. 4.37), compatible with an enhanced radial-field region that yields unusually large S2s passing the usual cuts.

The $\sigma(\phi)$ pattern is readily interpreted when compared with Fig. 4.34 and with the reconstruction-difference maps described in Fig. 4.38. Slices with a dramatic, highly localised inward scallop near the cathode (e.g. 3, 6, 12 o'clock) are accommodated by a concentrated charge on the lowest z patches; away from the cathode their walls track the average closely and the mean σ therefore remains moderate. In contrast, slices such as 9, 10 o'clock are consistently offset from

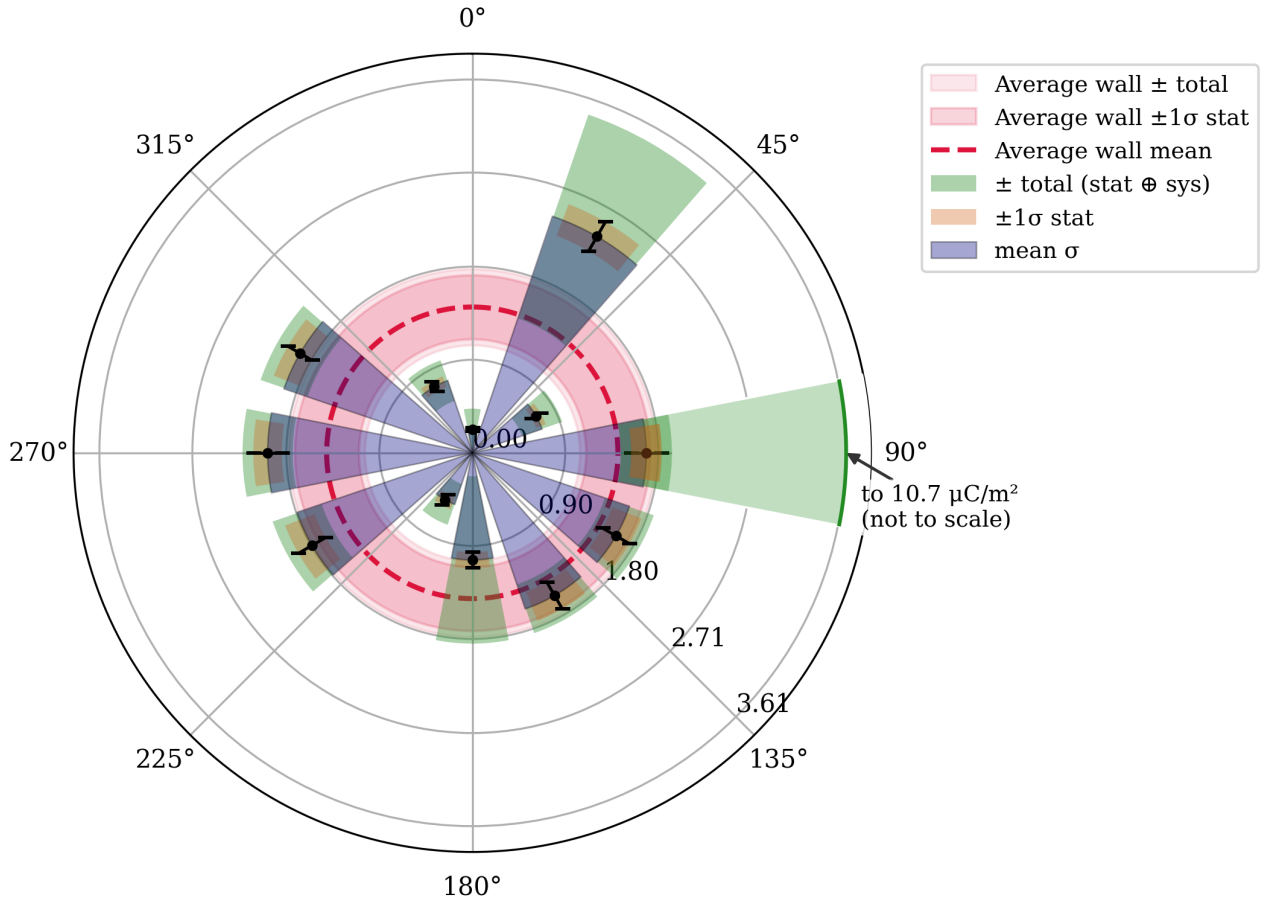


Figure 4.36: Per-slice calculated PTFE surface charge densities $\sigma(\phi)$. Navy wedges show the mean; brown bands with black error bars, the 1σ statistical error; green bands the total ($stat \oplus sys$) errors. The red dashed ring and pink band indicate the average-wall mean $-1.41 \mu\text{C}/\text{m}^2$ and its uncertainties. For 3 o'clock the total band is truncated; the arrow marks the full upper bound extent to $-10.7 \mu\text{C}/\text{m}^2$.

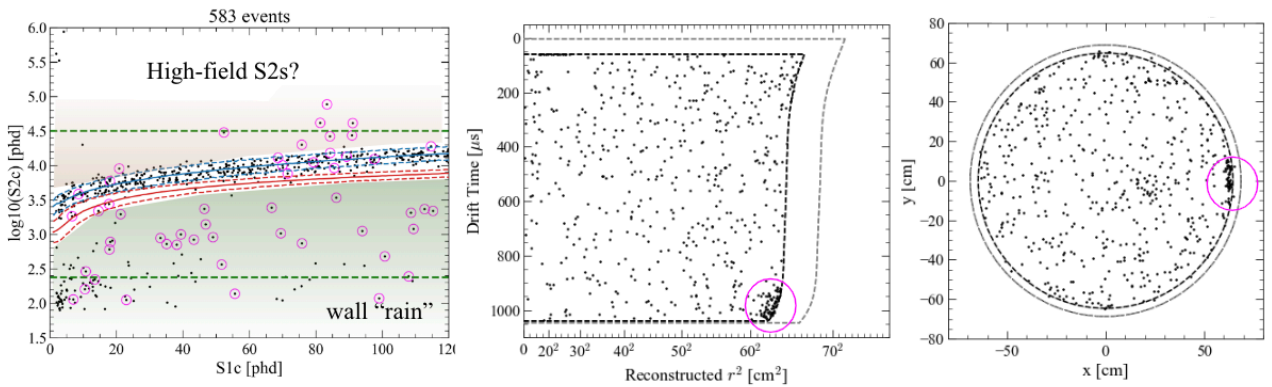


Figure 4.37: WS 2024 events after all analysis cuts showing the expected “wall-rain” population at low S2 (charge-loss events near the wall) and a subset with higher-than-expected S2. A localised cluster at large dt and large r appears near 3 o'clock (middle/right). This pattern is consistent with the 3 o'clock slice solution that predicts enhanced radial fields from a localised cathode-patch charge (Fig. 4.36).

the average over a wide range of drift times; reproducing that broad displacement requires charge that is distributed over several patches along z , yielding a comparable mean σ even without an extreme cathode excursion.

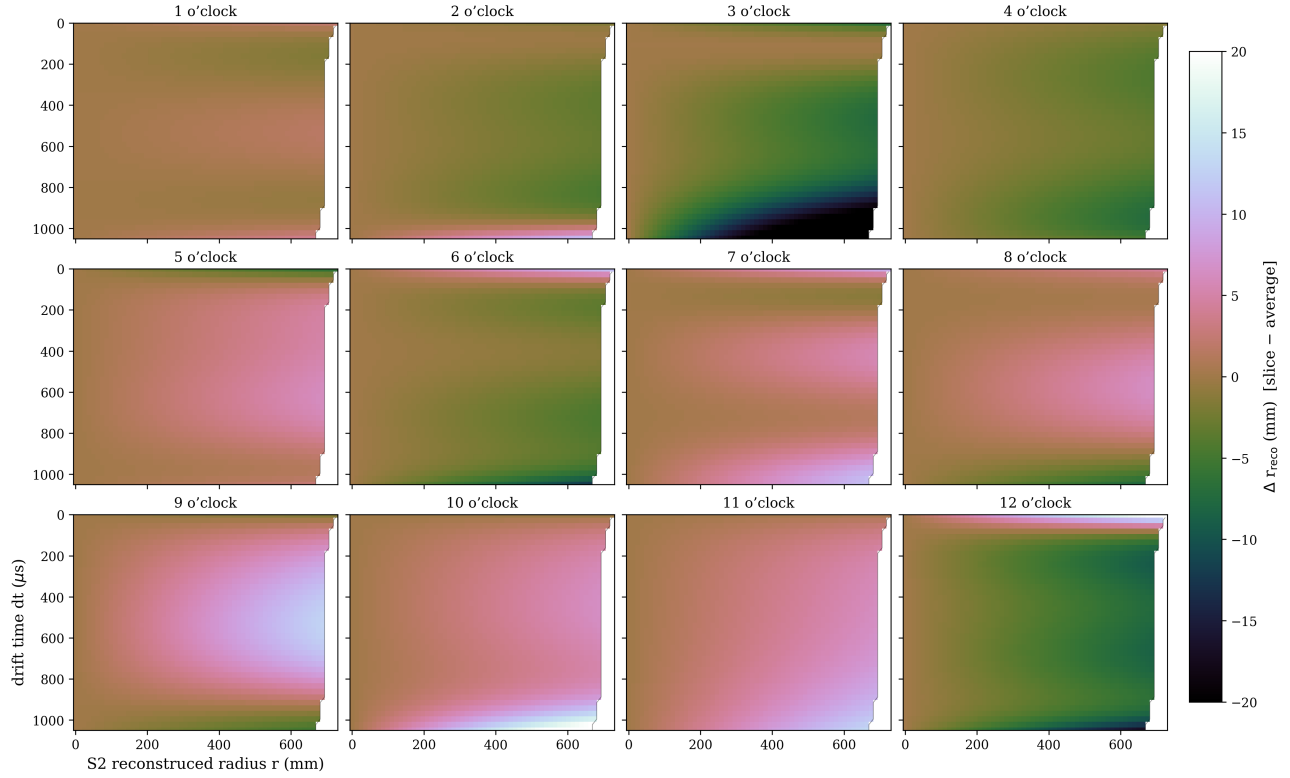


Figure 4.38: Bias in reconstructed S2 radius for each ϕ -slice relative to the azimuthally averaged map, $\Delta r_{S2}(\phi; r, dt) = r_{S2}^{\phi} - r_{S2}^{ave}$; the cathode corresponds to drifts near $1000 \mu s$, with the gate at $0 \mu s$ drift.

Methodological note: In this section each ϕ -slice is inverted in isolation to obtain a field solution that reproduces its wall contour. Since the true problem is 3D and the electric field superposes, neighbouring slices also contribute to the field in any given sector. The per-slice inversion therefore attributes the full distortion to that slice alone and will generally overestimate the absolute charge density needed there. We thus interpret the reported $\sigma(\phi)$ as an effective (upper-bound) normalisation that captures the correct sign, localisation, and relative ordering across ϕ ; the inferred S2-bias patterns are robust to this normalisation, whereas a global 3D fit with azimuthal continuity would redistribute, and typically reduce, the required charge among adjacent slices³⁴.

The impact of this azimuthal dependence on reconstruction is shown in Fig. 4.38, which maps the difference in reconstructed S2 radius from a slice-tuned field solution relative to the azimuthally averaged map,

$$\Delta r_{S2}(\phi; r, dt) = r_{S2}^{\phi} - r_{S2}^{ave}. \quad (4.48)$$

Across most of the volume the bias is at the few-mm level; for the most extreme slices it increases to $\sim 10 - 30 \text{ mm}$ at large drift times near the cathode and remains visible well inside the detector (to $r \sim 100 \text{ mm}$). The sign follows the

³⁴Put another way, solving each ϕ -slice independently forces that slice to “own” the whole distortion when in reality, its neighbours help out. So the absolute σ the fit returns is typically an upper bound. Relating back to Fig. 4.34, we also point out that broad, slowly varying offsets (e.g. near 9–10 o’clock) will be most reduced in a 3D fit, whereas sharply localised cathode push-ins (e.g. 3 o’clock) will remain largely concentrated and thus closer to the slice-wise estimate.

wall displacement: inward–scalped slices (e.g. 3, 12 o’clock) reconstruct smaller radii with the slice map than with the averaged map (negative Δr_{S2}), while persistently outward slices like 9, 10 o’clock show positive biases. Expressed relative to the local radius, these correspond to $\mathcal{O}(0.5 - 5)\%$ effects near the wall. Such biases propagate directly into fiducialisation, wall–cut acceptance, and background localisation, and therefore must be modelled in any analysis that averages over ϕ .

The physical origin of the asymmetry remains unclear: it shows no obvious correlation with geometric features (e.g. the HV umbilical), calibration–induced rate changes, or known PTFE charge–injection mechanisms such as breakdown or cathode emission (none observed). Addressing its cause, and how to mitigate it in future detectors, remains an open question. Although developed after the last WIMP search and therefore not used there, these corrections are ready for deployment in upcoming WIMP analyses and are likely to be even more critical for rare–event searches such as $0\nu\beta\beta$ decay.

4.8 The Skin

The Xe “skin” describes the volume of liquid xenon between the outer PTFE surface of the TPC field cage and the inner cryostat wall. Unique to LZ, it serves as both a mechanical interface and an active background rejection volume. It is optically isolated from the main TPC and contains approximately 2 tonnes of LXe, with dedicated

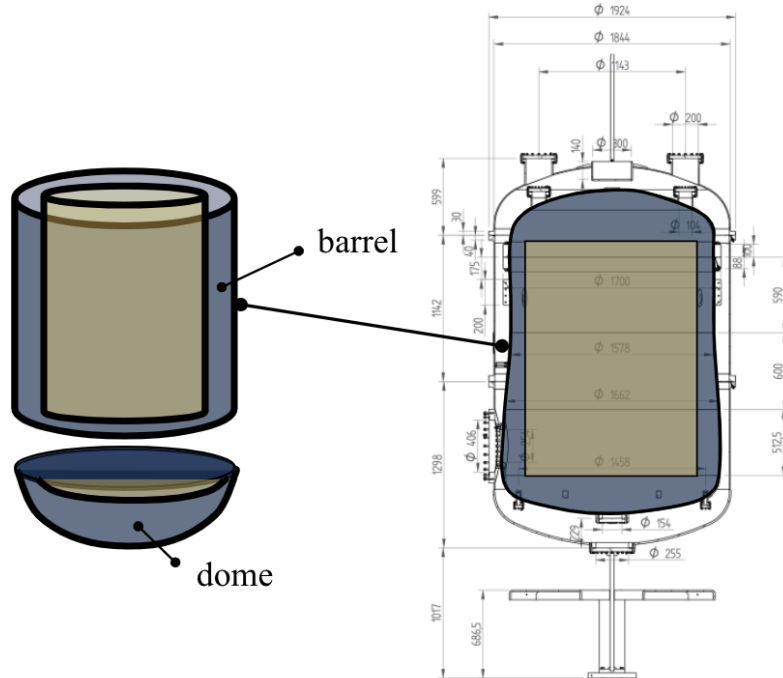


Figure 4.39: (Left) A simplified schematic of the skin volume (navy) identifying the “dome” and “barrel”. (Right) Technical drawing amended from [58] identifying the TPC volume (yellow) within the inner cryostat vessel; this visualises the true cross section of the skin. The TPC/ field cage boundary is not to scale.

PMT coverage in both the cylindrical side region and the dome region beneath the cathode. The concept of an instrumented skin volume was originally introduced by the XENON100 collaboration [177], but was not implemented in

XENON1T or XENONnT in order to minimise radon emanation from PTFE surfaces and to maximise the active target mass. In contrast, LZ adopted a fully-instrumented skin alongside a gadolinium-loaded outer detector (OD), enabling high-efficiency background rejection via prompt and delayed coincidence tagging³⁵. A neutron rejection efficiency of $89 \pm 3\%$ was measured during AmLi calibrations, increasing to $92 \pm 4\%$ when higher-energy radiogenic neutrons were included [49]. Gamma tagging efficiencies of $90.4 \pm 0.6\%$ (WS 2022) [179] and $78 \pm 5\%$ (WS 2024) [180] in the $10 - 78 \text{ keV}_{ee}$ range have also been reported, based on comparisons between tagged and untagged low-energy electron capture events from ^{127}Xe ³⁶.

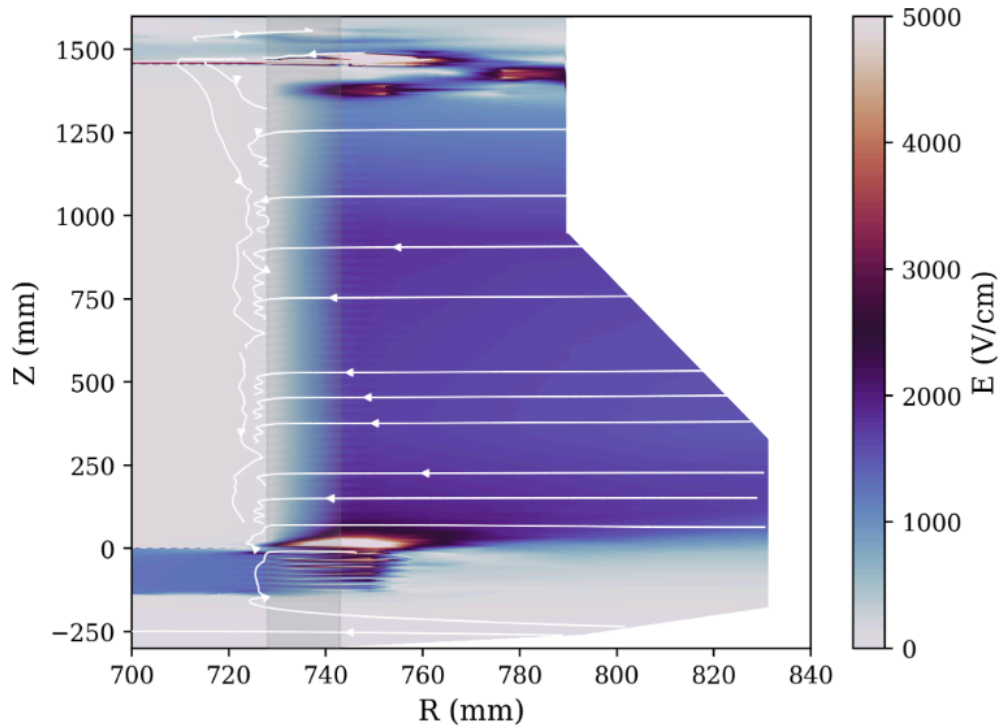


Figure 4.40: White streamlines, launched a few millimetres inside the field cage, pass uninterrupted through the PTFE wall (light grey box) and continue into the skin. Their continuity illustrates that, due to the dielectric match between PTFE and LXe and the presence of the shaping rings and resistor chain, the electric field remains smooth across the boundary. The heat map shows the electric field solution in the outer-TPC-skin region for the WS 2024 field configuration.

Beyond its role in background rejection, the skin provides a valuable opportunity to validate electric field models tuned to the “main TPC”³⁷ volume. Although optically isolated, the skin is electrically coupled to the TPC through shared PTFE panels in the field cage. The dielectric constant of PTFE (~ 2.1) is intentionally matched to that of LXe to reduce field non-uniformities (geometry-induced scalloping or general bending of field lines due to mismatched dielectric boundaries) near the field cage, crucial for maximising the fiducial volume; this same property ensures continuity of the electric field across the PTFE boundary, allowing field lines to extend smoothly from the TPC into the skin (Fig. 4.40). As a result, any perturbation to the electric field within the TPC, such as those arising from PTFE surface

³⁵The prompt veto targets gamma rays and fast neutron scatters by requiring a skin signal exceeding 2.5 phd in at least two PMTs within $0.25 \mu\text{s}$ of the TPC S1. The delayed veto targets radiogenic neutrons that thermalise and capture, typically producing delayed gamma cascades, and is defined by a skin signal above 300 keV within $600 \mu\text{s}$ of the TPC S1.

³⁶See Chapter 6 of both [179] and [180].

³⁷That is, the volume within the PTFE field cage, encapsulating the fiducial volume.

charge accumulation, must also affect the field configuration in the skin. A physically consistent field model must therefore reproduce not only internal observables, such as reconstructed wall positions or field profiles derived from $^{83\text{m}}\text{Kr}$ and $^{131\text{m}}\text{Xe}$ calibrations, but also the predicted field structure in the skin. This is particularly relevant given that the observed scintillation pulse shapes from various calibration sources deployed to characterise the skin are likely shaped by the combined effects of field leakage and the local geometry of the inner cryostat vessel.

4.8.1 Calibration Sources

LZ employs a set of commercial rod sources³⁸ that emit mono-energetic or nearly mono-energetic γ rays spanning two orders of magnitude in energy. Their key properties are summarised in Table 4.15. The energies are chosen to:

- cover the low-energy region ($\lesssim 200$ keV) where photoelectric absorption in LXe is significant and light-collection non-uniformities are most pronounced (^{57}Co , 122 keV);
- sample the intermediate regime around 0.5–1 MeV, where Compton scattering dominates and attenuation lengths are comparable to the skin thickness (^{54}Mn , 835 keV; ^{22}Na , 511 keV);
- provide high-energy anchor points above 1 MeV for linearity checks and optical-model validation (^{22}Na , 1274 keV; ^{228}Th , 2615 keV).

As ^{57}Co gammas ($\lambda_{\text{att}} \approx 3$ mm in LXe) are almost entirely absorbed in the skin, this source is ideal for mapping light-collection efficiency and verifying liquid-surface levelling via induced S2s when positioned above the liquid [75]. In contrast, ^{22}Na and ^{54}Mn gammas penetrate the skin and reach the TPC, enabling cross-calibration of the energy scale between volumes. The 2.615 MeV line from ^{228}Th (via ^{208}Tl decay) provides a high-energy reference for studying pulse-shape dependence on field strength and for validating linearity corrections.

Table 4.15: Rod γ -ray sources deployed for skin-energy calibration. Energies and branching ratios from [75].

Source	E_γ (keV)	Branching Ratio	Primary Calibration Role
^{57}Co	122	99.8%	Low-energy skin response; liquid-level tuning
^{54}Mn	835	99.9%	Mid-energy scale; position scans in skin/OD
^{22}Na	511 (ann.), 1274	89.8%, 99.9%	Coincidence timing; mid/high-energy anchors
^{228}Th	2615 (^{208}Tl)	36%	High-energy linearity, optical-model check

Fig. 4.41 shows single-scatter energy spectra recorded in the TPC, skin, and OD for two of the four sources: ^{54}Mn and ^{228}Th . In the following section, we examine how the mapped skin field alters the simulated ^{54}Mn and ^{228}Th spectra³⁹, review the present state of skin-specific tuning, and outline the remaining work required to separate field-induced effects from optical (g_1 , PDE) and modelling (NEST) uncertainties.

³⁸Eckert & Ziegler, encapsulated salts in acrylic rods, ~ 50 g, 15.9 mm $\times$ 74.9 mm, integrated with the Calibration Source Deployment (CSD) system.

³⁹This is due to availability of BACCARAT simulation inputs for these sources, which are then simulated incorporating the updated detector response parameters in LZLAMA allowing more direct comparison with data.

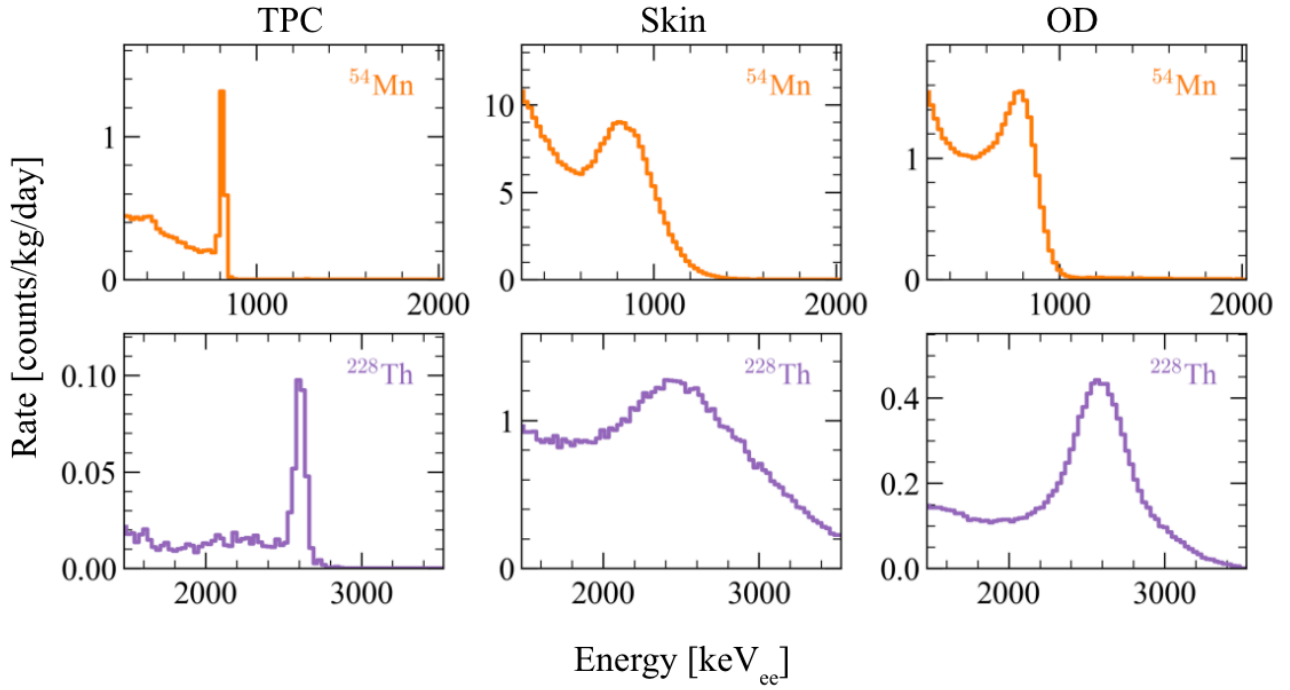


Figure 4.41: Single-scatter energy spectra from ^{54}Mn (835 keV), and ^{228}Th (2615 keV) recorded in the TPC (left) skin (middle) and the OD (right). Figure adapted from [75].

4.8.2 Consistency with TPC-derived Solution

As seen previously, the finite-element solution that reproduces drift trajectories inside the TPC extends naturally through the 15 mm-thick PTFE barrel into the skin xenon (inner radius 728 mm, outer 743 mm). Fig. 4.40 shows the resulting field map for WS 2024 as an example; away from a thin z-slice near-cathode and gate, the field in the skin barrel is essentially uniform at $E \approx 1.75 \text{ kV cm}^{-1}$. Only a narrow cathode fringe reaches $E \approx 10 \text{ kV cm}^{-1}$ at the cathode lip (Fig. 4.42 (left)).

Using NEST v2.0.3 we can calculate the photon yield $N_{ph}(E)$ for each calibration line. Relative to zero field, the 511 keV line, associated with the ^{22}Na source, is suppressed by 6.2% at 1.75 kV cm^{-1} . Pushing the field to the extreme 10 kV cm^{-1} lowers the suppression by only another 0.7% (0.8% for WS 2022), leaving the total reduction at 6.9%. For the higher-energy 2.615 MeV line, the field dependence is even weaker (5% at 1.75 kV cm^{-1} , < 0.5% extra at 10 kV cm^{-1}). In other words, the genuine E-field variation inside the skin cannot by itself move an S1 peak more than $\pm 1\%$ within the skin barrel volume. The field maps and corresponding NEST-derived photon yield suppression (relative to the zero-field case) at the various energies associated to the gamma decays of the calibration sources is shown explicitly in Fig. 4.43 for WS 2024.

A central goal of the present study is to move beyond purely empirical “shape-matching” and to identify which physical ingredients must change in the MC simulations (within LZLAMA) to reproduce the measured skin-source spectra. We therefore begin with the most recent empirical tuning⁴⁰, in which several high-level parameters were adjusted until

⁴⁰Thank you to M. Hernandez for his tuning studies.

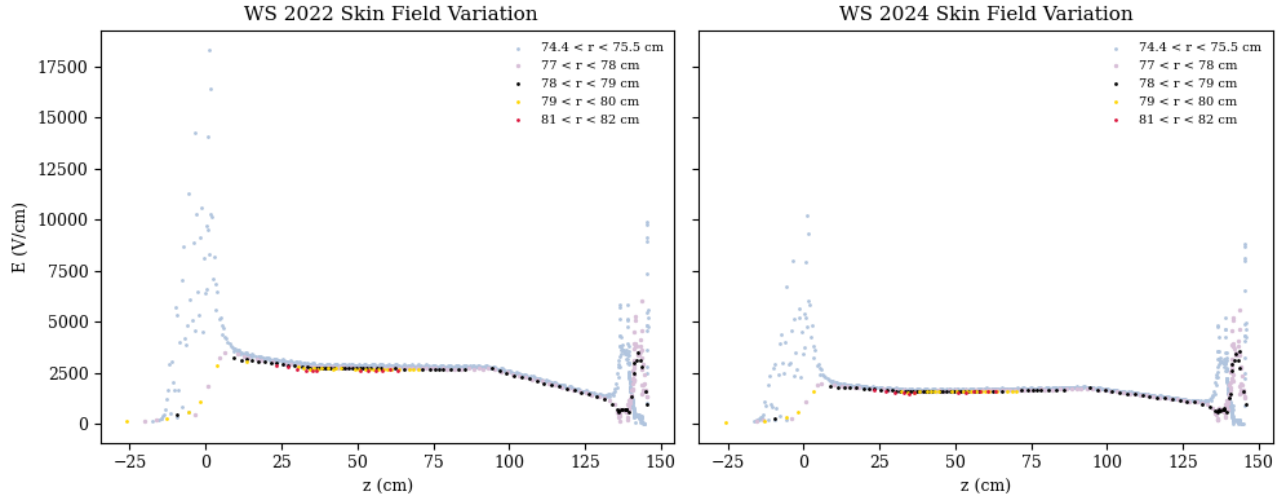


Figure 4.42: Skin field vs. height for (left) WS 2022 and (right) WS 2024. Each point is a finite-element mesh node; colours separate five cylindrical shells in radius (74.4 – 75.5 cm to 81 – 82 cm). Between $z \approx 5$ cm and $z \approx 90$ cm the barrel field is essentially flat at 1.75 ± 0.1 kV cm⁻¹ (WS 2024) and 2475 ± 1 kV cm⁻¹ (WS 2022), reflecting the uniform grading of the shaping rings and the near-perfect dielectric match between LXe and PTFE. Below $z \approx 5$ cm a sharp rise appears where field lines curl under the cathode - we label this the “cathode fringe” region. Above $z \approx 90$ cm the field falls steadily as the potential difference between the field cage and cryostat steadily decreases for a fixed stand-off distance.

simulation and data agreed. Table 4.16 lists the knobs that were varied, the role each plays in the MC chain, and what physical effect they are intended to mimic. Continuing from earlier discussions in §4.6 of tuning the TPC response, it is natural to question whether *additional charge accumulation on the outer PTFE wall* ($R \gtrsim 74.3$ cm) could lower the local drift field by the 15% ($\Delta E \simeq -260$ V/cm) that the empirical $0.847\times$ scale factor in table 4.16 presently delivers. In practice this hypothesis fails on both quantitative and qualitative grounds. The much smaller volume of the skin cannot supply enough charge to charge its wall. In WS 2022 (higher field regime), measurements of the skin rate registered an average of $R_{evt} \simeq 40$ Hz⁴¹ under a two-fold coincidence requirement. Taking an upper-bound ionisation yield of $N_e \approx 500$ electrons (or ions/holes) per event⁴², the maximum charge arrival rate at any surface is

$$I = eR_{evt}N_e \sim \mathcal{O}(10^{-15}) \text{ A}. \quad (4.49)$$

To reduce the radial field across the 40 – 90 mm LXe gap by 260 V cm⁻¹ one must then impose

$$\sigma_{req} = \Delta E \epsilon_0 \epsilon_r = 10^{-6} \text{ C m}^{-2}, \quad (4.50)$$

corresponding to more than

$$t = \frac{\sigma_{req} A}{I} \approx 10^{10} \text{ s} \quad (> 300 \text{ yrs}) \quad (4.51)$$

required to accumulate enough *positive surface charge* to yield the suggested empirical value. Moreover, field lines in the skin point radially outward toward the grounded cryostat; most electrons are swept to metal long before reaching PTFE. Positive ions, though directed toward the plastic, neutralise almost instantly, while electrons that do strike the PTFE can still remain trapped because of its negative electron affinity (lower electron trap energies than for holes

⁴¹This work was documented internally by Sivar Azadi (2022).

⁴²This takes into account the NEST-derived electron yield.

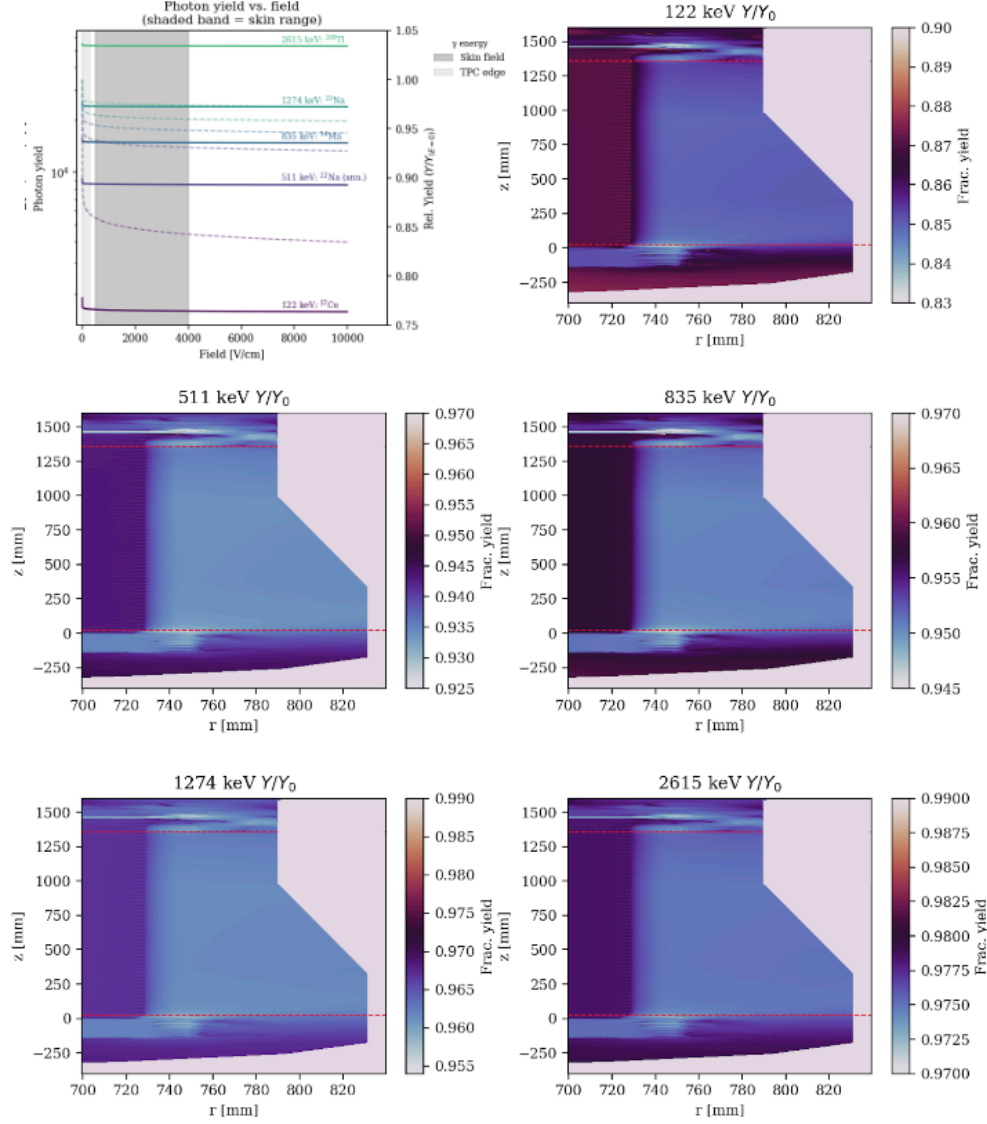


Figure 4.43: Impact of the WS 2024 field map on S1 light yield predicted by NEST v2.0.3. (**Top Left**) NEST yields for five calibration γ energies as a function of field; the plateau $\gtrsim 500$ V/cm is very evident for all of these energies and translates to the photon yield suppression maps of the skin (rest of the panels). Dashed lines show the suppression relative to zero field. (**Other Panels**) Dashed red lines mark the fiducial z limits. For most of the skin ($r > 74.3$ cm) volume ($\sim 95\%$) the fields lay in a regime where NEST predicts $< 1\%$ suppression (compared to an average) of S1 even at 122 keV for both WS 2022 and WS 2024. Larger deviations are only expected for fields near TPC drift fields, much lower than the average skin fields.

as discussed before). The net result is then, if there must be any charge accumulation, it is more likely due to a *much smaller negative surface charge density* than that possible on the inner PTFE wall (§4.6). Consequently the 15% renormalisation presently absorbed via the “field-scale” knob cannot be attributed to additional wall charging; it must likely be accommodated by optical parameters (g_1 , PDE normalisation, including potential QE measurements of PMTs), rather than predominantly by unmodelled (or mismodelled) electrostatics at the outer boundary. Dropping the ad-hoc 0.85 field-scale suppresses the NEST S1 yield by only $\sim 2.3\%$ in the barrel. That loss is recovered by a correspondingly small *increase* in the global photon-detection scale,

$$g_1^{\text{new}} = g_1^{\text{old}} \frac{Y(E_{0.85})}{Y(E_{\text{map}})} \simeq g_1^{\text{old}} (1.024), \quad (4.52)$$

i.e. a $+2.4\%$ adjustment for the current WS 2024 operating point⁴³. Such a shift is well within the $\pm 5\%$ systematic envelope usually assigned to g_1 and is most plausibly absorbed by optical uncertainties: slow drifts in PMT quantum efficiency, a small error in the global PTFE reflectivity at 175 nm or an overall mis-normalisation of the PDE map derived from α populations (high-LET, different topology and pulse shapes, occasional saturation) rather than ER γ calibrations. Further evidence comes from the WS 2022 ²²⁰Rn simulations in Fig. 4.44: moving from a uniform field to the TPC-tuned field map produces only a modest shift towards lower pulse area, whereas applying the α -derived $z - \text{PDE}$ together with a single global g_1 renormalisation produces the large systematic shift required by the data. Hence the empirical 15% renormalisation used in earlier tunings is best understood as an optical/PDE correction, not as evidence for unmodelled electrostatics at the outer boundary.

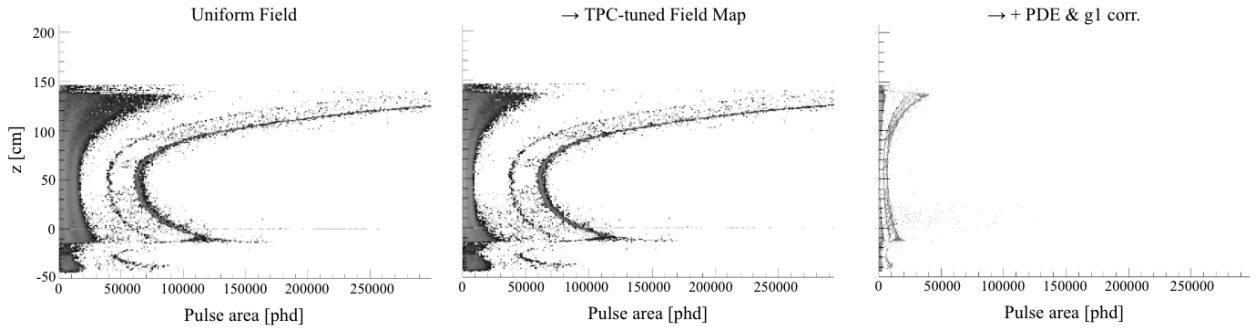


Figure 4.44: Effect of field and optical updates on Rn- α simulations in the skin (WS 2022). The plots show the pulse area- z spectrum for **(Left)** a uniform field assumption, **(Middle)** applying the TPC-tuned electrostatic field map and **(Right)** also applying an α -derived z -PDE correction and a single global g_1 renormalisation. The field map alone yields only a small leftward shift of the α bands; the dominant change comes from the PDE/ g_1 update, bringing the simulation much closer into the vicinity of the data.

Having established that optical effects dominate the absolute scale, we can cement our understanding of a residual depth-dependent PDE by comparing the measured ²²⁸Th and ⁵⁴Mn relative light yields to simulations using older and updated tuning of the PDE maps in WS 2024 (Fig. 4.45). The updated map much better reproduces the z -dependence across the barrel that is observed in data, but a coherent low- z deficit still remains. It is important here to note that the PDE map used was normalised at $z = 75 \text{ cm}$ and applied uniformly in depth; this is shadowed by the

⁴³The multiplicative factor varies between $+2.2\%$ (2615 keV) and $+2.6\%$ (835 keV); we quote the 511 keV mid-value.

low-residual difference in this z region. This residual grows smoothly towards the cathode consistent with a modest depth dependence of the effective PDE: changes in solid angle and incidence angle, reflections at the cathode lip, and absorption length variations tilt the S1 normalisation with z , once again inconsistent with the E-field effects in the skin's high-field plateau.

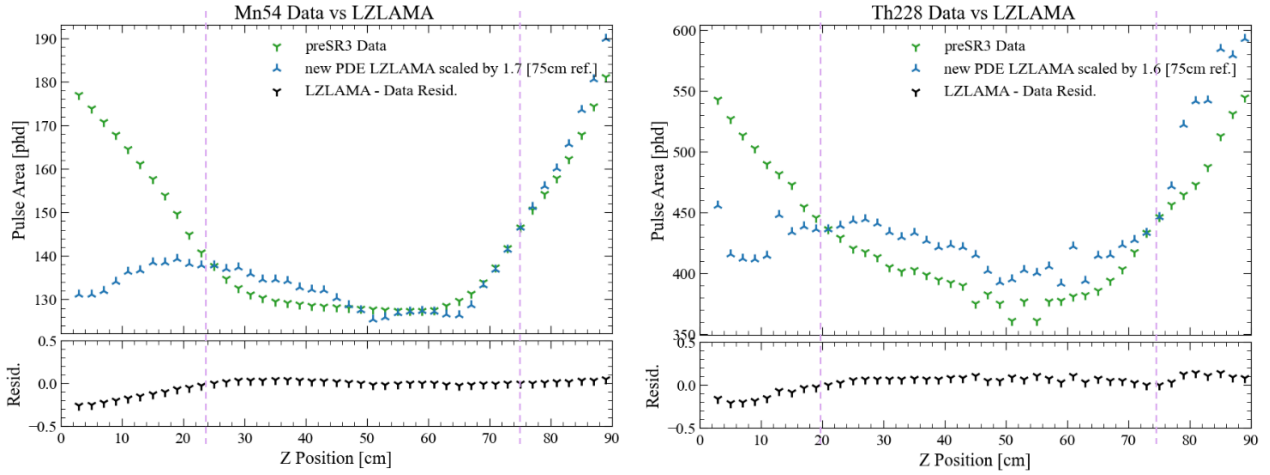


Figure 4.45: ^{54}Mn (left) and ^{228}Th (right) skin S1 pulse area vs. z : pre-WS 2024 data (green) and updated LZLAMA with the new PDE map scaled at the 75 cm reference (blue). Bottom panels show MC–data residuals. Vertical dashed lines mark the 75 cm anchor and the point where low- z divergences start to be noticeable. Modified from plots provided by M. Hernandez.

Taken together, these studies indicate that a modest depth-dependent PDE correction, augmented by a local term confined to the cathode-lip region, can reconcile the residual data–simulation differences in the skin. We therefore motivate a dedicated validation of $PDE(z)$, with emphasis on the complex geometry at the cathode base ring where occlusion and angular effects are largest. Practically, this means we anchor a correction $k(z)$ at a few depths (low- z , ~ 75 cm, high- z) using α -relative yields for shape and γ peaks for absolute scale, and we cross-check against independent observables (top/bottom asymmetry, effective attenuation length). Having firmly established the negligible S1 field dependence in the skin's high-field plateau (previously thought to be the reason behind such differences), this study strongly suggests that this is the most plausible route to transforming our understanding of the true skin yields in LZ.

4.9 Summary

Fields are the bedrock on which a dual-phase TPC stands. A fine-grained understanding is indispensable today, and the lessons learned here point the way to tomorrow: toward larger, cleaner, and more stable detectors. This chapter developed and validated an S2-reconstructed wall-motion–driven framework to reconstruct LZ's electric fields in situ, trace their temporal evolution, and characterise azimuthal non-uniformities, linking these directly to calibration, reconstruction, and fiducial definition.

We showed that LZ's fields evolve slowly during operations, with effects appearing strongest in the latest WIMP search, WS 2024. Central to this behaviour is the build-up and dynamics of negative surface charge, which has been historically hypothesised to accumulate on the PTFE wall. By tuning simulation wall profiles to calibration data and

performing eigenmode analysis of patch-based charge distributions, we addressed - explicitly and for the first time - the degeneracies among neighbouring z -patches. While absolute magnitudes can trade off between adjacent patches, the eigenvectors preserved the relative shape of the solution: in the case of WS 2024, they consistently favoured a highly localised cathode-proximal component. This approach has not been taken by other experiments; directly tackling these degeneracies shows that the profile of charge can be robust even when patch magnitudes can vary. This conclusion was powerful, already pointing toward a charge redistribution picture on PTFE rather than monotonic accumulation.

A second unexpected finding was the apparent receding of the ^{131m}Xe -derived S2 wall during a period of months during WS 2024. This was in-fact something that had not been observed in LZ's predecessors, and became a source of significant confusion given that hole attachment or discharging were disfavoured mechanisms given the electronegative nature of PTFE. The timescales and cross-checks were inconsistent with net discharging; instead, we observed month-scale migration of charge across the inner PTFE surface at roughly constant net density — the first explicit demonstration of this effect in a large dual-phase xenon TPC. This reframes wall charging as an evolving process and motivates time-aware field modelling, especially in the landscape of larger, new-generation experiments with increased wall surface areas, which will likely be more susceptible to such effects.

The framework also yields practical benefits. Along with an improved mapping of S2 reconstruction for WIMP searches, electron-lifetime estimates are now better anchored against field inhomogeneities, and the methodology is positioned to improve background rejection and exposure modelling as future detectors operate in regimes where charge/light yields and inferred lifetimes may be more susceptible to visible field- and energy-dependent variation (source-dependent). Azimuthal studies bound patch charges per ϕ slice and quantify associated reconstruction biases. Finally, the long-standing hypothesis that skin-region fields drive the observed data–simulation discrepancies is disfavoured; the studies strongly suggest that the answer lies in a depth-dependent $PDE \times g$, providing a more plausible resolution, clarifying both the limited utility of the skin as a tuning lever and the design sensitivities (cryostat geometry, PMT coverage, skin thickness) that merit attention.

In summary, this chapter goes beyond confirming wall charge: it introduces a degeneracy-aware inference of PTFE charging, provides the first evidence for large-scale redistribution over time, and propagates these effects into calibration and reconstruction. The methodology is designed to scale to a full 3D implementation (initiated in COMSOL where meshing is more easily handled than in LZEF) and establishes a generalisable tool for next-generation xenon TPCs, where rigorous field control will be mission-critical.

Table 4.16: Empirical “knobs” applied in the current LZ skin tuning, their technical effect in the MC simulations chain, the corresponding physical interpretation from a field-modelling perspective, and the principal degeneracies that make each knob difficult to disentangle from others.

Tuning knob	Implementation in sims.	Physics interpretation	Key degeneracies
<i>g1 adjustment</i> (0.0049 → 0.0041)	Global scale factor applied to every optical photon that reaches a PMT.	Absorbs <i>any</i> effect that changes the detector-wide average photon detection efficiency: drift of QE, overall reflectivity error, or a uniform error in <i>photon production</i> (e.g. field yield or <i>W</i> -value).	Exactly degenerate with the <i>absolute scale</i> of the PDE map and with a uniform offset in the field-yield curve.
α <i>z</i> -PDE map	Voxel-by-voxel weight derived from ^{222}Rn α events.	Corrects <i>spatial</i> structure in light collection or QE that was missed by the raw optical MC (e.g. small sensor tilts, cable shadows). No direct field dependence.	Indistinguishable from a real field gradient that has the same <i>z</i> -shape; cannot be separated using a single energy line.
<i>Linear noise term</i> (4.0%)	Adds a photon-count-proportional Gaussian broadening to S1.	Represents PMT gain variance and low-level electronic pickup; purely instrumental.	Degenerate with the NEST ER-width parameters—both broaden peaks without shifting the mean.
<i>Uniform field decrease</i> (multiply skin map by 0.847)	Every voxel in the skin field map is scaled by the same factor.	No obvious physical mechanism if HV set-points are known. Most likely compensates for an over-prediction of NEST light suppression at $E \gtrsim 1 \text{ kV cm}^{-1}$.	Trades directly against g_1 (global scale) and against the slope of the NEST field-yield curve.
<i>NEST ER-width parameters</i>	Tweaks intrinsic recombination-width parameters for ERs.	Encodes microphysics of recombination fluctuations not perfectly captured in default NEST.	Degenerate with linear noise and with small-scale PDE fluctuations.

“They knew she was a real princess, because she had felt the pea through twenty mattresses and twenty eider-down beds. Nobody but a real princess could be so sensitive.”

— Hans Christian Andersen, *The Princess and the Pea*

Part III

Backgrounds, Signals, and Data Interpretation

Enhancing WS 2022's Low-Mass Sensitivity

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DUAL-PHASE XENON TPCs achieve their lowest thresholds in conventional searches by requiring coincident scintillation (S1) and ionisation (S2) signals, enabling 3D position reconstruction and powerful electronic/nuclear recoil discrimination. However, this requirement excludes interactions that fall below the S1 detection threshold, limiting sensitivity to WIMPs below a few GeV/c^2 . In contrast, an S2-only search removes the S1 requirement, lowering the effective threshold to sub- keV energies and opening sensitivity to lighter dark-matter candidates, including standard spin-independent WIMPs, and coherent neutrino–nucleus scattering [46, 50, 60, 118]. This gain

in reach comes at the cost of qualitatively different backgrounds: without $S1$ information, drift-time-based fiducialisation information and ER/NR discrimination capabilities are lost, and the analysis must contend with accidental coincidences, surface and wall populations, and grid-related activity. In this chapter, we present a proof-of-concept $S2$ -only analysis using a subset of WS 2022 data, highlighting background-rejection methodologies for pathological populations in an $S2$ -only dataset and establishing baseline SI limits.

5.1 Backgrounds & Rejection Methods in an Ionisation-Only Search

The sensitivity of an ionisation-only ($S2$ -only) analysis is governed by how effectively non-signal populations are identified and removed especially in the low-energy regime.¹ Without an accompanying scintillation pulse, the event vertex along the drift direction is unconstrained and the usual $S1/S2$ ER/NR discrimination is unavailable. As a consequence, activity originating at boundaries and near the electrode grids, ordinarily suppressed by fiducialisation or pulse-shape selections, can imitate low-area $S2$ interactions and constitutes a dominant background. A dedicated re-optimisation of event selection is therefore required to suppress such pathologies while preserving acceptance for genuine low-energy bulk scatters. The development and validation of these rejection strategies form a principal objective of this chapter.

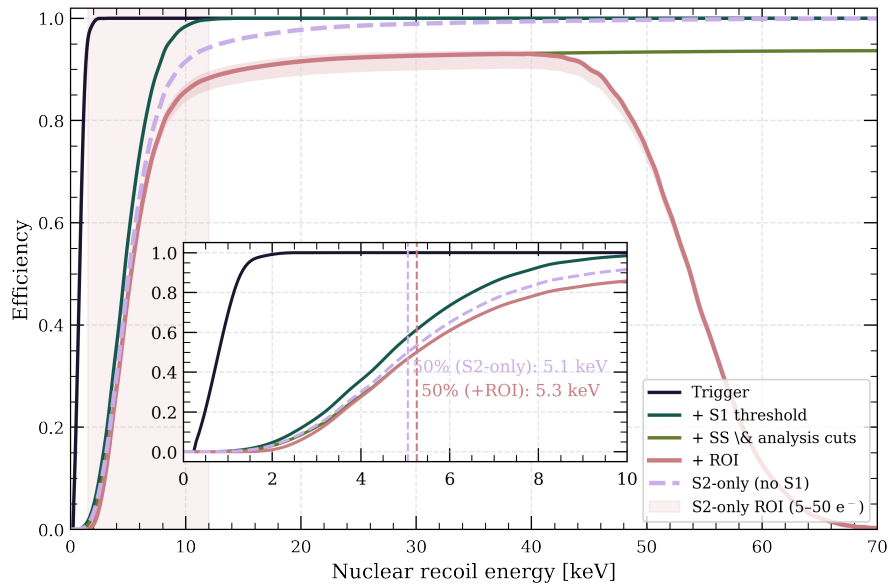


Figure 5.1: Selection efficiency versus nuclear-recoil energy for WS 2022: curves indicate the pure hardware trigger efficiency (black), + $S1$ threshold (green), + single-scatter selection as per the conventional WIMP search & analysis cuts (olive), and finally, + ROI cuts (rose). The $S2$ -only path with no $S1$ requirement is overlaid with preliminary data-quality cuts applied (violet dashed). The shaded region projects the $S2$ -only ROI (5 – 50 electrons, $\sim 300 - 3000$ phd) onto the energy axis. 50% efficiency points for $S2$ -only and +ROI (dashed verticals) are shown in the inset.

During WS 2022, data acquisition employed a digital filter tuned to $S2$ -like waveforms and achieved full efficiency for pulses corresponding to roughly six extracted electrons at a typical 5 Hz trigger rate [36]. In the standard $S1+S2$ WIMP analysis this trigger model was combined with an $S1$ requirement comprising a three-PMT coincidence and a

¹As with most rare-event searches.

per-channel threshold of >3 phd (Fig. 5.1). In the ionisation-only reanalysis presented here, the hardware trigger path and firmware thresholds are unchanged, but the offline $S1$ condition is not imposed. Accordingly, the hardware $S2$ detection efficiency is taken directly from the WS 2022 analysis, while all additional inefficiencies specific to $S2$ -only selection (arising from the absence of an $S1$ pulse and from offline event-quality requirements) are treated separately. The absence of an $S1$ threshold implies that the effective low-energy boundary is determined solely by $S2$ detection. We therefore adopt five extracted electrons (~ 300 phd) as the lower bound of our $S2$ -only region of interest (ROI), corresponding to the point at which the $S2$ trigger reaches (near-)unit efficiency. The upper bound is set at fifty extracted electrons (~ 3000 phd), beyond which the event rate is increasingly dominated by non-bulk populations associated with grid-adjacent and surface activity; in the $S2$ -only context, the loss of $S1$ -based handles permits a fraction of these events to masquerade as legitimate signal-like small- $S2$ interactions (cf. Fig. 5.12). The resulting ROI,

$$\text{S2-only ROI: } \{5, 50\} e^- \quad (5.1)$$

thus balances trigger completeness at threshold against contamination from grid- and surface-related pathologies, optimising acceptance for low-energy scatters in the bulk.

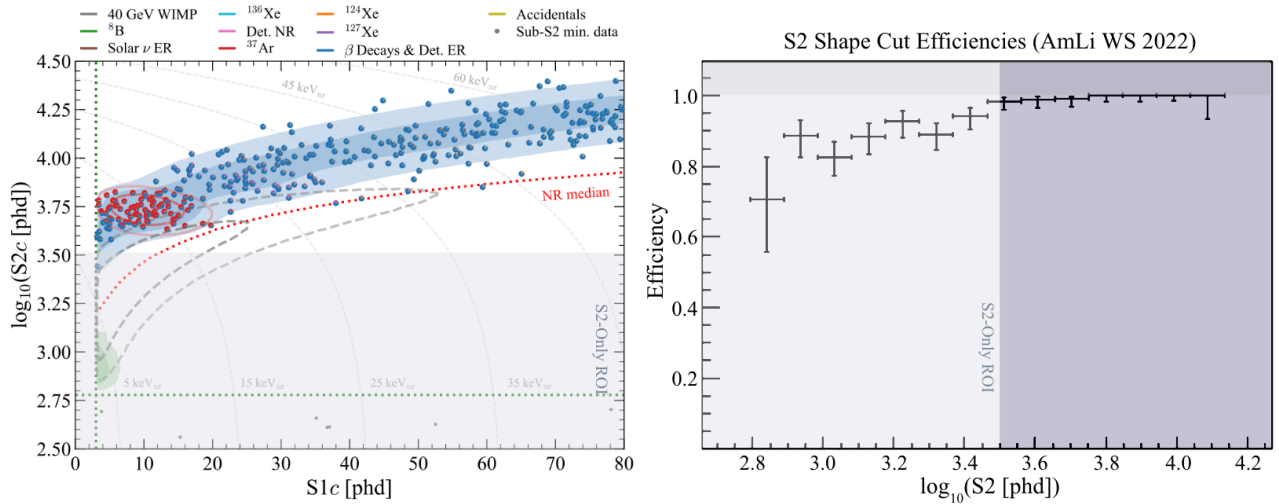


Figure 5.2: $S2$ -only threshold regime: placement of the ROI relative to the SS ($S1+S2$) phase space (**left**), where the ^8B signal contours start to appear, and the corresponding acceptance efficiencies evaluated on AmLi data as a function of corrected pulse area $S2c$ (**right**). Left-hand figure produced and modified using plotting code by A. Biekart.

Maximising sensitivity to low-mass WIMPs thus hinges on precise control of the detector response at the lowest accessible energies, where the standard $S1+S2$ selections lose acceptance and waveform systematics become most consequential (Fig. 5.2). In this threshold regime, small- $S2$ pulse topologies do not resemble simple boxcar-Gaussian smearings of the drift-time distribution: longitudinal diffusion is compounded by position-dependent fields, extraction and EL fluctuations, pile-up and other charge-collection effects, producing asymmetries and non-Gaussian tails in $S2$ morphology². As shown in Fig. 5.1, the lower edge of the $S2$ -only ROI corresponds to sub- keV_{nr} scatters, a

²In the standard $S1+S2$ analyses, pulse-shape selections rely on reduced quantities (AFT width descriptors as introduced in Chapter 3) that perform well at moderate energies. Near threshold, however, small $S2$ s are more sensitive to transport and interface effects so the corresponding RQ distributions broaden and overlap with pathologies (accidentals, gate/cathode emission). In the $S2$ -only context, the loss of $S1$ -based discrimination necessitates bespoke topology-based rejection tuned to this regime, with explicit control of signal acceptance evaluated via calibration data.

background-dominated corner of phase space. Consequently, competitive sensitivity requires a detailed characterisation of the threshold regime and, where needed, S2-only-specific selections. Table 5.1 summarises the final selection and addresses the dominant background contributors in turn, emphasising the additional handles introduced (or retuned) to maintain acceptance for genuine low-energy bulk scatters.

Cut group / name	Brief description (purpose)	Same as WS 2022?
LIVETIME (TEMPORAL VETOES)		
E/ph-train veto	Remove windows after large progenitor activity to suppress SE→S2 and SPE pile-up. For the S2-only search, we lower the threshold area.	R
Muon veto	Exclude periods after OD/skin-tagged muons (afterglow, correlated activity).	Y
Hot-spot veto	Mask flares in SE/S2 rates (grid-emission bursts). The spatial element of this cut has been modified slightly but the temporal cut remains the same.	R
High S1-rate veto	Remove short periods with pathological S1-rate spikes (reduces accidentals).	Y
Sustained-rate veto	Veto intervals with persistently high SPE rates.	Y
Burst-noise veto	Reject events during periods of higher electronics noise.	R
Bad-buffer veto	Discard events without valid pre/post-trigger buffers at the time of an event and an S2.	R
Gate-interval veto	Exclude times with high gate-tagged electron rates; searches for correlated SE/S1 emission within a gate-anode drift time interval of ($\sim 2.5 \mu\text{s}$); this is observed in about 10 – 28% of electron emission events.	N
Excess-area veto	Require summed pre-S2 area < S2 area to catch sustained high pulse rate events not caught by the e/ph-train and muon hold-offs.	R
PHYSICS (EVENT LEVEL)		
S2-only selection	Require at least one S2 and no S1 (defines S2-only class) within a given event window of an S2.	N
S2 window	Enforce timing of the chosen S2 within the full-drift window.	N
Prominent-S2	Select a single prominent S2; suppress merged/multi-scatter patterns.	N
Fiducial radius	Radial stand-off window to reduce high rates from wall leakage (dominated by Rn progeny).	N
Valid (x, y) (MERCURY χ^2)	Cut on quality of position reconstruction (§2.5); rejects glue-ring and wall events (high field region without a direct line-of-sight to PMTs) typically with longer tails and photoionisation shoulders.	Y
Field-cage resistor cut	Remove events consistent with “hot” resistor-chain activity (a very localised spatial cut).	Y
S2 PULSE-SHAPE (MORPHOLOGY)		
Absolute width window	Targets grid radiogenics (from cathode/ gate radioactivity). In principle this is as close to a fiducial z cut as we can get in an S2-only search.	N
Narrow S2	Width-based cut to remove unusually narrow S2s at short drift (near-liquid surface, gas events); designed to target accidental coincidences in the S1+S2 search.	Y
Early-peak	Another width-based cut designed to suppress merged S2s especially near extraction-region where leakage of gas events is not unlikely.	Y
S2 TBA	Top/bottom asymmetry requirement to remove above-anode / EL-region events.	Y

Table 5.1: Summary of selections in the WS 2022 S2-only analysis, grouped by function. “Same as WS 2022?” indicates whether the implementation is unchanged (Y), completely new (N), or retuned without significantly changing cut logic (R) relative to the S1+S2 WIMP search. Exact thresholds and functional forms for these cuts are not given here but will be described for *select cuts* in subsequent sections.

Within the few–tens of electrons characteristic of the S2-only window, the spectrum receives contributions from both electronic- and nuclear-recoil processes. Monoenergetic ER features arise from Auger cascades in activation and

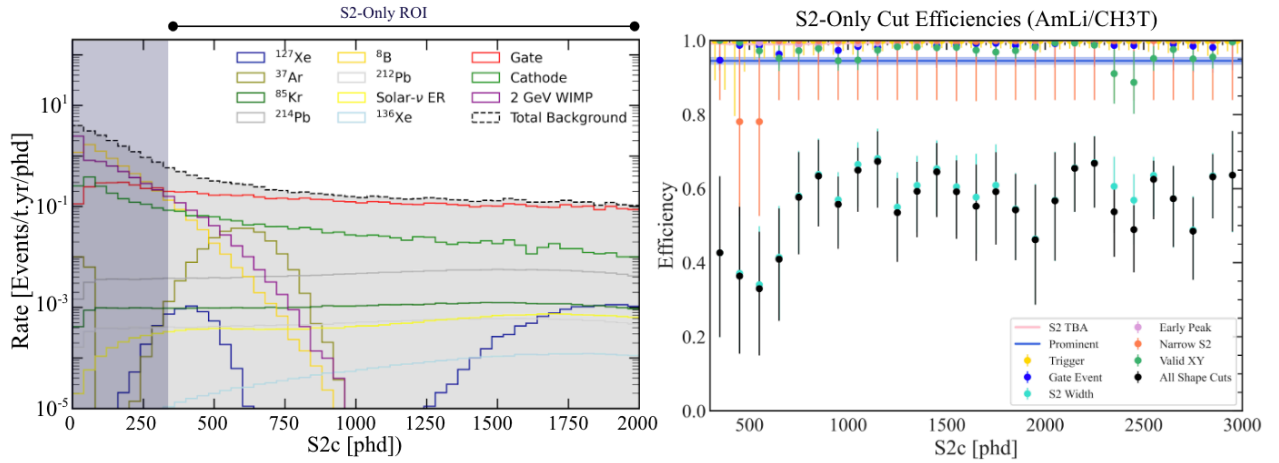


Figure 5.3: Background composition and selection acceptance in the S2-only analysis. **(Left)** Differential rate versus corrected S2 area, showing contributions from grid radiogenics (gate and cathode according to the model in [115], which dominate), various intrinsic ER lines from β decays, solar- ν ER, and a $2\text{ GeV}/c^2$ WIMP template; the dashed curve is the total. The shaded band marks the S2-only ROI. **(Right)** Acceptance of the principal S2-only selections in AmLi/CH₃T calibration data as a function of $S2_c$; coloured points are single-cut efficiencies (e.g. trigger, prominent S2, TBA, width), and black points show the combined “all shape cuts.” Error bars are statistical. The current cut-tunings represent a combined effort towards developing a robust framework to reject pathological backgrounds in an extended S2-only search and hence report only preliminary efficiencies to deliver a proof-of-concept result. Efficiency panel courtesy A. Wang and T. Pershing, background panel reproduced using plotting code from D. Hunt.

trace isotopes (notably ^{37}Ar and ^{127}Xe), while a broad β continuum from radon progeny and ^{85}Kr extends to low energies; after the livetime and topology selections of Table 5.1, these components are sub-dominant in rate in our ROI (Fig. 5.3). Nuclear recoils in LZ predominantly lie above this energy range; the only irreducible NR source proximate to threshold is coherent elastic neutrino–nucleus scattering from solar ^8B . In contrast, near-surface activity associated with the electrode grids (gate and cathode) yields abundant isolated S2s of small area and, in the absence of $S1$ -based constraints, constitutes the dominant background in S2-only data (cf. Fig. 5.3 and Fig. 5.12). These considerations motivate the structure of the remainder of the chapter, where we discuss (i) suppression of *accidental coincidences*, (ii) a data-driven *fiducial radius* to mitigate *wall leakage*, and (iii) rejection of *grid radiogenics* using S2 morphology and associated quality selections.

5.1.1 Accidental Coincidences

Dual-phase xenon TPCs deliver extraordinary sensitivity, yet their many interfaces and subsystems also introduce inhomogeneities that generate isolated light (iS1) and charge (iS2) pulses that are not reliably predictable from first principles (Fig. 5.4). We call accidentals the spurious single-scatter candidates formed when an iS1 and an iS2 from uncorrelated processes occur within one maximum drift time and are mistakenly paired by reconstruction. The composition and rates of iS1/iS2 vary with operating conditions, and near threshold the reconstruction can merge or mislabel pulses, making these backgrounds particularly problematic at low energy - the exact regime of an S2-only search. In practice, several iS2 sources — charge-loss near the wall, delayed electrons after S2s, and interactions near the liquid surface or in gas — preferentially produce small-area S2s with narrow, boxy shapes that are hard to reject without sacrificing genuine events. In this section, we outline how these S2 topologies³ can be selected for to reject a significant

³We do not discuss isolated S1s here as they are not relevant to our analysis but further details on the full range of isolated-pulse sources are discussed in [36, 152, 181].

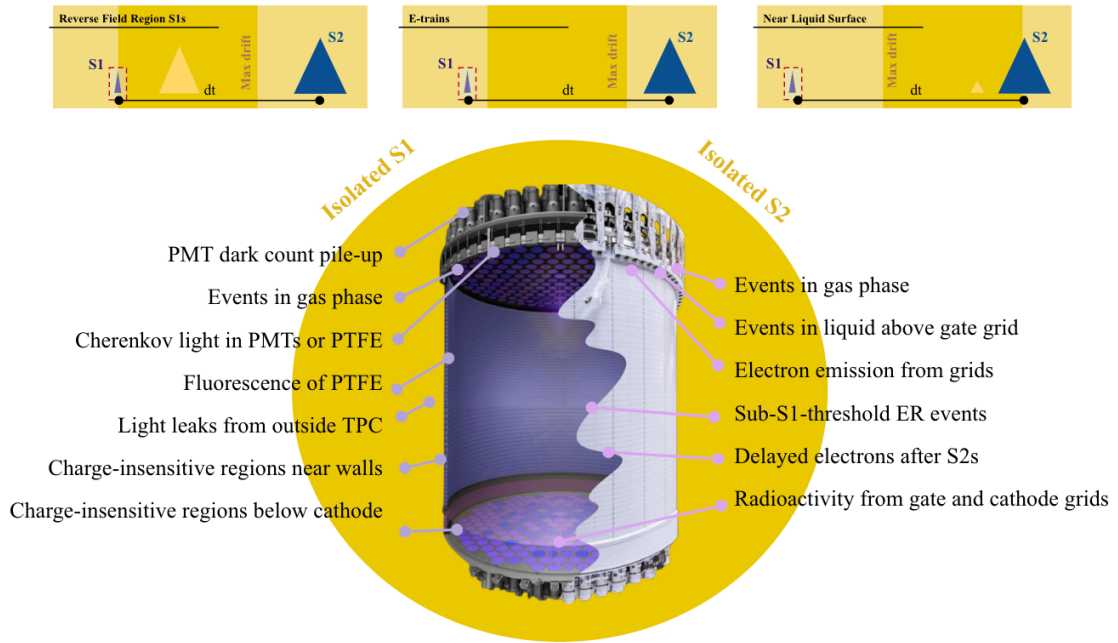


Figure 5.4: Known sources of isolated pulses (iS1/iS2) that can form accidental coincidences. The top cartoons illustrate representative geometries—RFR S1s, electron-train emission, and near-liquid-surface events—whose pairings within one drift length can masquerade as genuine single scatters. Also shown are UDT populations (S1–S2 with drift time $> dt_{max}$), which provide a clean accidental sideband for tuning and diagnostics.

source of isolated S2s known to be present in the WS 2022 dataset.

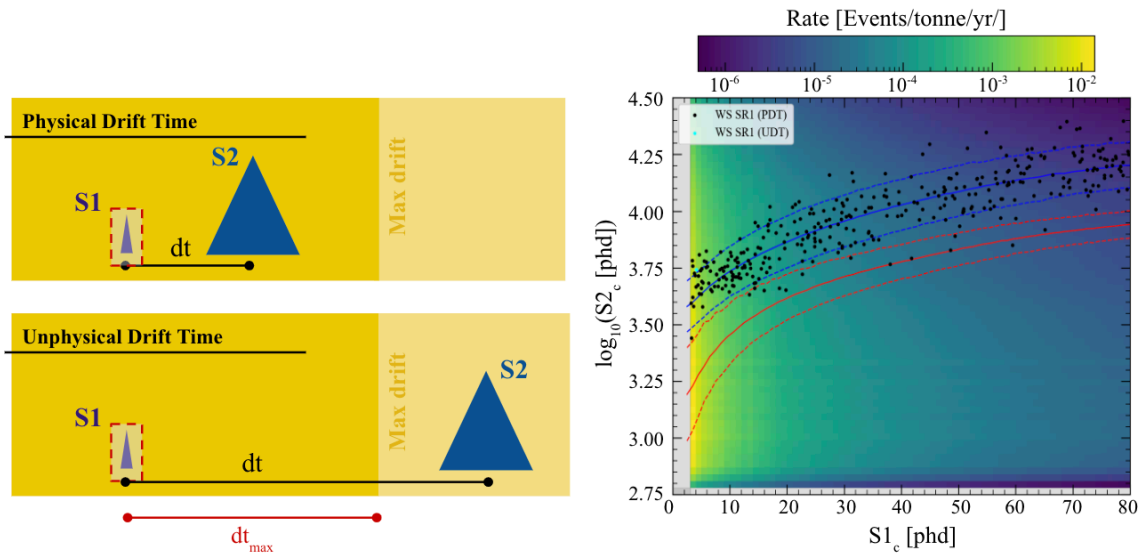


Figure 5.5: (Left) schematic of physical (PDT) vs unphysical (UDT) drift-time pairings used to identify genuine accidentals. (Right) ACS accidentals PDF with UDT/WS data passing all data quality cuts overlaid.

To characterise accidentals we use two complementary, data-driven ingredients established in WS 2022. Fig. 5.5 helps to visualise these. First, unphysical-drift-time (UDT) events, or S1-S2 pairs which otherwise look like legitimate SS

events but with reconstructed drift time longer than the cathode-to-gate maximum ($\sim 951 \mu s$), provide a clean rate anchor because such pairs cannot arise from a single physical interaction. Second, “ChopStitch”-ed accidentals (ACS), constitutes a high-statistics dataset generated by randomly pairing real iS1 and iS2 pulses selected from data, reprocessing the stitched waveforms through the full chain, and constructing a separable 2D PDF in $(S1_c, \log_{10}(S2_c))$ from the 1D S1 and S2 spectra. Consistency tests then show no statistically significant S1–S2 correlation introduced by the chain, and UDT points overlaid on the ACS PDF validate the modeling. This overall expectation is then normalised using the UDT rate and cross-checked against a first-order estimate of the accidentals rate $\Gamma_{acc} \approx \Gamma_{iS1} \Gamma_{iS2} t_{drift}$, with Γ_{iS1} , Γ_{iS2} measured directly from data. Within the WS 2022 ROI, this procedure yields 1.22 ± 0.26 (Fig. 5.6) accidental events (translating to only 0.18 ± 0.04 events [152] within the $\pm 1\sigma$ NR band), and after the pure-S2 shape selections are applied, the rejection efficiency increases to $> 99.6\%$ ⁴.

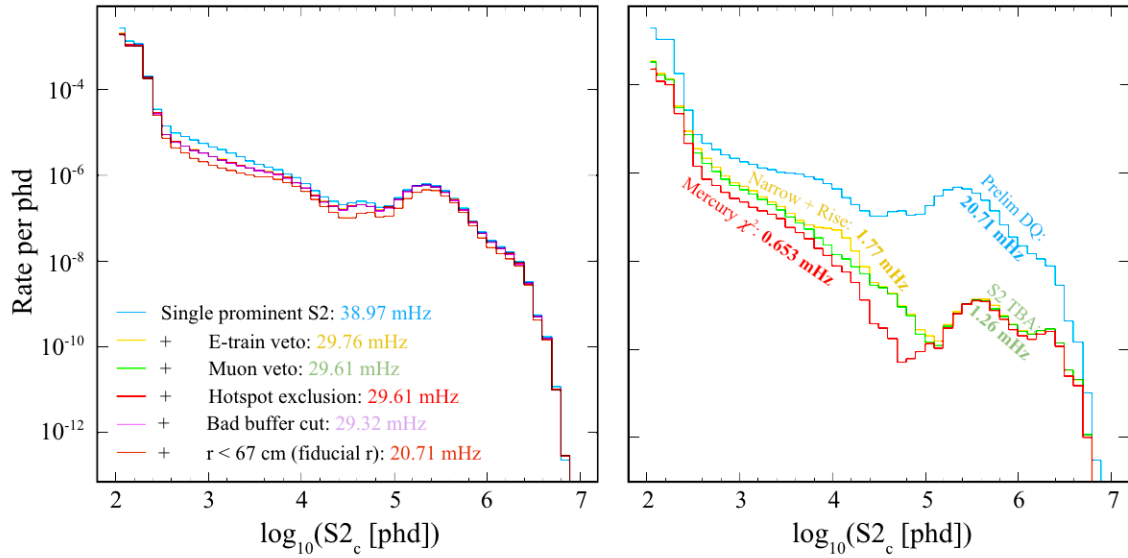


Figure 5.6: (Left) Rate per phd versus $\log_{10}(S2 \text{ [phd]})$ various preliminary data quality cuts. These cuts are not tuned to target the iS2 population and therefore do not have much of an impact on their rates. **(Right)** Impact of S2 shape selections (applied sequentially); the “narrow width” and “rise time” cuts provide the dominant suppression of the residual iS2 background across the full S2 range.

Fig. 5.6 shows two salient features. The iS2 rate is highest at small pulse areas ($\log_{10}(S2_c \text{ [phd]}) \lesssim 3$), consistent with near-surface, gas-adjacent, and delayed-electron topologies. Across the full S2 range, the narrow width and rise time selections provide the dominant suppression of the WS-2022 iS2 background while maintaining high calibration acceptance. These observations show that a morphology-driven strategy is effective at removing a significant proportion of accidental events, despite not having access to any S1-derived RQs.

In the WS 2022 S2-only analysis we therefore apply a two particularly effective S2 shape cuts designed to reject near-liquid-surface pathologies while preserving bulk-like S2s: (i) a narrow-width lower bound versus $\log_{10} S2_c$ and (ii) an early-peak time bound versus $\log_{10} S2_c$ (this is shown to have high degeneracy and performs marginally better in the

⁴Similar methodology has been used for WS 2024 [49] but we only discuss WS 2022-related examples here as we only target this dataset for our S2-only analysis.

low S2 regime than the rise time cut and so replaces it). The waveform archetypes motivating these cuts are thus shown in Fig. 5.7, depicting a near-liquid-surface event in which a small pre-pulse lies within a sub- μs window ahead of the main S2 and is sometimes merged by the pulse finder; originating within a few millimetres of the surface, such events accrue little longitudinal diffusion and thus yield narrow S2s with a steep leading edge. The second waveform shows an S2 with an extended flat-top/shoulder immediately after onset, characteristic of near-extraction/gas topologies where strong electroluminescence photoionises species near the gate/anode (including the glue ring, a region of high electric field deviations and an indirect optical pathway to the PMTs), releasing additional electrons over several microseconds; the sustained injection produces a boxy plateau and a pronounced early peak. These two morphologies are the targets of the narrow width and early peak observables used in the analysis.

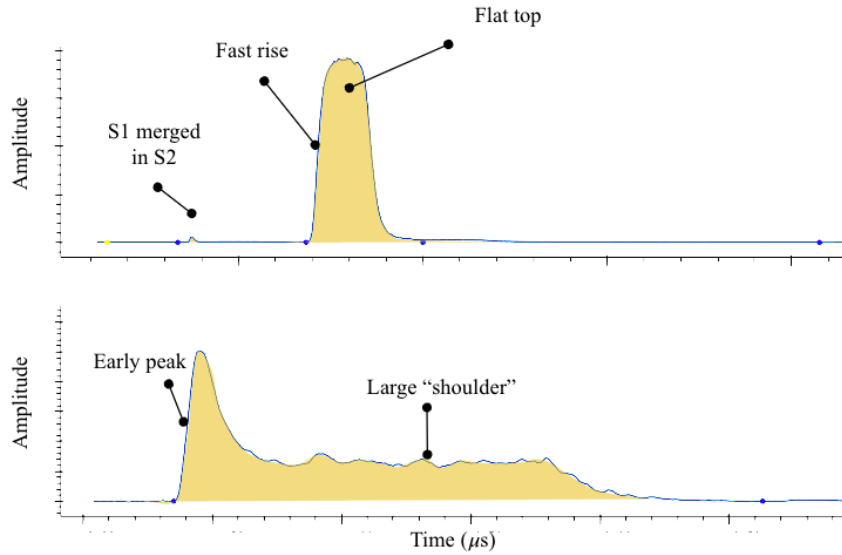


Figure 5.7: Representative S2 morphologies. **(Top)** near-liquid-surface S2 with fast rise and flat top (small S1 merged). **(Bottom)** near-extraction/gas S2 with early peak and extended shoulder—features targeted by the narrow width and early peak cuts.

We adopt RMS width as the S2 shape metric, having the cleanest separation between isolated S2/UDT populations and calibration SS (DD , CH_3T) among the width-like observables tested (AFT intervals, FWHM, RMS pulse widths). After standard data-quality cuts to remove periods with e-trains, grid emission, muon activity, and other noise [36], we scan a lower RMS threshold as a function of $\log_{10}(S2c)$ and build efficiency maps for “good” data and rejection maps for accidentals. The 99% acceptance contours of DD/CH_3T and the $\geq 60\%$ rejection contours of iS2/UDT are then fit with simple lines in RMS , $\log_{10}(S2c)$ space and the contours are subsequently scanned near these boundaries to maximise rejection while preserving acceptance across the full S2 range. This procedure yields the working boundary

$$RMS [ns] > 17 \log_{10}(S2c) + 390 \quad (5.2)$$

with $S2c$ the corrected S2 area; the boundary is visualised by overlaying all datasets in width- $\log_{10}(S2c)$ space and by 2D efficiency heatmaps used to derive it. Independent validation with AmLi shows near-flat, $\approx$ unity acceptance in the WIMP ROI, and most residual low-S2 pulses ($\lesssim 2.5$) that survives the cut sits below the physical S2 threshold and

is outside the S2-only analysis region, so no additional tightening is applied.

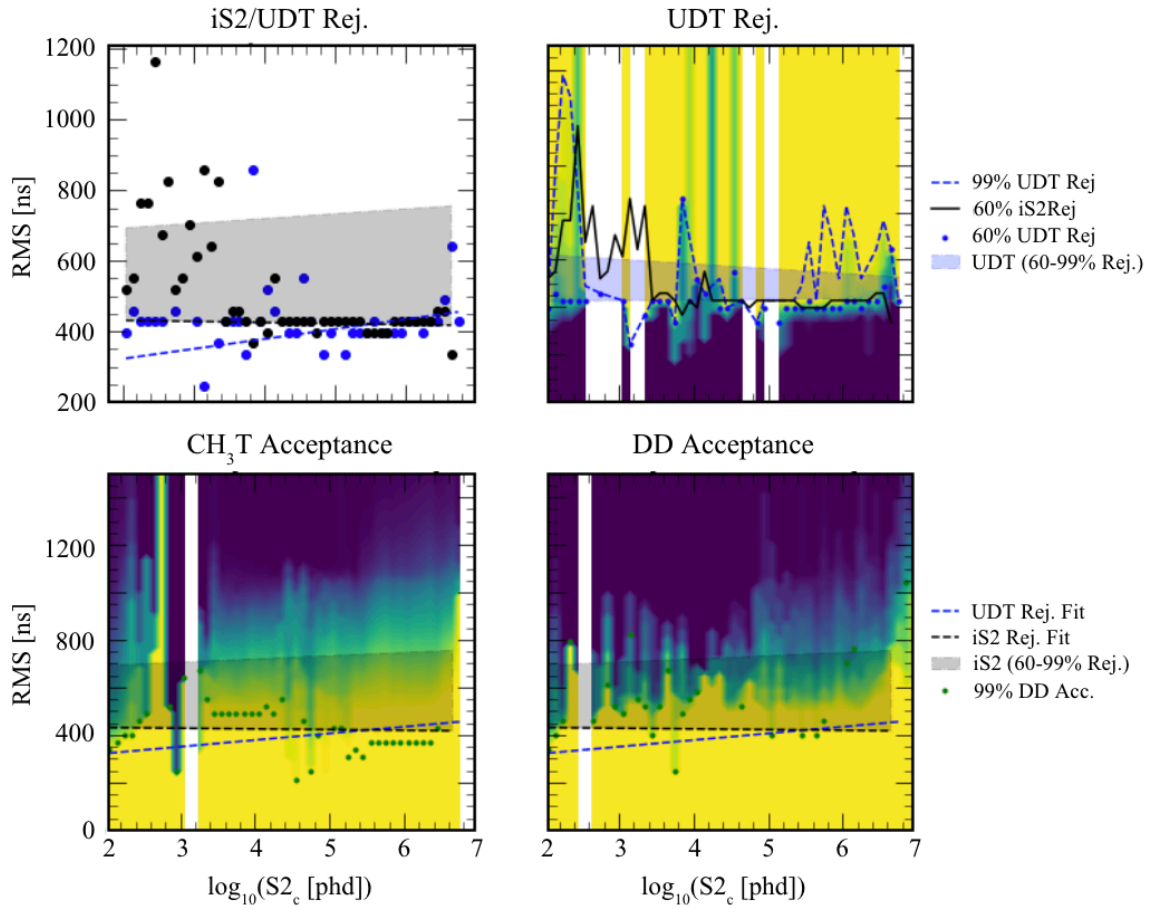


Figure 5.8: Heat maps of efficiencies (yellow = 100%, dark blue = 0%) for varying values of RMS as a function of $\log_{10}(S2_c)$ for the different datasets. Linear fits have been applied to the various acceptance (rejection) contours within the calibration (accidentals) data. There is no required S1 threshold applied to the data.

Using the same envelope-fit procedure as for the width scan, the early peak boundary is then implemented as another area-dependent minimum on the S2 FWHM:

$$FWHM [ns] > 60 \log_{10}(S2_c) + 880, \quad (5.3)$$

which reproduces the performance of the rise-time variant $\{(AFT_{05} - AFT_{01})^5$ Fig. 5.9 shows the AmLi acceptance for both the combined narrow width and early peak selection: acceptance remains essentially flat and near unity across the WIMP ROI, with the dip near $\log_{10}(S2_c) \sim 4.2$ (above the S2 ROI) attributable to limited statistics. Example waveforms also illustrate typical rejected morphologies and a residual borderline case.

With accidental leakage controlled by these S2-shape selections combined with the $S2\ TBA$ cut and the absolute S2 width window (the full S2 shape cut suite described in table 5.1), the leading residual backgrounds in the S2-only

⁵Used as a trio of shape cuts in the main WS 2022 analysis, each more sensitive to its own set of features and working as a sequential set of fine-tuning selections which combined reported a rejection efficiency $> 95\%$ while maintaining near-unity signal acceptance.

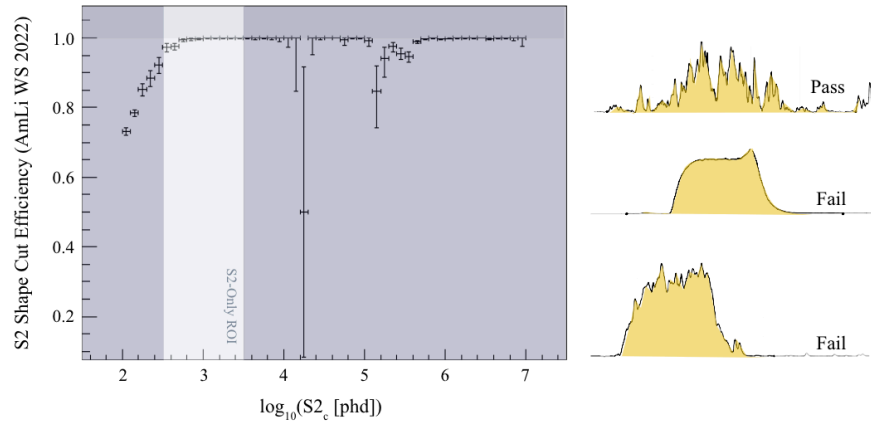


Figure 5.9: AmLi acceptance of the combined S2-shape cuts. Acceptance of the narrow-width + early-peak combined as a function of $\log_{10}(S2_c)$ for WS-2022; the unshaded band marks the S2-only ROI. Acceptance is $\gtrsim 99\%$ across the ROI. **(Right)** example ROI waveforms: top passes (residual accidental-like morphology: these pulses tend to still pass through the shape cuts with visually different morphology to that the cuts were trained to target), middle/bottom fail as intended.

dataset arises from charge-loss near the PTFE wall and related near-surface topologies as well as grid radiogenics. We discuss these in turn in the rest of the chapter.

5.1.2 Wall Events

Defining a fiducial volume is a critical component of background rejection in rare-event searches with TPCs. Radioisotope plate-out on PTFE surfaces and distortions of the electric field at the detector boundary both give rise to populations of events that reconstruct at large cylindrical radius R , which cannot be treated as part of the uniform active volume. In the standard SS analysis, this problem is addressed by defining a fiducial boundary as a function of drift time, $R_{SS}(dt \Leftrightarrow z)$, which follows small geometric and electrostatic variations with depth. In practice this boundary corresponds to approximately $R \simeq 68 \text{ cm}$; if expressed as a static cut, the SS fiducial radius would therefore be a circle (or cylinder) of roughly this radius. Events within this boundary are retained as the fiducial volume for SS analyses.

For an S2-only analysis, the definition of a fiducial radius requires a dedicated treatment. First, S2-only events are intrinsically of lower energy and are more susceptible to reconstruction biases near the TPC wall, where charge transport and extraction are less efficient (§4.2.1). As a result, wall-related backgrounds contribute a larger fraction of the total event rate in this regime and are perhaps a more critical background too. Second, the (x, y) position reconstruction relies exclusively on the distribution of electroluminescence light in the top PMT array. At low S2 areas this reconstruction is prone to broadening due to spurious fields and proximity to PTFE, increasing the risk of charge trapping and signal degradation; this leads to radial smearing and enhanced apparent leakage of wall events into the nominal bulk region. Finally, because the S2-only analysis is designed to remain agnostic with respect to a specific dark matter spatial prior, it is preferable to define the fiducial boundary in a manner that is fully data-driven rather than relying on simulation or extrapolation from the SS analysis.

The S2-only fiducial radius is therefore determined directly from the measured areal event rate as a function of radius. This distribution is modelled as the combination of a flat bulk component and an exponentially rising wall tail, with the transition between the two providing a natural definition of the fiducial boundary. This strategy offers several advantages: it employs the correct Poisson statistics of binned counts, it anchors the cut to features observed directly in the data rather than to simulation, and it produces well-defined confidence intervals that can be propagated into subsequent analyses. The following subsections describe the construction of the likelihood model, the change-point scan used to identify the onset of the exponential rise, the use of bootstrap resampling to obtain confidence bands, the independent determination of the tail-onset radius, and the final conservative choice of fiducial cut adopted for the S2-only analysis.

Likelihood model and change-point fit

The areal event rate as a function of cylindrical radius was modelled using a piecewise parametrisation that captures both the flat bulk distribution and the exponential rise due to wall leakage. The expected rate density is defined as

$$\lambda(R) = B + L \exp\left(\frac{R - R_0}{\lambda_0}\right) \Theta(R - R_0), \quad (5.4)$$

where B is the bulk rate level, L is the amplitude of the exponential rise, λ_0 is the characteristic scale length, and R_0 is the candidate change-point radius. The expected number of events in annulus i , of area A_i , is then $\mu_i = \lambda(R_i)A_i$, and the corresponding likelihood is the product of independent Poisson terms,

$$\mathcal{L}(B, L, \lambda_0; R_0) = \prod_i \frac{\mu_i^{n_i} e^{-\mu_i}}{n_i!}, \quad (5.5)$$

with observed counts n_i . This form correctly accounts for statistical fluctuations even in low-occupancy bins.

A scan over candidate values of R_0 was performed, minimising the negative log-likelihood with respect to (B, L, λ_0) at each point. The optimal change-point R^* was selected using the Akaike Information Criterion (AIC), which balances goodness-of-fit against model complexity. This procedure identified the best-fit transition point as

$$R^* = 50.1 \text{ cm}, \quad (5.6)$$

corresponding to the onset of the exponential rise in the observed distribution.

Bootstrap confidence bands

To assess the stability of the fitted change-point, parametric bootstrap resampling was employed. Pseudo-datasets were generated by drawing Poisson counts from the fitted expectation μ_i , and the full change-point scan was repeated for each realisation. This ensemble provides both an empirical distribution of R^* and a family of fitted radial models. From these resamples, the 68% confidence interval was determined, yielding

$$R^* = 50.1^{+0.3}_{-0.2} \text{ cm}. \quad (5.7)$$

The spread of resampled models was displayed as a shaded band in the radial distribution plot (Fig. 5.11), demonstrating that the inferred changeover is well localized and robust against statistical fluctuations.

To further illustrate both the stability and impact of the change-point determination, Fig. 5.10 summarises three complementary diagnostics. Panel (a) shows the cumulative retained fraction of events as a function of radial cut, which makes explicit the exposure trade-off as the boundary moves inward. Panel (b) displays the bootstrap distribution of R^* obtained by refitting pseudo-datasets drawn from the best-fit model; the narrow spread confirms that the inferred change-over is statistically well localised. Panel (c) shows pull residuals versus radius, demonstrating that the piecewise “bulk+exponential” model describes the data at the Poisson level across the bulk, with coherent deviations only where the wall tail turns on.

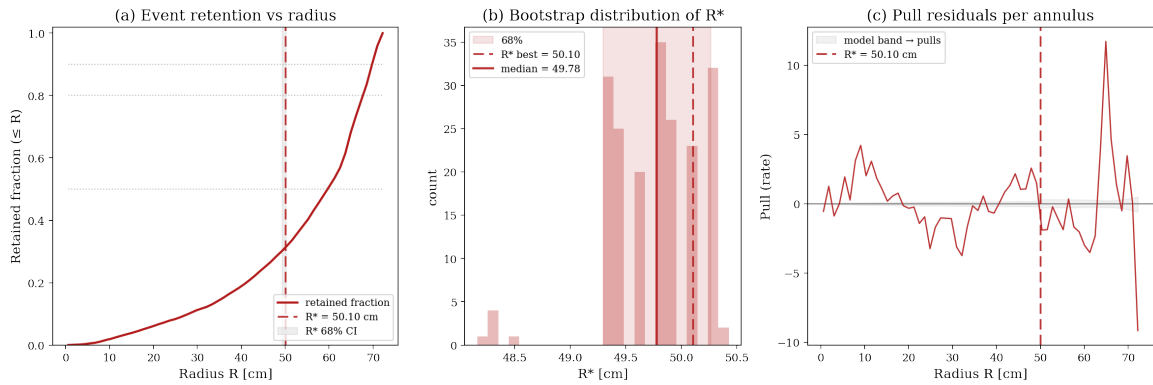


Figure 5.10: Diagnostics for the S2-only fiducial boundary. (a) Fraction of events retained by a radial cut at R in the sideband tuning dataset; vertical lines/bands mark R_{tail} and their 68% intervals, and the adopted R_{cut} . (b) Bootstrap distribution of the change-point R^* with median and best-fit values; the 68% central interval is shaded. (c) Pull residuals of the piecewise “bulk+exponential” model versus radius.

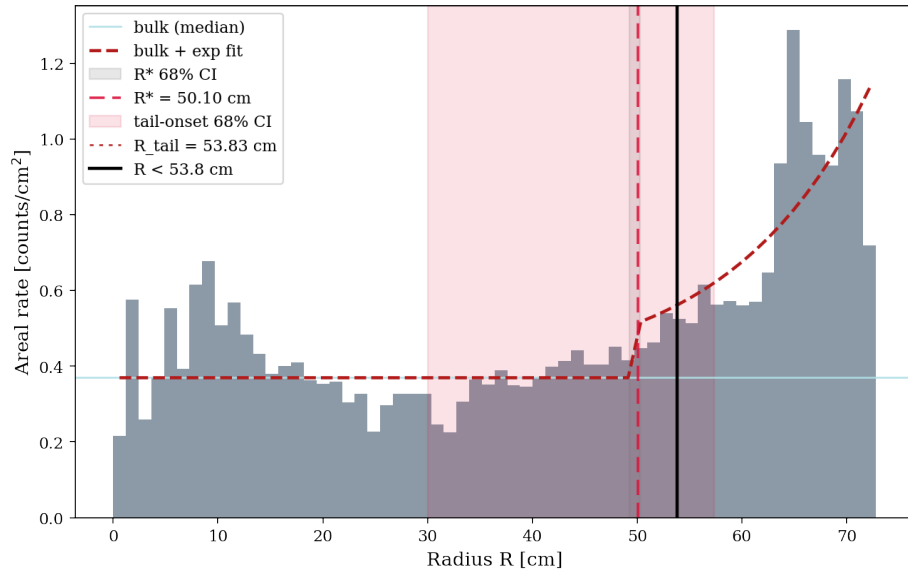
Independent tail-onset method

As an orthogonal validation, an “outer” radial region ($30 \leq R \leq 65$ cm) was fitted independently with the exponential form above, anchored to a fixed baseline. From this fit, a tail-onset radius R_{tail} was defined as the point at which the rate exceeded the bulk level by $\sim 1.5 \sigma$. This criterion ensures that the threshold is determined relative to the statistical uncertainty on the bulk estimate, rather than from the exponential slope alone, and also validates the solution is consistent with the change-point band shown in figures 5.11 and 5.10.

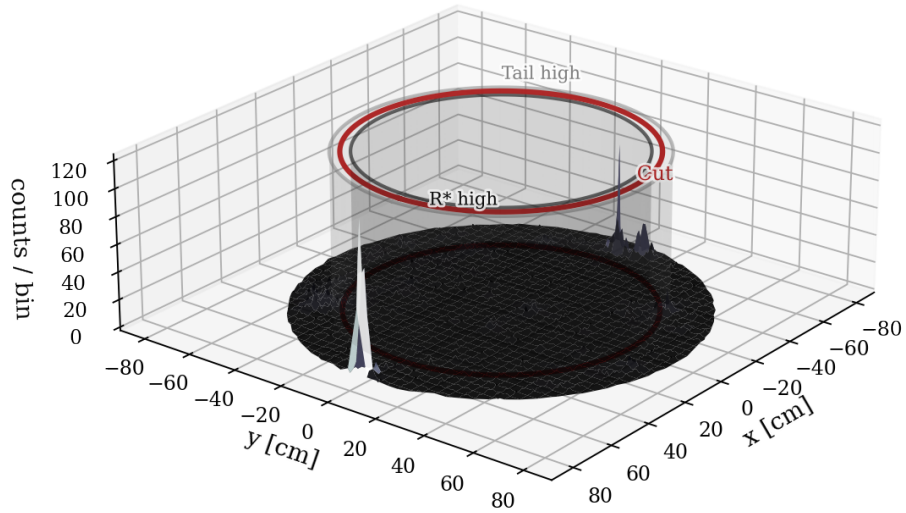
The procedure yields

$$R_{tail} = 53.8^{+3.4}_{-8.3} \text{ cm}, \quad (5.8)$$

with uncertainties propagated through parametric resampling of the fitted parameters. While broader than the profile-likelihood interval for R^* , this estimate provides a conservative bound beyond which wall leakage is unambiguously dominant.



(a) Areal event rate as a function of reconstructed radius. A piecewise bulk+exponential fit (red dashed) is applied to identify the onset of wall leakage. The bulk plateau is shown as a cyan line, with shaded bands indicating the 68% confidence intervals for the inferred change-point radius R^* (grey) and the exponential tail onset (light red). The final fiducial cut is placed at $R_{cut} = 53.8 \text{ cm}$ (black vertical line), just beyond the exponential onset radius R_{tail} .



(b) Three-dimensional view of the reconstructed (x, y) event density, with hollow cylindrical shells overlaid to illustrate the fitted bands. The dark band marks the inferred R^* interval, the lighter shell indicates the tail-onset region, and the crimson wire ring shows the final radial cut. This representation highlights how the fitted confidence intervals translate into geometric rejection in the detector volume, ensuring that the maximal possible “uniform” bulk region is retained. The elevated event rates near $\phi \simeq 0$ coincides with the resistor chain location and a region of known elevated surface activity, indicating a physical azimuthal asymmetry.

Figure 5.11: Radial wall-event rejection in the S2-only analysis.

Final fiducial cut definition

The two approaches are deliberately complementary: the change-point likelihood identifies the statistical transition from bulk to wall-dominated behaviour, while the tail-onset criterion defines a conservative boundary relative to the bulk level. To ensure robustness, the final S2-only fiducial radius was defined as $R_{cut} = \max(R^*, R_{tail})$. For this dataset, the resulting value was

$$R_{cut} \approx 54 \text{ cm}. \quad (5.9)$$

This choice ensures that wall-related backgrounds are strongly suppressed while retaining the majority of the uniform bulk volume. This more conservative boundary then retains 38.1% of S2-only events⁶ (Fig. 5.10a), while suppressing the wall population visible beyond $\sim 50 \text{ cm}$ (figures 5.10c, 5.11a,b). Taken together, these results demonstrate that the likelihood-based method provides a rigorous data-driven definition of the fiducial boundary for the S2-only analysis.

5.1.3 Grid Radiogenics

The electrode grids represent a persistent near-surface background in dual-phase xenon TPCs. Radon progeny plating onto the gate and cathode wires establishes long-lived ^{210}Pb contamination in secular equilibrium with its $^{210}\text{Bi}/^{210}\text{Po}$ daughters, producing continuous α/β activity on the electrode surfaces (see chapter 3). In a conventional S1+S2 (SS) analysis these populations are efficiently tagged and rejected: the paired signals provide a direct depth coordinate via drift time (discussed extensively in §4.6.3), revealing clear clustering at the detector boundaries, with further distinct signatures in their occupancy of $\log_{10}(S2) - \log_{10}(S1)$ visualised in Fig. 5.12 and S1 TBA space (§4.4.2). Indeed, the efficiency of these variables also underpins the background identification used in Chapters 3 and 4; without them, the detailed mapping of charge transport and field non-uniformities would not have been possible.

For an S2-only analysis, however, these handles are absent. Any emission with an undetected or suppressed S1 is indistinguishable from a genuine low-energy bulk event unless residual differences in the S2 pulse itself can be exploited. Microphysics considerations suggest such differences should exist. The strong field gradients in the vicinity of grid wires suppress recombination, favouring charge-only signatures with non-Gaussian shapes or longer tails. Near the gate, the short drift paths and reduced diffusion are expected to yield narrower S2 widths; near the cathode, the distorted reverse-field region and extended drift can broaden the S2 beyond that expected from bulk events. Yet, in practice these distinctions are not clean. Calibration data show that the width distributions of gate, cathode, and bulk events overlap substantially, with the tails from grid radiogenics blending into the continuum of bulk single scatters. The effect is exacerbated at higher drift fields, where diffusion is reduced and the separation between populations is subsequently further diminished. Thus, while the physics provides a qualitative picture of where grid events should appear, their quantitative discrimination requires a careful, data-driven treatment very different from that used in a conventional S1+S2 search.

For this reason, an S2 width-based metric, is used as the primary observable in a challenging regime where there is no S1 and hence, no drift time variable to be exploited. Fig. 5.13 demonstrates that an area-independent, static cut would work well for this purpose⁷. The aim is simple: by defining a width window, removing events below

⁶Note that this acceptance rate increases when further preliminary data quality-based cuts are applied to remove other types of backgrounds too, justifying the seemingly high rejection rate.

⁷In fact, comparison of background rejection vs signal acceptance efficiencies using an area-dynamic cut shows marginal differences and therefore the simpler static cut is chosen, much like that used in the XENON1T [118] analysis.

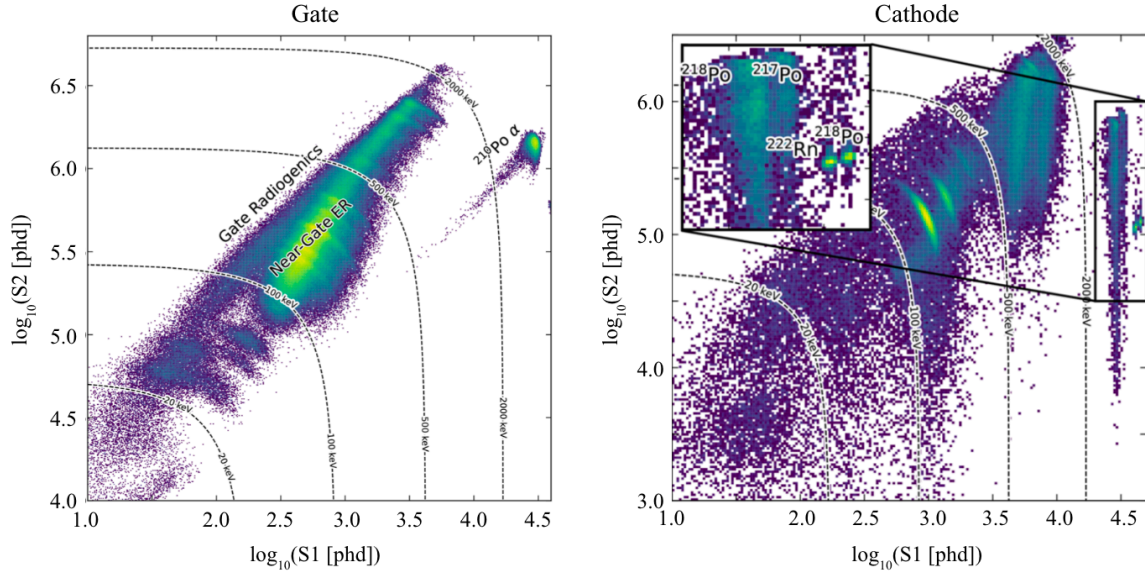


Figure 5.12: Grid radiogenics visible in $\log_{10}(S2)-\log_{10}(S1)$ space, near the gate (**left**) and near the cathode (**right**). Dashed curves indicate empirical ER energy contours. In SS data these populations are cleanly tagged using a combination of S1 and S2-based cuts. Near the gate, a broad near-gate ER band sits above the bulk ER locus due to suppressed recombination in the high-field wire region, while a compact $^{210}\text{Po } \alpha$ cluster appears at large S1 and S2. In comparison, the reverse-field region and wire geometry lead to partial charge collection for cathode-adjacent interactions, producing a low- $S2$ tail at fixed S1. In $S2$ -only, those handles are absent and the same populations can leak into the signal region masquerading as signal-like events. Figure courtesy: D. Hunt.

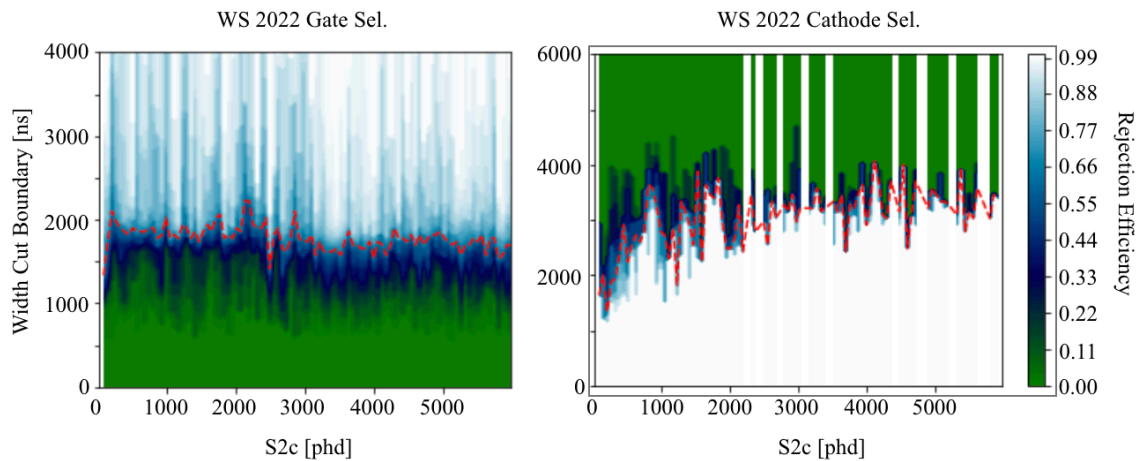


Figure 5.13: Cut boundary scan showing the rejection efficiency of selected populations of tagged gate (**left**) and cathode (**right**) events in the chosen subset of WS 2022 data used for tuning cuts. The 90% rejection efficiency boundary is shown for both populations in the cut boundary- $S2c$ area parameter space. This motivates a broadly flat/ static width cut.

a lower bound (gate-like) and above an upper bound (cathode-like), we try to suppress as large a fraction of grid backgrounds as possible while maintaining a high signal-like event acceptance rate. This strategy parallels the wall-event treatment in §5.1.2: it is anchored to data, exploits only observables available in the S2-only regime, and allows uncertainties in the cut placement to be propagated directly to the sensitivity calculation. In the following, we detail the optimisation of this width window and quantify the achievable rejection of gate and cathode backgrounds in WS 2022, critical in an S2-only analysis.

Defining the training dataset

To tune a static width cut for an ionisation-only selection, we use calibration data to define signal-like and background-like populations, then optimise two boundaries in width–depth space. We first choose a width observable with strong, monotonic depth dependence; throughout we adopt $AFT\ 90 - AFT\ 10$, which “most cleanly” increases with drift time across the inspected calibration datasets. In reality, any of the symmetric AFT width definitions explored in the context of diffusion measurements in chapter 3 would have worked well, however it was found that $AFT\ 90 - AFT\ 10$ spanned a greater range of widths whilst maintaining a similar “collimation” in its mean width’s evolution with drift time. This is explicitly shown in Fig. 5.14 for the AmLi dataset.

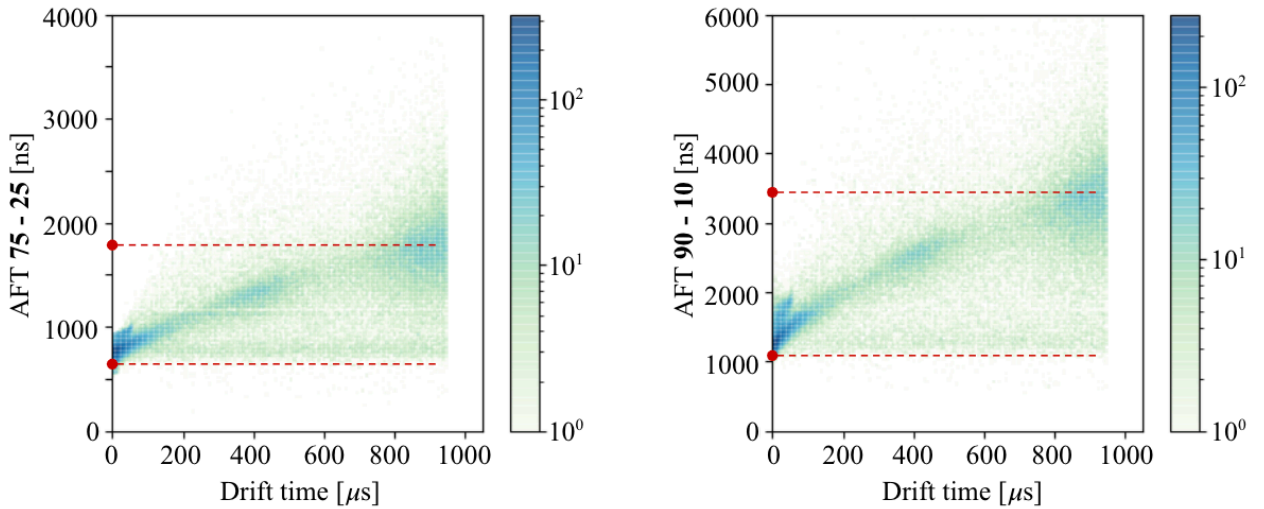


Figure 5.14: Comparison of two S2 width observables versus drift time in AmLi calibration data; $AFT75 - 25$ (left) and $AFT90 - 10$ (right). Both metrics show a clear monotonic dependence on depth, but the latter spans a wider dynamic range of widths without compromising on its $\Delta AFT(dt)$ band width. Since it captures a larger fraction of the S2 pulse - including sensitivity to the tails - this metric may provide marginally clearer separation and may enhance background rejection while preserving high signal acceptance. For this reason, $AFT90 - 10$ is chosen for the width cut optimisation.

To avoid imprinting spatial or energy biases on the tuning, we rely on a combination of AmLi and CH₃T data. AmLi provides high statistics with broad coverage in z (albeit deployed in discrete azimuthal patches near the wall via the CSD tubes [75]), while CH₃T, LZ’s lowest-energy injected source, anchors pulse-shape behaviour in the few-electron regime with a much more uniform distribution; with a low rate in the S2 ROI ($3 - 50\ e^-$), it complements rather than dominates the optimisation. Before scanning cut boundaries, events are re-weighted to be uniform in $(r, dt, S2\ area)$,

matching the spatial and spectral expectations for a dark-matter signal and removing any residual geometric/reconstruction non-uniformities in the calibrations that could otherwise bias the tuning. This “flat-fielding” process can be visualised in Fig. 5.15. Background templates are drawn from the same datasets using drift-time–tagged gate and cathode populations. The lower width bound is primarily tuned to reject gate events (narrower widths at small dt), while the upper bound controls cathode leakage (broader widths at large dt due to diffusion). We then maximise a background-dominated sensitivity metric over the [lower, upper] plane to obtain the final cut.

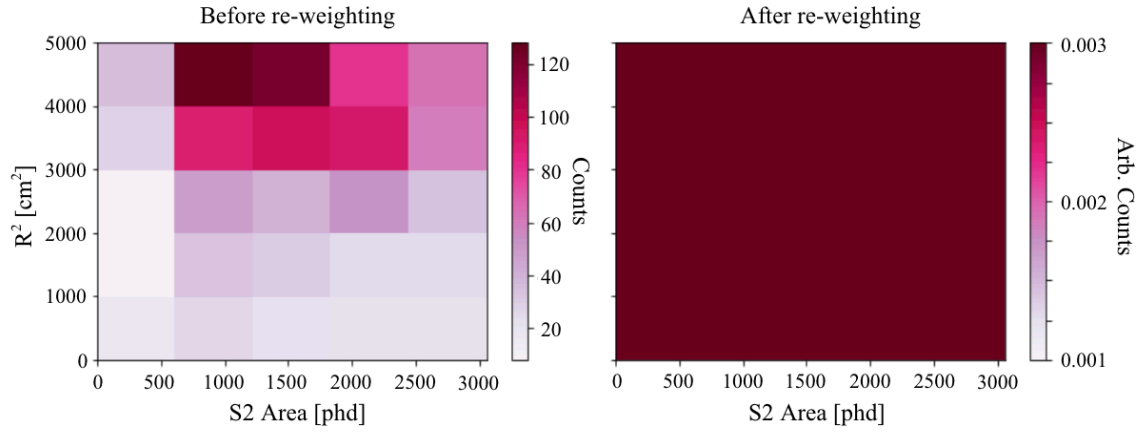


Figure 5.15: Illustration of the event re-weighting procedure, shown here in two dimensions for clarity. **(Left)** the raw event distribution in $(R^2, S2 \text{ area})$ space; **(Right)** the same distribution after applying weights $w = 1/(N_{\text{events in bin}} \times N_{\text{bins}})$. The full procedure is in fact applied in three dimensions $(R^2, S2 \text{ area}, dt)$ prior to cut tuning to remove geometric and spectral biases in the optimisation of the width cut.

Choosing a Signal:Background metric

As this chapter is intended as a proof-of-concept of S2-only performance based on the first WIMP-search dataset, we employ a simple cut-and-count approach to derive a conservative upper bound on sensitivity. To make this optimisation meaningful, the signal–background metric is selected to mirror the counting significance and to guide the placement of width cuts toward the best expected limit.

In a Poisson counting experiment with expected signal s and background b , the principled objective for cut optimisation is the profile-likelihood (Asimov) median discovery significance [62]

$$Z_A = \sqrt{2 \left[(s + b) \ln \left(1 + \frac{s}{b} \right) - s \right]}, \quad (5.10)$$

which follows from the asymptotics of the likelihood-ratio test. In the background-dominated regime ($s \ll b$) with well-constrained b , Z_A reduces to the familiar proxy $S/\sqrt{B}$; hence $S/\sqrt{B}$ is an excellent stand-in for our scan, selecting virtually the same working region as Z_A ⁸. This is explicitly shown in Fig. 5.16, where a direct comparison of this metric and the Asimov significance shows $\leq 3\%$ deviation in the background-dominated regime ($s/b \leq 0.2$), confirming that the proxy is statistically consistent for our use case.

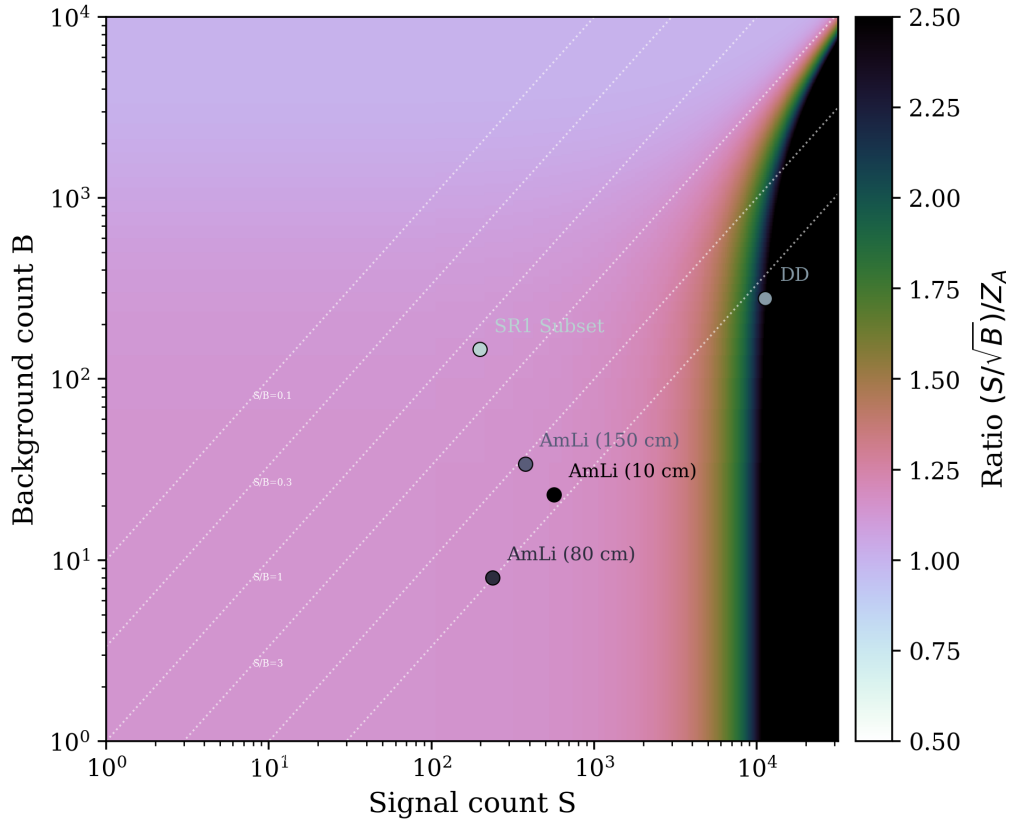


Figure 5.16: Agreement between the small-signal proxy $S/\sqrt{B}$ and the Asimov median discovery significance Z_A across expected signal S and background B . The heatmap shows the ratio $(S/\sqrt{B})/Z_A$; markers indicate post-preselection counts for AmLi (deployed from three positions 10/ 80/ 150 cm), the WS 2022 subset used for tuning, and one DD dataset used to evaluate cut efficiencies. In the background-dominated wedge relevant for the WIMP search ($s/b \leq 0.2$), the deviation is small: $\max | \frac{S/\sqrt{B}}{Z_A} - 1 | \approx 3.2\%$ (mean $\sim 0.6\%$). Larger ratios in the NR calibration samples reflect their signal-dominated nature ($s/b \gg 1$), where $S/\sqrt{B}$ overestimates the true significance.

For completeness, we also consider the widely used discovery/limit-neutral figure of merit that does not assume a specific s : the Punzi figure of merit [182],

$$Z_{\text{Punzi}} = \frac{\varepsilon_s}{a/2 + \sqrt{b}}, \quad (5.11)$$

with ε_s the signal efficiency and a the target discovery threshold (e.g. $a = 3$, i.e. 3σ). Since ε_s and the choice of a set the overall scale, we use Punzi primarily as a *ranking* cross-check rather than an absolute significance. In our application we expect $s \ll b$, for which $S/\sqrt{B}$ is well motivated and closely tracks the Asimov significance; we therefore adopt $S/\sqrt{B}$ as the primary optimisation metric. For completeness we also compare to $S/\sqrt{S+B}$, which becomes relevant only when S is not small compared to B . This last quantity must be used with caution: when tuning on calibration samples that are intentionally signal-rich, optimising $S/\sqrt{S+B}$ can favour looser cuts that appear to perform better on those samples but do not translate to the truly background-dominated WIMP-search dataset, where $S/\sqrt{B}$ remains the more robust choice.

⁸If background systematics (captured by an uncertainty σ_b) are non-negligible, the corresponding Asimov expression penalises this. A full treatment amends Z_A to include a nuisance constraint in the likelihood; a common conservative approximation is $Z \approx s/\sqrt{b + \sigma_b^2}$.

Cut Optimisation

After re-weighting the training samples, we apply a final “conditioning” step that encodes the expected relative occurrence of gate vs. cathode backgrounds. This step is physics-driven: the model combines (i) intrinsic activities of ^{218}Po , ^{214}Pb , ^{214}Bi and ^{214}Po ; (ii) detailed grid geometry (pitch/diameter) and surface roughness, which impact energy reconstruction and pulse topology, especially for small S2s; and (iii) spatial variations of the EL yield, light-collection efficiency (LCE), and extraction efficiency near the electrodes [115]. The model has been validated across multiple datasets⁹, and we use it to align our selection with realistic background composition. The result is an estimate of the *expected* rate of gate contamination relative to the cathode background using time-normalised S2-only width spectra. This is shown in Fig. 5.17, with an explicit calculation of the per-bin gate-to-cathode rate ratio $r_i = R_i^{\text{gate}} / R_i^{\text{cathode}}$ with Poisson uncertainties calculated from effective counts.

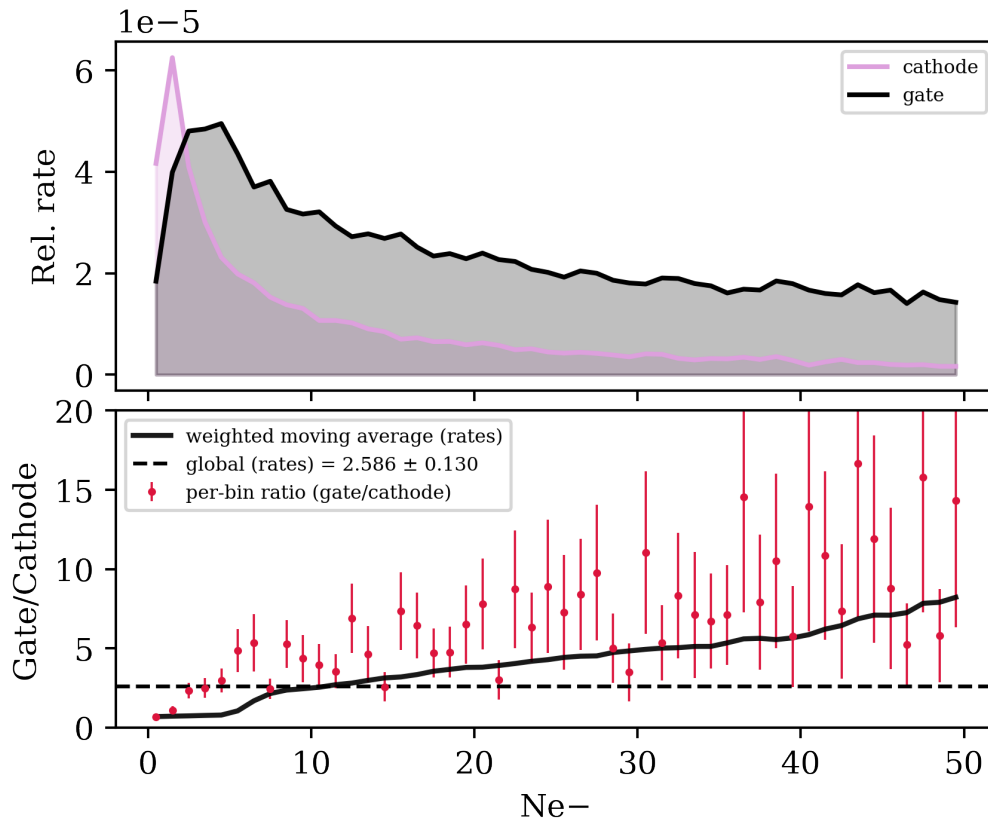


Figure 5.17: Gate vs. cathode rate model. (Top) time-normalised S2-only size spectra (gate: black; cathode: plum). (Bottom) per-bin gate/cathode rate ratio with Poisson errors (red) and weighted moving average (black); the dashed line shows the global rate ratio κ_{rate} . The rising tail indicates stronger gate contamination at large N_{e-} and guides the choice of S2-width cut to prioritize gate rejection.

For a first-pass weighting scheme, we summarise the overall “imbalance” by the global rate ratio

$$\kappa_{\text{rate}} = \frac{\sum_i R_i^{\text{gate}}}{\sum_i R_i^{\text{cathode}}}, \quad (5.12)$$

⁹A dedicated paper by R. Linehan is in revision.

and use a weighted moving average of r_i to visualise trends as a function of Ne^- . The S2 width cut is then tuned to preferentially suppress gate events while controlling cathode loss, by minimising κ_{rate} or, equivalently, maximising the chosen weighted significance Z with $B_\alpha = \alpha G + C$ to penalise gate events more strongly when desired.

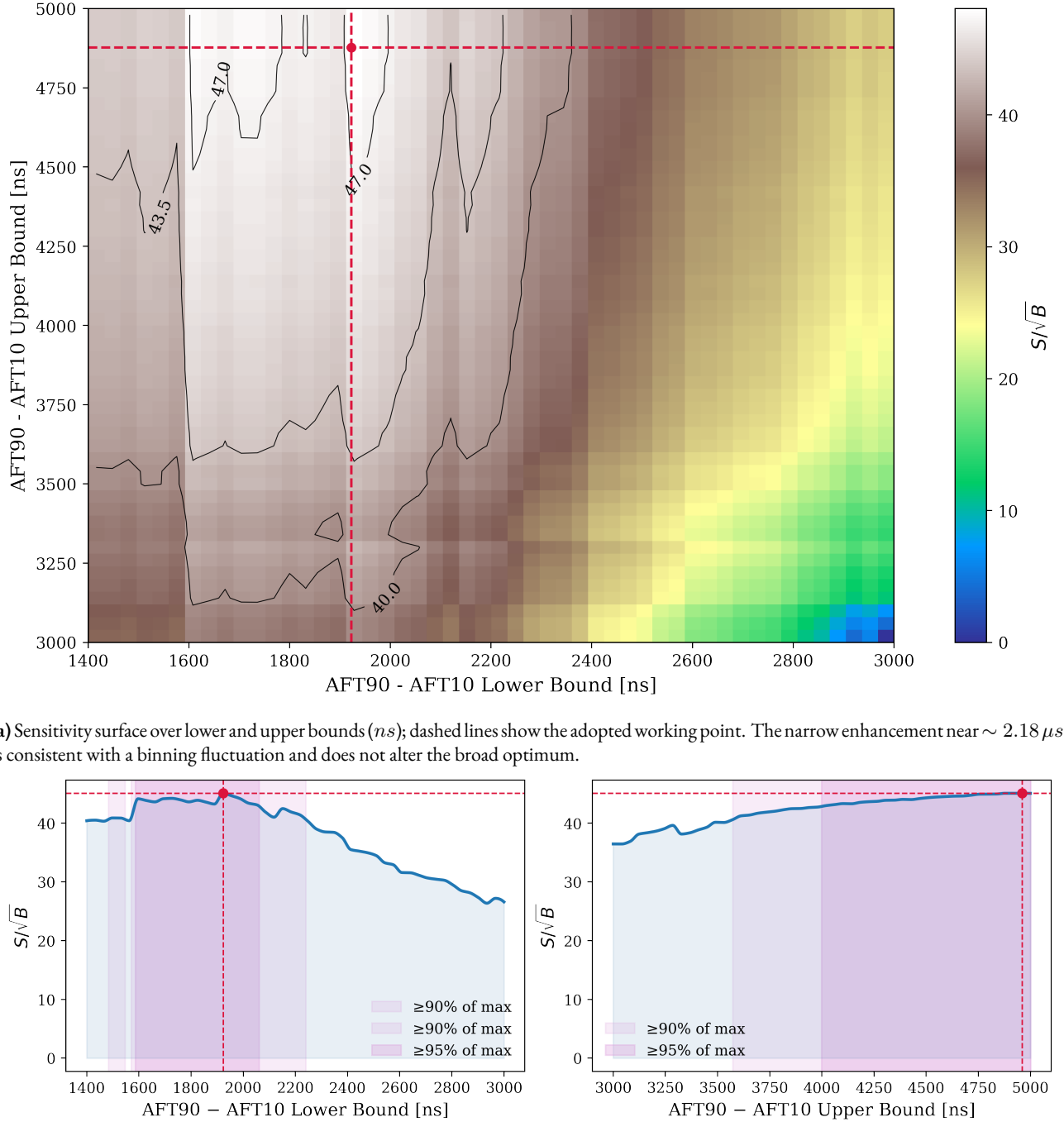


Figure 5.18: Optimisation of static S2-width bounds using $AFT\ 90 - AFT\ 10$ and the metric $S/\sqrt{B}$ with a gate-cathode priority factor $\alpha/\beta = 2.586$. Varying this weighting between 2 – 8 (as per the weighted average ratio span in Fig. 5.17) does not affect the lower bound optimisation but can shift the upper bound up to $\sim 5000 ns$.

Fig. 5.18 shows the optimisation surface for the width window $[w_{lo}, w_{hi}]$ using the gate-cathode priority factor $\alpha/\beta = 2.586$. The maximum in $S/\sqrt{B}$ is not sharply localised: there is a broad plateau in which many neighbouring choices deliver essentially the same sensitivity. As expected, the *lower bound* is driven by gate leakage and exhibits a gentle maximum centred near $w_{lo} \sim 1.9 \mu s$; a narrow spike around $2.18 \mu s$ coincides with a bin of very low background and is treated as a binning artefact rather than a physically meaningful optimum. The *upper bound* mainly controls cathode leakage and is comparatively flat for $w_{hi} \gtrsim 3.3 \mu s$, with only a mild rise toward the edge of the scan. Varying the gate–cathode priority within 2–8 leaves the preferred *lower* boundary essentially unchanged and shifts the *upper* boundary modestly upward, consistent with the picture that gate dominates the narrow-width region while cathode populates the diffusion tail.

Given the breadth of the plateau, the final choice is a balance between conservatively protecting signal acceptance and being stricter against background leakage. We therefore place the cut near the centre of the high-sensitivity region,

$$1900 < (AFT_{90} - AFT_{10}) < 4880 \text{ ns} \quad (5.13)$$

which is stable with respect to small variations in the weighting and binning and sits within the $\gtrsim 90\%$ – $\gtrsim 95\%$ of maximum $S/\sqrt{B}$ bands visible in the 1D slices. As discussed previously, for completeness and as an extra validation, we also scan the $S/\sqrt{S+B}$ proxy, which becomes relevant in regimes where S is not small compared to B . As anticipated for our signal-rich calibration samples, this metric prefers a more permissive lower bound and yields an optimum at $[1265, 4959]$ ns being looser on gate rejection while leaving the upper bound effectively unchanged. Finally, because the Punzi figure of merit depends on the efficiency normalisation and on the chosen discovery threshold a , we use it only as a *ranking* cross-check rather than an absolute significance. Across the full (w_{lo}, w_{hi}) scan the Spearman rank correlation between Punzi and $S/\sqrt{B}$ is $\rho = 0.982$, indicating near-identical ordering. A Punzi-style optimisation would therefore select essentially the same width window, and we retain $S/\sqrt{B}$ as the primary objective (validated against Z_A).

5.2 Results from a Preliminary Ionisation-Only Search

Having defined the background-rejection strategy, we translate the surviving event count into a statistical limit. For this demonstration we adopt a simple cut-and-count framework: for a given signal model and an S2-only region of interest, we generate toy Monte Carlo realisations of the expected number of signal events under different trial cross-sections, including the impact of systematic variations. Each toy represents a possible experimental outcome assuming that particular cross-section, and the fraction of toys yielding fewer events than the observed count after all selections taken from the unblinded WS 2022 dataset within the S2-only ROI, defines the corresponding p –value. Scanning this p –value as a function of cross-section identifies the point at which the model would produce outcomes less probable than 10% of toys, from which we derive the 90% confidence-level upper limit. We thus use a left-tail test (deficit of events): $p = Pr(N_{toy} \leq N_{obs} | \sigma)$, with the ROI and selections fixed *a-priori*; the 90% CL upper limit is then obtained by interpolating the first crossing $p(\sigma) = 0.10$ in $\log(\sigma)$.

5.2.1 A Spin-Independent S2-Only Upper Limit

Fig. 5.19 presents a preliminary 90% CL upper limit on spin-independent (SI) WIMP-nucleon scattering obtained with an S2-only analysis of a subset of LZ WS 2022 data (proof-of-concept). Using data from the unblinded dataset of $0.1199 \pm 0.0010 \text{ t} \cdot \text{yr}$ ($43.82 \pm 0.36 \text{ t} \cdot \text{d}$) and scaling to the full WS 2022 exposure, the best reach occurs near $m_\chi \approx 17 \text{ GeV}$ with $\sigma^{90} \approx 9.97 \times 10^{-45} \text{ cm}^2$. The limit is derived with the cut-and-count framework described above, using toy-based left-tail p -values and a fixed, *a-priori* ROI; no formal background model is fitted and systematic variations enter only via the toy smearing. As expected for this first pass, based on limited exposure

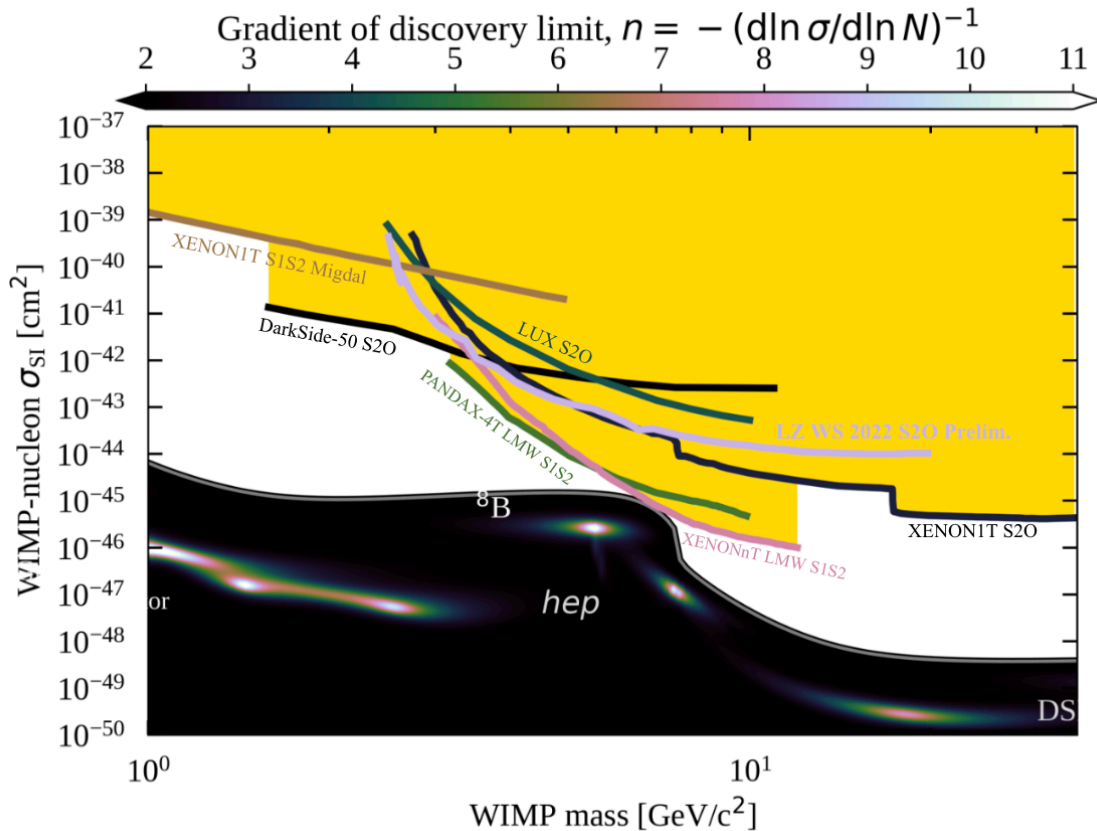


Figure 5.19: 90% C.L. limit on spin-independent WIMP-nucleon scattering set by a proof-of-concept ionisation-only analysis using data from a subset of LZ’s first science run, WS 2022, scaled up to the full projected exposure for this dataset (lilac line). Results from other recent experiments either competitive in the same parameter space or featuring S2-only searches of their own are shown, including S2-only analyses from LUX [46] (green) and DarkSide-50 (black) [183], and XENON1T [118] (also including a Migdal search). Recent results from PandaX-4T (lightgreen) [38] and XENONnT (pink) [59] have also been included, due to their proximity to the neutrino fog, with the heatmap [61] showing sensitivity.

and baseline, hand-tuned selections, the curve is not yet competitive with the best published results, but it already tracks the envelope of existing S2-only constraints across the few-*GeV* mass range and demonstrates a solid baseline for LZ even with conservative selections. We do not quote an “expected” sensitivity band at this stage, as no background model has been fitted; the current toy studies capture only signal-model systematics. However, with full-dataset tuning, explicit modeling of background components (e.g., accidentals, gate/cathode radiogenics, and solar ^8B), a consistent uncertainty treatment, and multivariate rejection (e.g., BDTs based on width/shape variables used in this study), a profile likelihood ratio analysis is expected to yield significantly improved sensitivity—especially in low-field data (WS

2024) where gate-cathode separation is enhanced (Fig. 5.20).

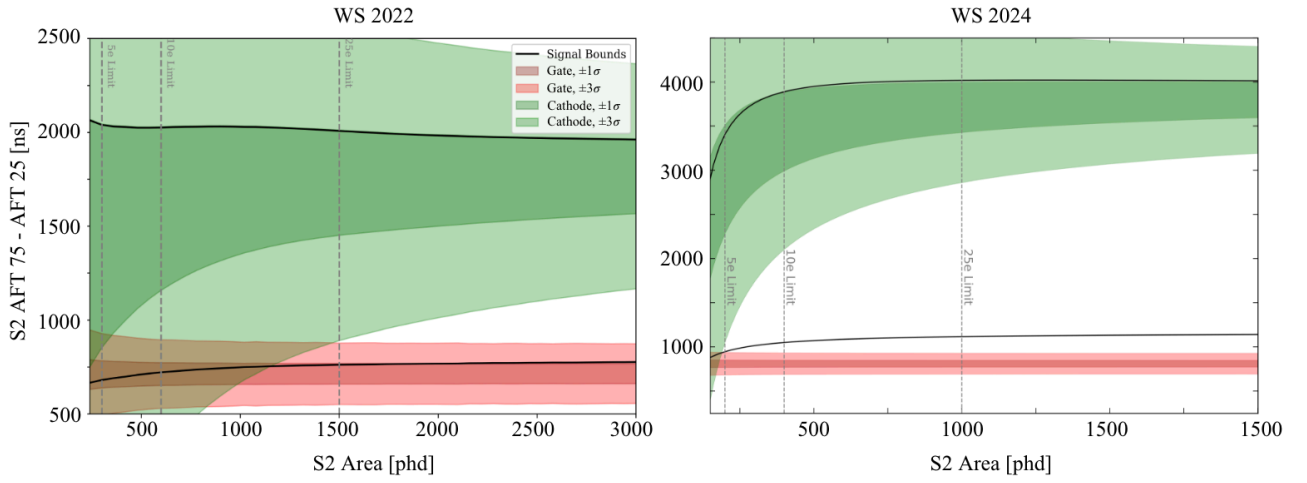


Figure 5.20: Separation of gate (red) and cathode (green) activity from bulk events (the region of interest for the signal search) is tightly coupled to the operating drift field. Although standard S1+S2 analyses often use ~ 300 V/cm to minimise ER leakage into the NR band, the lower-field regime of WS 2024 (**right**) yields improved discrimination between our principal pathological background and bulk, signal-like events seen in calibration data for an S2-only search.

The present curve should therefore be interpreted as a conservative baseline that validates the S2-only analysis framework and motivates the forthcoming likelihood-based result. A dedicated S2-only group is actively developing the key components outlined above. To ensure statistical rigour and avoid bias, the current unblinded WS 2022 subset used for cut tuning will be frozen and used solely as a training/tuning sample. Final limits and sensitivity estimates will be performed only on a statistically disjoint evaluation sample comprising the remainder of WS 2022 and the full WS 2024 exposure. Multivariate methods will be trained exclusively on the tuning sample (with cross-validation), and all model hyper-parameters will be fixed *a-priori* before evaluation on the hold-out dataset. The upcoming full S2-only analysis presents unique challenges, but with LZ's demonstrated capabilities, the parallel efforts on a solar 8B analysis, and the proof-of-concept result presented in this study, the outlook for ionisation-only searches is very promising.

“The man who moves a mountain begins by carrying away small stones.”

— Confucius

Part IV

Pathways to Next-Generation Detectors

6

Design of the XLZD Fieldcage & Skin

Contents

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6.1 Introduction

THROUGHOUT THE PRECEDING CHAPTERS, we have shown that dual-phase xenon time projection chambers function as light/charge cameras, capturing, in just a few microseconds, the entire chronology of a particle interaction. The detector’s electric fields control every step: the drift field is intimately connected to the electron transit time (and z -position); the extraction and electroluminescence fields define the S2 size and uniformity; and the field strength between the electrodes (particularly in the forward field region) governs the local recombination probability, linking detector response directly to xenon microphysics. Field quality therefore is key, underpinning position reconstruction, energy calibration, electron-/nuclear-recoil discrimination, and ultimately the discovery reach of any rare-event search.

The current generation of detectors has pushed each frontier in turn. LZ, with 7 t of active liquid xenon target (~ 5.5 t fiducial), now sets the world’s most stringent limit on spin-independent WIMP scattering with $\sigma_{SI}^{90\%} = 2.2 \times 10^{-48} \text{ cm}^2$ at a WIMP mass of 40 GeV/c^2 after a 4.2 ty exposure [49]. XENONnT and PandaX-4T have looked instead toward the low-energy horizon, registering the first ^8B solar-neutrino recoils through coherent elastic neutrino–nucleus scattering ($\text{CE}\nu\text{NS}$) at 2.7σ [59] significance and thus stepping squarely into the “neutrino fog” that will one day bound every WIMP search. Each result is, in its own way, a declaration of maturity for the dual-phase xenon technique, and an invitation to think bigger.

XLZD unifies the hardware expertise and data-analysis experience of the LZ and XENONnT collaborations to build the next logical step: the largest dual phase TPC-based detector to date, with 60 *t* or 80 *t* of active LXe [53]. A drift field of 300 V/cm optimises NR acceptance against accidentals rejection/ ER background discrimination, while an extraction field of at least $\gtrsim 3 \text{ kV cm}^{-1}$ secures $> 97\%$ charge extraction¹. The baseline instrument is projected to reach a 3σ discovery sensitivity of $\sigma^{SI} \approx 3 \times 10^{-49} \text{ cm}^2$ at 40 GeV/ c^2 after a 500 *ty* exposure [53], effectively touching the neutrino floor in the traditional high-mass WIMP corridor.

In its 80 *t* configuration, XLZD will also contain some 5.3 *t* of natural ^{136}Xe , enough to chase neutrinoless double- β decay well beyond today's frontier. KamLAND-Zen's combined limit of $T_{1/2}^{0\nu} > 3.8 \times 10^{26} \text{ yr}$ sets the benchmark [184]; XLZD aims two orders of magnitude higher, with projected exclusion exceeding 10^{28} yr within ten calendar years [53, 185], which could help to settle the very nature of the neutrino (Dirac or Majorana). Sub-*keV* (including “S2-only”) thresholds further extend the physics reach to sub-*GeV* dark-sector particles, solar axions, ALPs (axion-like particles), low-energy *pp* neutrinos, and even core-collapse supernova neutrinos [186].

Realising this physics program requires two advances in tandem: increased target mass and reduced backgrounds. As *CEνNS* increases inexorably with target size, every other background (krypton, radon, surface radioactivity) must fall correspondingly [187]. XLZD therefore inherits and amplifies not only hardware but also the ultra-clean construction protocols, radon-reduced facilities, and continuous purification techniques refined in LZ and XENONnT. The choice of veto configuration is a central part of this optimisation, with current-generation detectors demonstrating contrasting design priorities.

The remainder of this chapter documents the UK-based contributions that transform these ambitions into engineering reality. §6.2 quantifies the electric-field constraints driving grid geometry, high-voltage design, and extraction efficiency. §6.3 follows these requirements into the cryostat and skin-veto layout, where mechanical, thermal, and background-rejection considerations converge. §6.4 concludes with an outlook on ongoing R&D highlighting how the combined LZ & XENONnT expertise will deliver a detector whose ultimate sensitivity is limited only by nature itself.

6.2 The Design Specifications

In this section, design specifications are outlined drawing directly on the operational experience of LZ, complemented by insights from the preceding chapters of this thesis. Together, they update and extend literature benchmarks, quantifying the electric-field requirements and design tolerances that govern the performance of large dual-phase TPCs. These specifications serve not only to frame the underlying physics constraints — from discrimination and breakdown limits to extraction and grid stability — but also to inform one preliminary XLZD design concept, deliberately modelled on the proven success of the LZ field cage architecture.

¹To be discussed further in §6.2.

6.2.1 ER/NR Discrimination-Motivated Constraints on Drift Field

The leakage of electronic recoils into the nuclear recoil signal region remains a benchmark figure of merit for xenon TPCs, encapsulating how well backgrounds can be rejected, across experiments. It can be approximated as the gaussian tail

$$L = \frac{1}{2} \operatorname{erfc} \left(\frac{\Delta\mu}{\sqrt{2}\sigma_{ER}} \right), \quad (6.1)$$

where $\Delta\mu$ is the ER-NR median separation in the $\log_{10}(S2) - S1$ space (or for a parameter space representing $\log_{10}(S2/S1)$) and σ_{ER} is the width of the ER band. Leakage, or the occurrence of ER events which fluctuate downward into the NR band, thus reflects *both* the *mean separation* (drift-field dependent) and the *band width* (driven by photon and electron statistics). Three detector-level quantities dominate:

- Drift field E

Increasing the drift field suppresses ER recombination, increasing ER S2 and reducing ER S1, while NR yields remain comparatively field-insensitive. This increases $\Delta\mu$ up to a point, but at very high fields the ER S1 becomes photon starved, broadening σ_{ER} . At very low fields, ER and NR bands converge, reducing $\Delta\mu$. The net effect is a non-monotonic or u-shaped dependence of leakage on field, with a reasonably broad plateau at a few-hundred V/cm [97, 188, 189].

- Light-collection efficiency g_1

This sets the number of emitted photons per S1. The fractional S1 noise scales as

$$\frac{\sigma_{S1}}{S1} \sim \frac{1}{\sqrt{g_1 N_\gamma}}, \quad (6.2)$$

such that a larger g_1 narrows the ER width without altering $\Delta\mu$. As leakage lives in the tail of the error function, even modest improvements in g_1 can exponentially suppress leakage [188]. High g_1 is particularly important at high fields where S_1 is intrinsically small; however, there is of course an anti-correlation between S_1 and S_2 for any same-energy interactions.

- Extraction efficiency p_{ext}

The extraction efficiency (g_2 per unit SE gain) is the probability that a drift electron is extracted from the liquid surface into the gas phase in a dual phase TPC. Sub-unity extraction introduces binomial fluctuations in S2, with relative variance

$$\frac{\sigma_{S2}^2}{S2^2} \sim \frac{1 - p_{ext}}{p_{ext} N_e}. \quad (6.3)$$

This broadens the ER band in $\log_{10}(S2/S1)$ without improving separation. Raising p_{ext} therefore reduces leakage steeply up to $\sim 95\%$, after which the gain saturates.

Putting these together, a practical first-order response-level width model is

$$\sigma_{ER}^2 = \underbrace{\frac{A}{g_1}}_{\text{S1 photon statistics}} + \underbrace{\frac{B}{p_{ext}} \frac{1 - p_{ext}}{p_{ext}}}_{\text{extraction binomial (S2)}} + C, \quad (6.4)$$

with $\Delta\mu(E)$ encoding the field-driven separation.

To validate this approximation, we turn to literature.

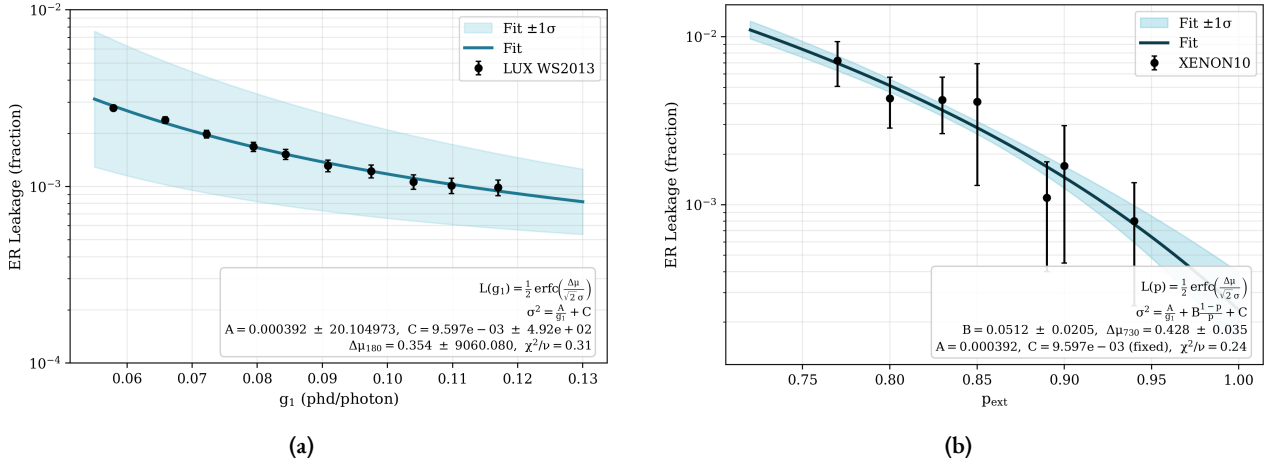


Figure 6.1: ER leakage fraction as a function of (a) light-collection efficiency (proxy) g_1 (LUX WS 2013) and (b) extraction efficiency p_{ext} (XENON 10). Shaded bands show the 1σ confidence intervals of the fits. Both dependencies confirm the expected scalings: leakage in these datasets fall approximately exponentially with g_1 reflecting narrowing S1 statistics, and decreases non-linearly with p_{ext} consistent with the expected binomial variance. These single-variable fits are used to constrain the response model applied to the full field-dependent dataset.

- **g_1 scan (LUX WS 2013, $E = 180$ V/cm, $p_{\text{ext}} = 0.54$).**

We fit

$$L(g_1) = \frac{1}{2} \operatorname{erfc}\left(\frac{\Delta\mu_{180}}{\sqrt{2}\sqrt{A/g_1 + C}}\right), \quad (6.5)$$

to the dedicated leakage-vs- g_1 scan [188] (Fig. 6.1). The description is good ($\chi^2/\nu = 0.31$ for 7 dof) and captures the expected monotonic, convex decrease with g_1 . Although A , C , and $\Delta\mu$ are partially degenerate, the trend is unambiguous: increasing g_1 narrows the ER band ($\sigma_{\text{ER}} \propto 1/\sqrt{g_1}$), raises $\Delta\mu/\sigma_{\text{ER}}$, and exponentially suppresses L .

- **Extraction scan (XENON10, $E = 730$ V/cm, $g_1 = 0.073$).**

With A and C fixed from the g_1 fit, we model

$$L(p_{\text{ext}}) = \frac{1}{2} \operatorname{erfc}\left(\frac{\Delta\mu_{730}}{\sqrt{2}\sqrt{A/g_{1,\text{fix}} + B(1-p_{\text{ext}})/p_{\text{ext}} + C}}\right), \quad (6.6)$$

obtaining $B = 0.051 \pm 0.021$ and $\Delta\mu_{730} = 0.428 \pm 0.035$ PE with $\chi^2/\nu = 0.24$ for 5 dof [190].

The dependence is strongly non-linear: leakage improves rapidly as p_{ext} rises from ~ 0.8 to ~ 0.95 and then saturates as $p_{\text{ext}} \rightarrow 1$, consistent with the $(1 - p_{\text{ext}})/p_{\text{ext}}$ term.

These single-axis fits confirm the scalings $\sigma_{\text{ER}} \propto 1/\sqrt{g_1}$ and $\sigma_{\text{ER}} \propto \sqrt{(1-p)/p}$. Once $g_1 \gtrsim 0.11$ and $p_{\text{ext}} \gtrsim 0.90 - 0.95$, leakage is primarily determined by $\Delta\mu(E)$. Cross-experiment comparisons then reveal a broad “plateau” around $90 - 360$ V/cm [36, 83, 188] exactly as predicted within NEST [97]. This motivates the joint response fit model we use in this section

$$L(E, g_1, p_{\text{ext}}) = \frac{1}{2} \operatorname{erfc}\left(\frac{\Delta\mu(E)}{\sqrt{2}\sqrt{A/g_1 + B(1-p_{\text{ext}})/p_{\text{ext}} + C}}\right), \quad (6.7)$$

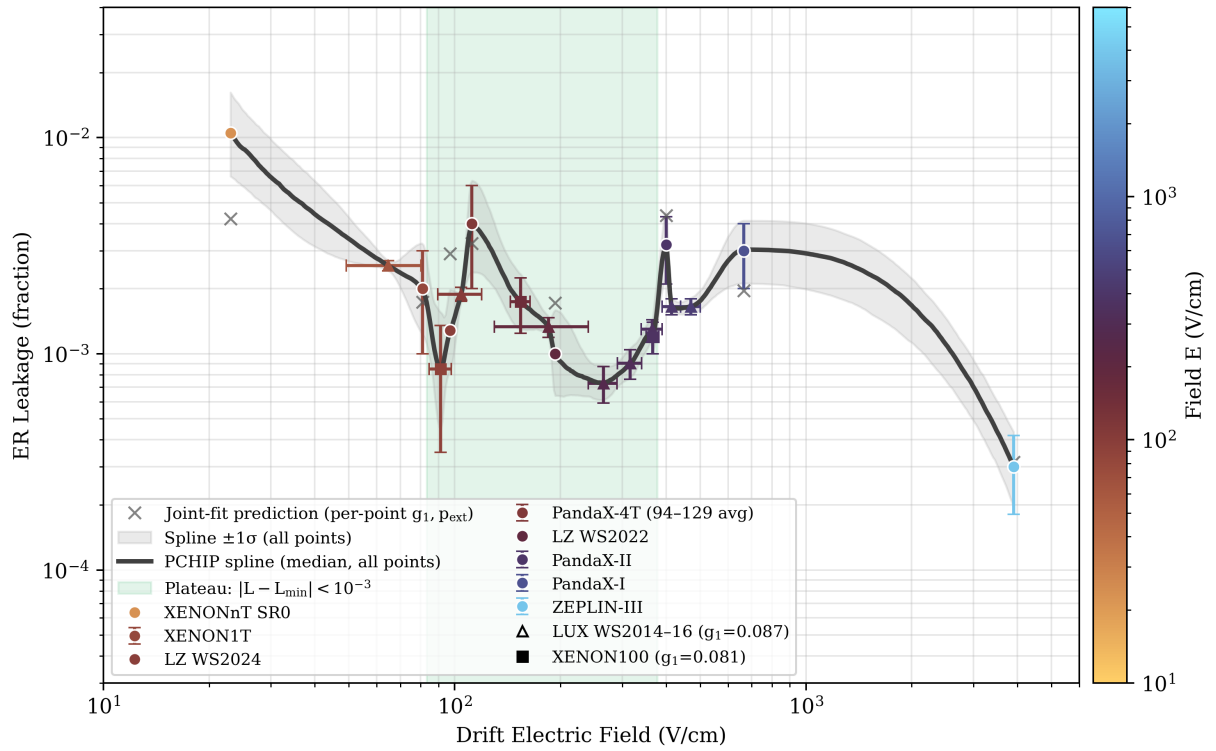


Figure 6.2: ER leakage fraction versus drift field, combining literature points and LZ data. Markers (with errors) are colour-coded by experiment (legend); uncertainties are shown where available in literature, the LZ WS 2024 point is based on a preliminary calculation using simulated data as described in §4.6.3 (this should be interpreted as a ballpark estimate). The black curve is a non-parametric PCHIP spline through *all* points; the grey band is its 1σ interval from MC resampling of the reported errors. Grey “x” denote predictions of the joint response proxy, evaluated at each experiment’s (E, g_1, p_{ext}) , which track the data. The green band marks the field range where the spline remains within $|L - L_{\min}| < 10^{-3}$ of its global minimum, identifying a broad discrimination operating band ($\sim 95\text{--}300$ V/cm).

used strictly as a proxy for the stable operating band for XLZD². In Fig. 6.2³, the grey “x” markers are the model predictions evaluated at each experiment’s own (E, g_1, p_{ext}) . Although this region is often described as an “ER discrimination plateau” in the literature, the data in Fig. 6.2 do not imply a strictly flat field dependence. Instead, they show an empirical minimum in the leakage fraction spanning the $\sim 95 - 300$ V/cm range, populated by multiple experiments. This range is therefore not a physical plateau but a well-characterised operating regime in which several detectors have achieved stable discrimination performance. Outside this interval - particularly at much higher drift fields where only an isolated ZEPLIN-III point exists - the behaviour is far less constrained experimentally. For XLZD, this empirically validated minimum provides a pragmatic operating target: maximise g_1 , stabilise $p_{\text{ext}} \gtrsim 0.90$, and choose a drift field near ~ 300 V/cm (with ± 100 V/cm tolerance) or within a similarly well-populated region where ER leakage is predictable and robust against small fluctuations.

6.2.2 Extraction Efficiency

Efficient extraction of electrons at the liquid-gas interface is essential for stable dual-phase xenon operation. The electron extraction efficiency (EEE) exhibits a steep, sigmoid-like dependence on the electric field in liquid xenon:

²The intention here is to validate the trends in historical data and motivate design parameters, not to derive a first-principles leakage model. A full treatment would propagate uncertainties and model experiment-specific backgrounds/selection effects.

³The data in this plot has been compiled and digitised in places from various papers: XENONnT SR0 [83], XENON1T [97], LZ WS 2022 [36], PandaX-4T [51], PandaX-II [191], PandaX-I [97], ZEPLIN-III [192], LUX [97, 188], XENON100 [188, 193].

efficiencies are $\approx 50\%$ at $2 - 3 \text{ kV/cm}$, rise rapidly through the $3 - 6 \text{ kV/cm}$ interval, and plateau near unity above $\approx 7 \text{ kV/cm}$ [194–196]. Early measurements by Gushchin et al. [194] established this behaviour, later confirmed in PIXeY [196], which observed $\approx 50\%$ efficiency at $2.5 - 3 \text{ kV/cm}$ and $\gtrsim 95\%$ at $\geq 7 \text{ kV/cm}$. In-situ measurements in large detectors follow the same trend: LUX obtained $49 \pm 3\%$ at $\approx 3.5 \text{ kV/cm}$ during its 2013 run and $73 \pm 4\%$ at $\approx 4.2 \text{ kV/cm}$ in 2015-16 [129]. LZ reported $\approx 80\%$ efficiency at $\approx 4 \text{ kV/cm}$ [36, 197], while PandaX-4T reached $\approx 90\%$ at $\approx 6 \text{ kV/cm}$ [198]. By contrast, XENONnT operated at $\approx 2.9 \text{ kV/cm}$, yielding only $\approx 50\%$ extraction [83]. Collectively, these benchmarks demonstrate that fields below $\approx 3 \text{ kV/cm}$ impose severe penalties, whereas operation above $\approx 4.5 \text{ kV/cm}$ secures efficiencies $\geq 80 - 90\%$.

The extraction field may also influence delayed-electron backgrounds. Electrons that fail to extract can be transiently trapped at the interface and later released in bursts on millisecond timescales. However, the microphysical origin of these delayed single-electron signals remains unresolved. Possible mechanisms include unextracted electrons trapped beneath the liquid surface, impurity capture and re-emission in the bulk, or photoionisation of impurities and surfaces [199–201]. In the surface-barrier framework, electrons must surmount a potential of order $\sim 0.35 \text{ eV}$ to escape into the gas [202], offering a natural explanation for the observed EEE curve. Nonetheless, LZ and XENON studies caution that bulk impurity processes may contribute comparably, and that no single hypothesis yet provides a complete description [203].

Experimentally, there is evidence that higher extraction fields can suppress at least part of the delayed component. LUX observed a clear reduction in delayed-emission amplitude when raising the field from 3.5 to 4.2 kV/cm [204]. In LZ, power-law tails were largely insensitive to the precise extraction field setting, though a small residual surface-trapping contribution could not be excluded [203]. The XENON program further identified both surface and bulk contributions, with the delayed rate correlating weakly with electron lifetime but strongly with prior S2 activity [83]. Operationally, such signals impose substantial cost: PandaX-4T reported live-time losses of $23 - 34\%$ in Run 0 and $26 - 33\%$ in Run 1 due to post-S2 vetoes [38], while LZ retained $\approx 86\%$ live-time after similar exclusions. XENONnT instead adopted predictive modelling to mitigate delayed electrons without long veto windows [83], though this approach also benefits from reducing the surface component at the source. For XLZD, the implications are clear even without a definitive microphysical attribution. If higher extraction efficiency suppresses even a subdominant contribution to delayed electrons, operating on the high-EEE plateau offers dual benefits: maximising prompt charge collection and reducing the live-time cost of electron-train backgrounds. This provides additional motivation for aiming at extraction fields in the $4 - 6 \text{ kV/cm}$ regime ($8 - 12 \text{ kV}$ anode–gate), beyond the primary requirement of high charge yield.

For XLZD, these considerations can be expressed in engineering terms. Continuity of the displacement field requires

$$\epsilon_{LXe} E_l = \epsilon_{GXe} E_g, \quad (6.8)$$

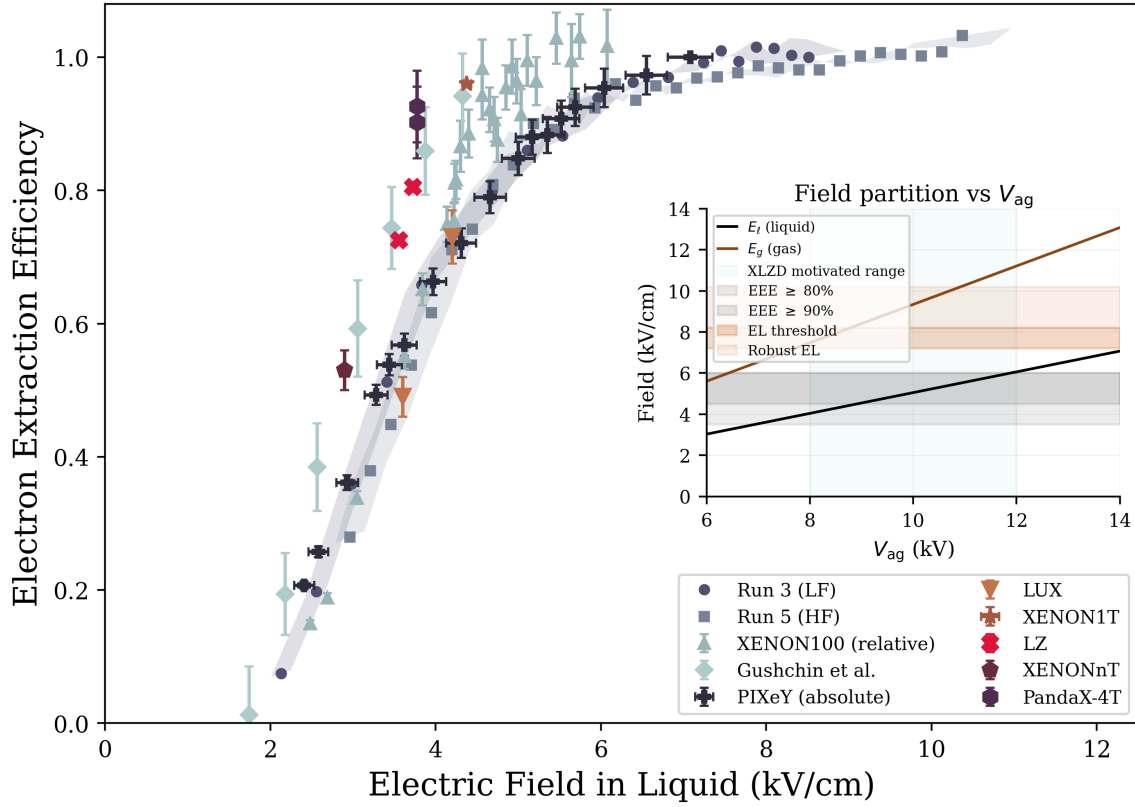


Figure 6.3: EEE versus extraction field in liquid xenon. Black/grey points show Run 3 (low field) and Run 5 (high field) measurements taken with the XeNu apparatus [84] with a semi-transparent 2D envelope built from the quoted x/y uncertainties; literature measurements are overlaid (XENON100 [176], PIXeY [196], Gushchin *et al.* [194], LUX [178], XENON1T [176], LZ, XENONnT [37], PandaX-4T [198]). The inset maps the anode–gate voltage to fields in liquid and gas for liquid gap $t_\ell = 5$ mm, gas gap $t_g = 8$ mm and $\epsilon_{\text{LXe}} = 1.85$ at $p \approx 1.79$ bar, with the XLZD-motivated range $V_{\text{ag}} = 8\text{--}12$ kV highlighted. This corresponds to $E_\ell \simeq 4.0\text{--}6.1$ kV/cm and $E_g \simeq 7.5\text{--}11.2$ kV/cm, placing operation on the high-efficiency plateau ($\gtrsim 90\%$), while fields $\lesssim 3$ kV/cm risk significant losses.

so that $E_g \approx 1.85 E_\ell^4$. With $t_\ell = 5$ mm liquid and $t_g = 8$ mm gas gaps⁵, the anode–gate potential distributes as

$$V_{\text{ag}} = E_\ell(t_\ell + \frac{\epsilon_{\text{LXe}}}{\epsilon_{\text{GXe}}}t_g). \quad (6.9)$$

Representative values are shown in table 6.1. Level fluctuations of ± 0.5 mm perturb E_ℓ by only $\approx 2 - 3\%$, ensur-

Table 6.1: Anode–gate voltage and corresponding extraction fields for a 5 mm liquid and 8 mm gas gap, assuming $\epsilon_{\text{LXe}}/\epsilon_{\text{GXe}} = 1.85$.

V_{ag} (kV)	E_ℓ (kV/cm)	E_g (kV/cm)	Expected EEE
8	4.00	7.50	$\sim 80\%$
10	5.00	9.38	$\sim 90\%$
12	6.00	11.25	$\gtrsim 95\%$

ing stability provided the operating point lies on the plateau of the efficiency curve. At $10 - 12$ kV, the gas field corresponds to $E_g/p \simeq 5.2 - 6.3$ kV cm⁻¹ bar⁻¹ at ~ 1.8 bar, comfortably above the proportional-scintillation

⁴Note that in literature it is common to see ϵ_{LXe} quoted as anything between $1.85 - 1.96$. Older measurements tend to prefer the higher values.

⁵These values are adopted as representative values based on the demonstrated LZ anode–gate geometry, and are used here for illustrative purposes rather than as optimised design parameters; the emphasis of this section is on the resulting field constraints rather than on the precise gap dimensions.

threshold of $\approx 4 \text{ kV cm}^{-1} \text{ bar}^{-1}$. Too low a voltage compromises both electron extraction and S2 yield; too high a voltage elevates gas fields and wire-surface stresses. Taken together, current literature and operational experience motivate aiming for extraction fields of $4 - 6.1 \text{ kV/cm}$ in liquid ($\approx 8 - 12 \text{ kV}$ anode–gate for $5/8 \text{ mm}$ gaps) in XLZD. This range achieves $\geq 90\%$ efficiency, potentially mitigating a source of delayed-electron backgrounds (and their associated live-time penalties), and maintains a gas field that ensures stable proportional scintillation while preserving HV and grid safety margins.

6.2.3 Grid Deflection

Electrostatic loading of the gate and anode grids leads to measurable mechanical deflection, which in turn modifies the extraction region geometry. These deformations, though typically at the sub-millimetre scale, have direct consequences for electroluminescence uniformity, S2 resolution⁶, and the onset of localised high-field regions, and therefore constitute a key design specification for XLZD.

Departures from the nominal geometry are undesirable for several reasons. First, they compromise the uniformity of the electroluminescence region, leading to position-dependent variations in the S2 signal. Second, the broadening of the electroluminescence layer degrades S2 pulse resolution, particularly for large energy depositions. Finally, sag-induced enhancement of the local surface field on the wires increases the likelihood of spurious electron emission and electrical breakdown. The magnitude of these effects depends directly on the mechanical response of the mesh, which to first order can be expressed by the scaling relation for the maximum wire deflection z_{max} :

$$z_{\text{max}} \propto \frac{E^2 p L^2}{\tau}, \quad (6.10)$$

where E is the applied field, p the mesh pitch, L the unsupported length, and τ the wire pre-tension. This expression emphasises the competing design requirements: minimising sag demands both fine pitch and high pre-tension, which must be balanced against mechanical feasibility and optical transparency.

Fig. 6.4 illustrates the consequences of representative deflections obtained from simulation. Increasing sag reduces the average photon yield, broadens the temporal width of S2 signals, and enhances the maximum surface fields on the gate wires while also increasing the risk of non-uniformities in S2 pulse shape. These dependencies demonstrate the necessity of maintaining stringent tolerances on grid planarity in large-scale dual-phase detectors.

A dedicated analytical framework was developed in this thesis to describe grid deflection more rigorously. A simplified catenary model provides a baseline estimate, but neglects higher-order terms in the elastic–electrostatic balance. By contrast, a full Euler–Lagrange formulation incorporating both electrostatic pressure and wire elasticity reproduces the measured sag of prototype meshes with improved accuracy. Fig. 6.5 compares open-air measurements of prototype grids performed at SLAC with the predictions of both models. The superior agreement of the Euler–Lagrange treatment (a set of non-linear coupled differential equations) validates its use as the reference model for XLZD design. The design requirement that follows is unambiguous: grid sag must be limited to $\mathcal{O}(0.1 - 1 \text{ mm})$ in order to preserve extraction and electroluminescence uniformity, mitigate local field enhancement, and safeguard high-voltage

⁶Also discussed in the context of diffusion and drift velocity measurements in chapter 3.

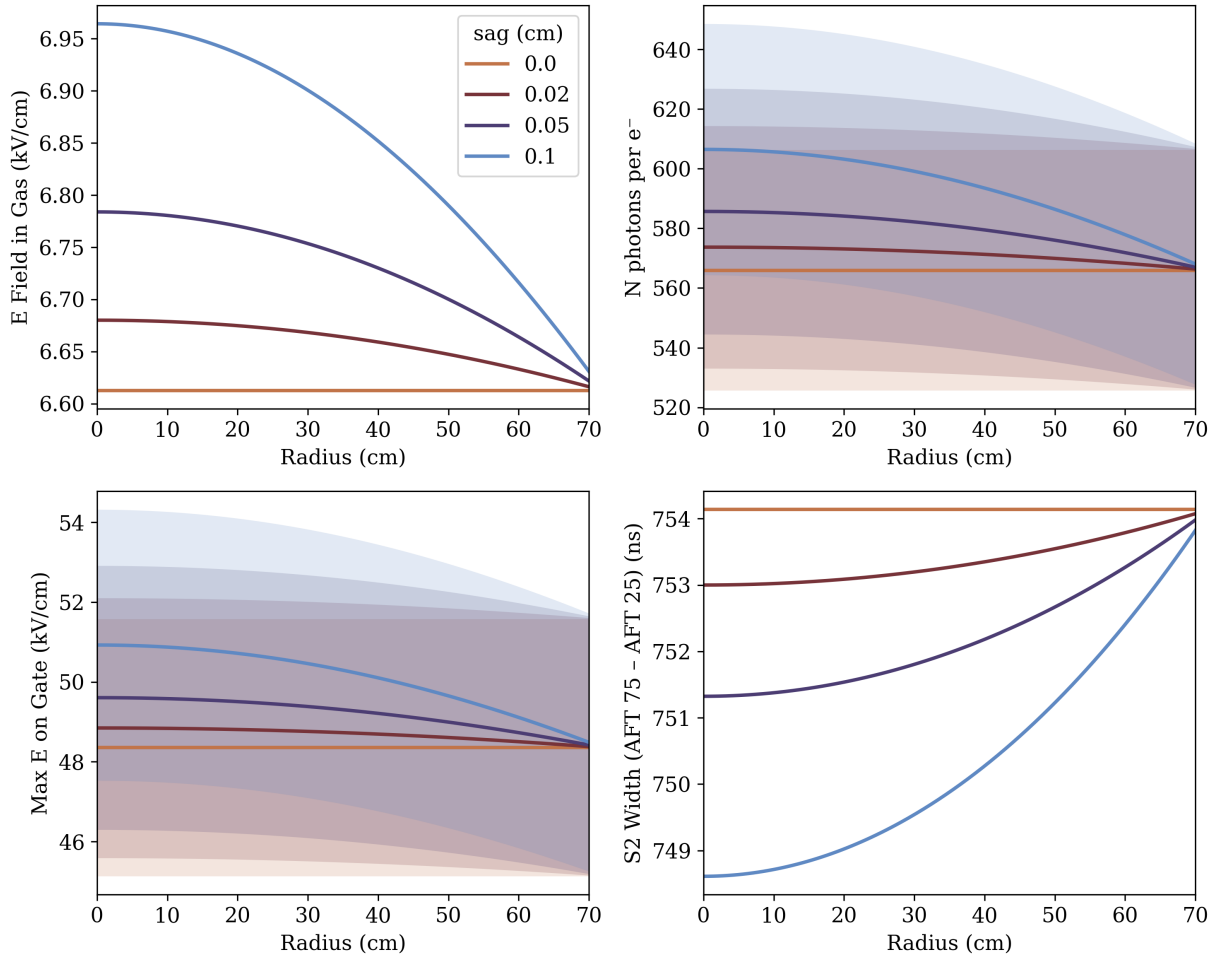


Figure 6.4: Simulated impact of grid deflection (gate deflection only) on electroluminescence region performance for WS 2024's field configuration. Panels show (a) gas field, (b) photon yield per extracted electron (§A), (c) maximum surface field on gate wires [156], and (d) SE pulse width (σ_0 modelling gas transit time only for an extracted SE rather than longitudinal diffusion effects), for nominal geometry and representative sag values. Even sub-millimetre deflections measurably degrade yield and resolution while elevating local surface fields, establishing the need for strict grid planarity tolerances in XLZD.

stability. The complete derivation of the catenary and Euler–Lagrange models is reported in completion in an internal analysis/technical note written by the author and hence, has not been repeated here [130]. Together this provides quantitative guidance on grid pre-tensioning requirements for XLZD as well as for future large-scale dual-phase TPCs.

6.2.4 Thermodynamic Constraints: LXe Density and the Saturated Interface

The operating point of a dual-phase TPC is determined by the thermodynamic coexistence line of liquid and gaseous xenon. Stable operation requires the temperature and pressure to follow the saturation curve, ensuring a stable and flat liquid-gas interface. For xenon, this curve is well measured, with a typical operating point near 174 K and ~ 1.8 bar absolute, corresponding to a liquid density of [205]

$$\rho_{\text{LXe}}(174 \text{ K}, 1.79 \text{ bar}) \approx 2.93 \text{ g cm}^{-3}. \quad (6.11)$$

The equilibrium vapour pressure is governed by the Clausius-Clapeyron relation,

$$\frac{dP}{dT} = \frac{L}{T\Delta v}, \quad (6.12)$$

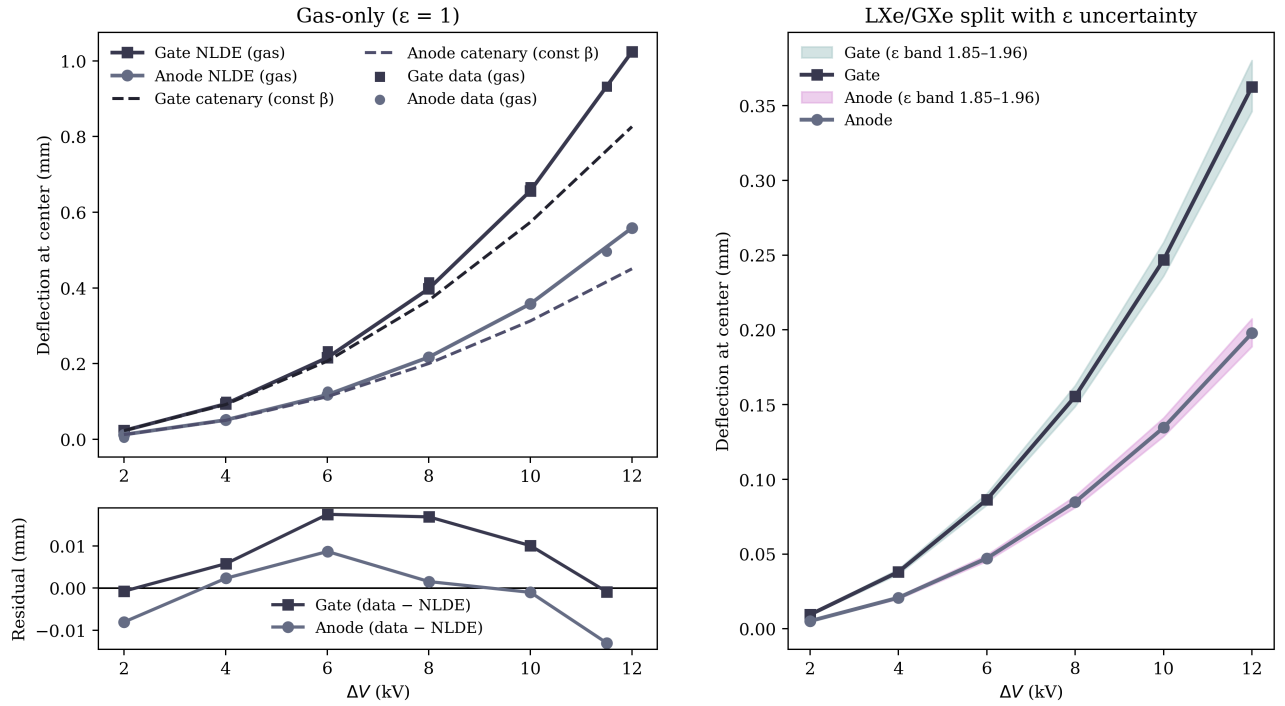


Figure 6.5: Measured electrostatic deflection of prototype grids in open-air tests at SLAC [115], compared with predictions from the simplified catenary model and the full Euler–Lagrange formulation [130]. The superior agreement of the Euler–Lagrange model validates its use in XLZD design studies and provides quantitative guidance for grid pre-tensioning specifications in future large dual-phase detectors. Bands overlaid represent the propagated uncertainty in the measured value of the dielectric constant of LXe and its effect on the maximum deflection expected in a dual-phase environment.

where L is the latent heat of vaporisation and Δv the molar volume different between gas and liquid. Integrating this relation yields the saturation curve $P_{sat}(T)$, which defines the allowed operating band for dual-phase detectors (Fig. 6.6).

In dual-phase operation, the xenon liquid–gas interface is stabilised only when the detector is operated at or very close to this “coexistence” curve. Deviations in temperature from the saturation point at fixed pressure modify both the macroscopic geometry of the gas gap and the microscopic smoothness of the interface, with direct consequences for charge extraction and proportional scintillation.

- **Superheating ($\Delta T > 0$)**

When the liquid is held above its saturation temperature, the interface becomes metastable. Surface waves that are normally damped can grow into corrugations. The effective normal electric field is reduced when the interface is tilted at a local angle, leading to a decrease in extraction efficiency ε_{ext} . At higher temperatures, bubble nucleation can occur, further disrupting the uniformity of the interface.

- **Sub-cooling ($\Delta T < 0$)**

Cooling below the saturation temperature decreases the equilibrium vapour density, leading to a partial collapse of the gas gap above the liquid. The total anode–gate separation is fixed mechanically, consisting of a $\approx 5\text{ mm}$ liquid layer and an $\approx 8\text{ mm}$ gas layer in LZ, but only the gas thickness g governs proportional scintillation. With fixed anode–gate voltage, the gas field rises as g shrinks, but once g is too small the light yield Y falls below threshold.

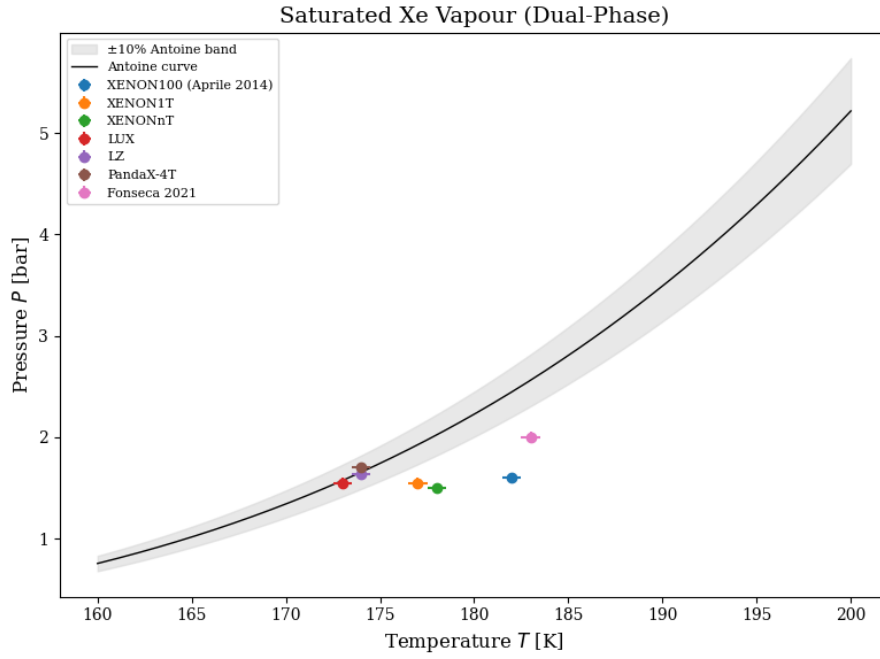


Figure 6.6: Saturated vapour pressure of xenon as a function of temperature, with a $\pm 2.5\%$ band around the coexistence curve. Operating points of recent dual-phase detectors (LZ [36], XENON1T/nT [127, 206], PandaX-4T [207]) are indicated for reference. The preliminary XLZD design adopts 174 K and 1.79 bar as its nominal operating condition, ensuring stable dual-phase equilibrium and a well-defined liquid–gas interface.

- **Stable operation** ($\Delta T \simeq 0$)

At the saturation point, the interface remains flat, the gas gap thickness is constant, and both extraction efficiency and proportional scintillation yield remain at their optimal values.

In addition to defining the operating point in $T - P$ space, the saturated density of liquid xenon directly fixes the geometry required to achieve a given active mass for the TPC. For a cylindrical active region, the drift height is obtained directly from the liquid xenon density at the chosen operating point:

$$h = \frac{M_{\text{active}}}{\rho_{LXe} \pi r^2}, \quad (6.13)$$

with r the active radius. Taking $r = 1.50 \text{ m}$ and $\rho_{LXe} = 2.93 \text{ g cm}^{-3}$ at 174 K, 1.79 bar, the required drift height for a 60 t active mass is

$$h(60 \text{ t}) = \frac{60 \times 10^3}{2.93 \times 10^3 \times (1.5)^2 \pi} = 2.90 \text{ m}. \quad (6.14)$$

Scaling to 80 t increases the height by a factor of 4/3, giving

$$h(80 \text{ t}) = 3.86 \text{ m}. \quad (6.15)$$

While equations 6.14 and 6.15 fix the drift height for the chosen 60 t and 80 t active targets, it is instructive to view this in the broader context of scaling. Fig. 6.7 shows the aspect ratio h/d as a function of active xenon mass for a fixed active diameter $d = 3.0 \text{ m}$ at $\rho = 2.93 \text{ g cm}^{-3}$. A $\pm 1\sigma$ band is indicated, combining density variations from small T, P excursions about saturation and a $\pm 5 \text{ mm}$ tolerance on the field cage radius. Existing xenon TPCs (and the

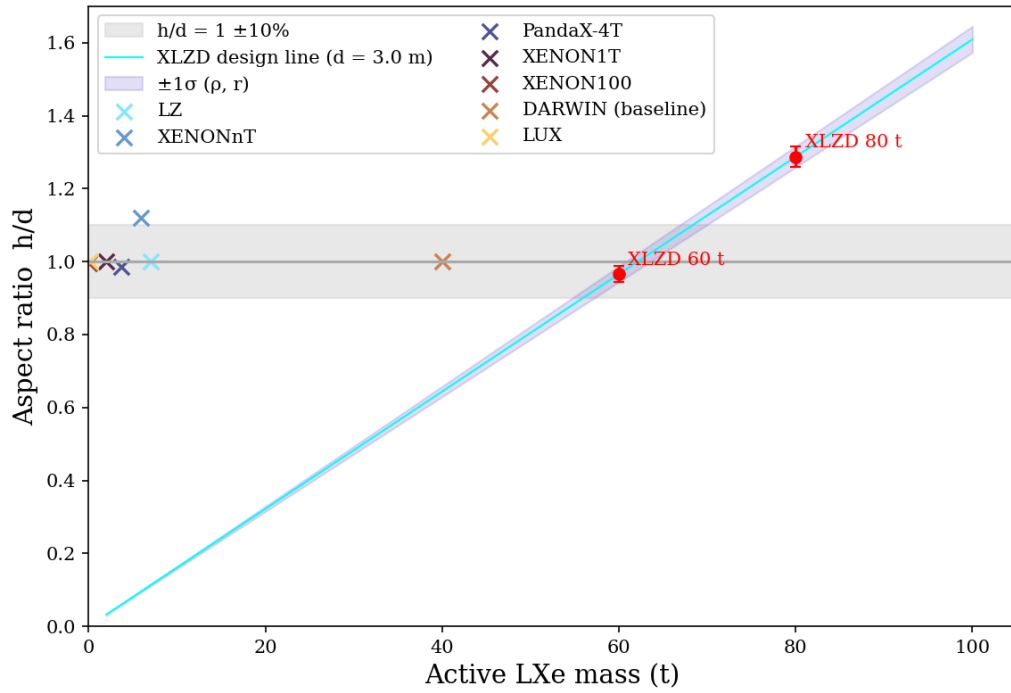


Figure 6.7: The XLZD design scaling for $d = 3.0 \text{ mm}$ is shown by the cyan line, with shaded bands derived from estimated $\pm 2\%$ density and $\sim \pm 5 \text{ mm}$ radius uncertainties. Crosses show various experiments and their respective parameters overlaid in this parameter space. The grey band denotes the balanced-cylinder regime, $h/d = 1 \pm 10\%$.

DARWIN experiment’s design baseline [186]) are overlaid for comparison. All large-scale instruments cluster around $h/d \sim 1$, with XLZD 60 t and 80 t lying at 0.97 and 1.29 respectively. The figure makes clear that the 60 and 80 t XLZD designs fall naturally within the “balanced” aspect ratio band, favouring good charge transport, low diffusion, and efficient optical collection. This motivates the discussion of aspect ratio as a design driver in §6.2.5).

Finally it must be noted that the xenon skin and cryostat taper introduce an additional, geometry-dependent volume which modestly increases the total xenon inventory above the active target mass. A detailed accounting of this annular volume, including the top and bottom taper thicknesses, is deferred to §6.3 where the engineering optimisation of the field cage and cryostat is presented.

6.2.5 Aspect Ratio

The aspect ratio of a dual-phase xenon TPC,

$$a \equiv h/d, \quad (6.16)$$

with h the drift height and d the active diameter encapsulates several of the most critical design parameters: the maximum drift time (and thus the required electron lifetime), the light collection efficiency (LCE) and corresponding PMT coverage, and the cathode potential required to sustain the drift field. Large-scale dual-phase detectors to date have adopted near-balanced geometries; XENON100 [177], LUX [54], XENON1T [92], PandaX-4T [208], XENONnT [127], and LZ [58] all operate with $h/d \simeq 1 \pm 0.1$. This convergence reflects the fact that a (near-) balanced cylinder provides the most robust compromise between charge transport, optical performance, and high-voltage stability. XLZD’s baseline design likewise falls within this regime (Fig. 6.7). In the following, we close the

Table 6.2: Aspect-ratio trade-offs for a cylindrical dual-phase TPC. Each item is mapped to the geometry where the effect is most constraining. Cross-references point to subsections where the constraint is quantified or discussed.

Theme	Tall TPC ($h \gg d$)	Short TPC ($h \ll d$)	Balanced ($h \simeq d$)
Charge transport (drift time, lifetime)	Long $t_d^{\max} \Rightarrow$ high τ_e requirement; larger longitudinal diffusion; stronger z -dependence. §6.2.5, §3.2	Short $t_d^{\max} \Rightarrow$ relaxed τ_e ; reduced diffusion; easier stability. §6.2.5, §3.2	Meets survival goals without extreme τ_e ; diffusion acceptable. §6.2.5
Cathode HV headroom / breakdown	Higher $V_{\text{cath}} \simeq E_d h$; tighter margins for breakdown / emission. §6.2.5	Lower V_{cath} for same E_d ; improved HV stability. §6.2.5	Within demonstrated HV ranges at design E_d . §6.2.1, §6.2.5
Grids: sag, fields, emission	Not height-driven per se; risk grows with <i>diameter</i> (span) and wire tension/pitch. §6.2.3, §6.2.5	Same note: governed by span/tension, not h . §6.2.3, [130]	Keep d moderate $\Rightarrow$ manageable sag and surface fields. §6.2.3
Optical transfer (LCE, uniformity)	Longer mean path to PMT planes; lower absolute LCE; stronger z -non-uniformity. §6.2.5	Vertical path short, but radial transport dominates; stronger <i>radial</i> non-uniformity unless coverage increased. §6.2.5	Near-unity h/d yields demonstrated LCE ~ 7 –12% with best spatial uniformity. §6.2.5
PMT coverage, dark noise, PMT radioactivity	Fewer PMTs per unit mass, but optical penalties may dominate. §6.2.5	More PMTs per unit mass to preserve uniformity $\Rightarrow$ higher aggregate dark rate and PMT γ budget. §6.2.5	PMT count scales naturally with mass; noise/background tax minimised. §6.2.5
Wall/PTFE surfaces & fiducial volume	At fixed mass, departures toward extreme h/d increase S/V as geometry forces growth of one dimension. §6.2.5, §4.6	Small $h \Rightarrow$ higher $S/V \Rightarrow$ more PTFE per mass (Rn plate-out, charging). §6.2.5	$S/V = 4/d + 2/h$ minimised near balance; reduced PTFE-related backgrounds and charging risk. §6.2.5, §4.6
Thermal / dual-phase envelope	Taller columns can amplify sensitivity to T – P excursions (level, S2 path). §6.2.4	Shallower gas gap control easier; very wide d complicates levelling and edge optics. §6.2.4	Operate on saturation curve with flat interface and constant gas gap. §6.2.4

loop on field-motivated design requirements, also making the case for why a balanced aspect ratio remains optimal for next-generation detectors (table 6.2).

Charge transport and electron lifetime

The principal cost of increasing the drift height h in a dual-phase xenon TPC is the corresponding rise in the maximum drift time,

$$t_d^{\max} = \frac{h}{v_d(E)}, \quad (6.17)$$

which in turn sets the minimum electron lifetime τ_e required for acceptable charge survival. Using the drift-velocity parametrisation established in Chapter 3, we evaluate $t_d^{\max}$ for the XLZD baseline drift of 3.0 m and the 80 t case of 3.86 m , across representative fields of 23, 97, 193, and 310 V/cm . The results are summarised in Table 6.3. Achieving 90% survival requires lifetimes in the range of 18 – 50 ms depending on field and drift height, while 99% survival would demand lifetimes in excess of 200 ms .

A global view of this parameter space is shown in Fig. 6.8, which maps survival probability as a function of drift height and lifetime for the same four fields. Overlaid are typical lifetimes reported by previous large-scale TPCs, including XENONnT, LZ, PandaX-4T, LUX, and Xenoscope. These comparisons illustrate that state-of-the-art detectors achieve $\tau_e \sim 10$ – 15 ms yielding 80 – 88% survival over 1.3 – 1.5 m drifts, while earlier instruments/

Electron survival probability vs drift height and lifetime

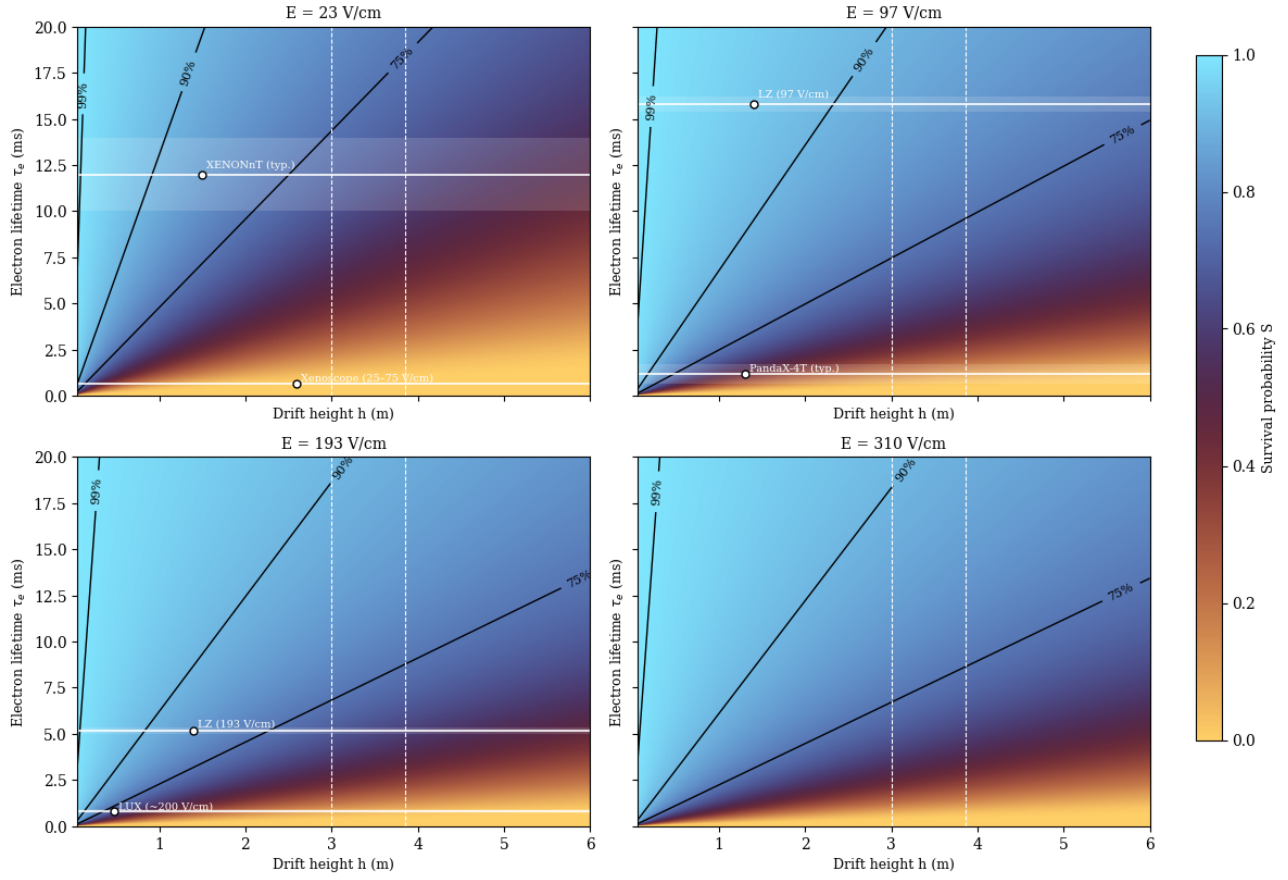


Figure 6.8: Electron survival probability S as a function of drift height h and electron lifetime τ_e for four representative drift fields. Contours indicate survival levels of 75%, 90%, and 99%. Vertical dashed lines mark the XLZD design drifts of 3.0 m and 3.86 m, while horizontal lines show typical lifetimes achieved in previous experiments (white markers) projected to XLZD's design heights. The plots highlight how survival improves with field and lifetime, but degrades with increasing drift height, quantifying the charge-transport penalty of tall geometries.

Table 6.3: Drift times and electron-lifetime requirements for XLZD at two candidate drift heights. Requirements are computed from $S = \exp(-t_d^{\max}/\tau_e)$ with $\tau_e \gtrsim t_d^{\max}/|\ln S_\star|$ for target survival $S_\star$. Drift times use the Chapter 3 fit for $v_d(E)$.

E (V/cm)	h (m)	$t_d^{\max}$ (ms)	τ_e for 90% (ms)	τ_e for 99% (ms)
23	3.00	4.13	39.2	411
23	3.86	5.31	50.4	529
97	3.00	2.15	20.4	214
97	3.86	2.76	26.2	275
193	3.00	1.97	18.6	195
193	3.86	2.53	24.0	252
310	3.00	1.93	18.3	192
310	3.86	2.49	23.6	247

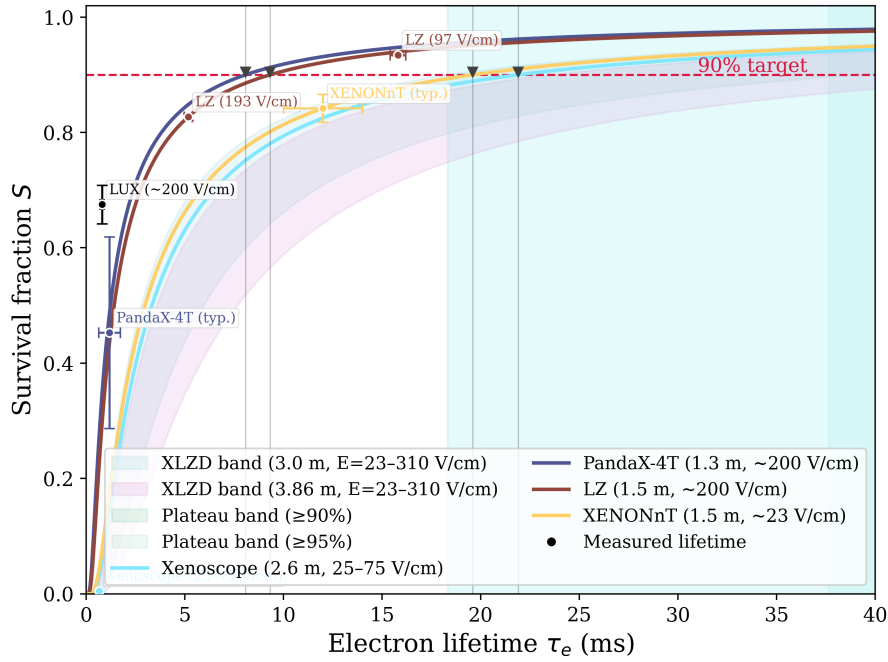


Figure 6.9: Electron survival probability S as a function of electron lifetime τ_e . Shaded bands show the range spanned by XLZD drifts of 3.0 m and 3.86 m for fields between 23 – 310 V/cm. Curves for previous detectors (Xenoscope, PandaX-4T, LZ, XENONnT) are overlaid for comparison, with the 90% survival target indicated. The same $> 90\%$ survival threshold for XLZD’s target dimensions have also been shown (green band).

R&D efforts (e.g. LUX, Xenoscope - still ongoing) operated at sub- ms values. Extrapolating these measured lifetimes to XLZD’s longer drifts implies survival fractions of 60 – 80% at the lowest fields, rising to 85 – 90% at fields above 97 V/cm.

The scaling is made more explicit in Fig. 6.9, which shows survival as a function of τ_e for different detector geometries. Increasing the drift height inevitably lowers the survival fraction for any given lifetime, while operating at higher drift fields shortens t_d^{max} and thus partly compensates. However, the upper bound on field is set by the competing requirements of stable high-voltage operation and optimal ER/NR discrimination (see §6.2.1), so the achievable improvement is limited.

Finally, Fig. 6.10 places these requirements in historical context, showing the steady increase in measured lifetimes across successive xenon TPCs. The observed progression from sub- ms in early detectors to $\sim 15 ms$ in current large-scale experiments supports the feasibility of XLZD’s targets, but also underscores the need for continuous advances in purification and high-voltage stability to sustain multi-meter drifts. From an aspect ratio point of view, shorter TPCs with $a \lesssim 1$ is ideal; tall TPCs would require even higher electron lifetimes than those calculated in this discussion if a good survival fraction is to be achieved, posing a significant challenge.

Optical transfer efficiency and TPC PMT coverage penalty

Scintillation photons in LXe are emitted isotropically; their detection probability is governed by the mean path to a PMT and the number of reflections en-route. Departures from a balanced cylinder tend to degrade either absolute

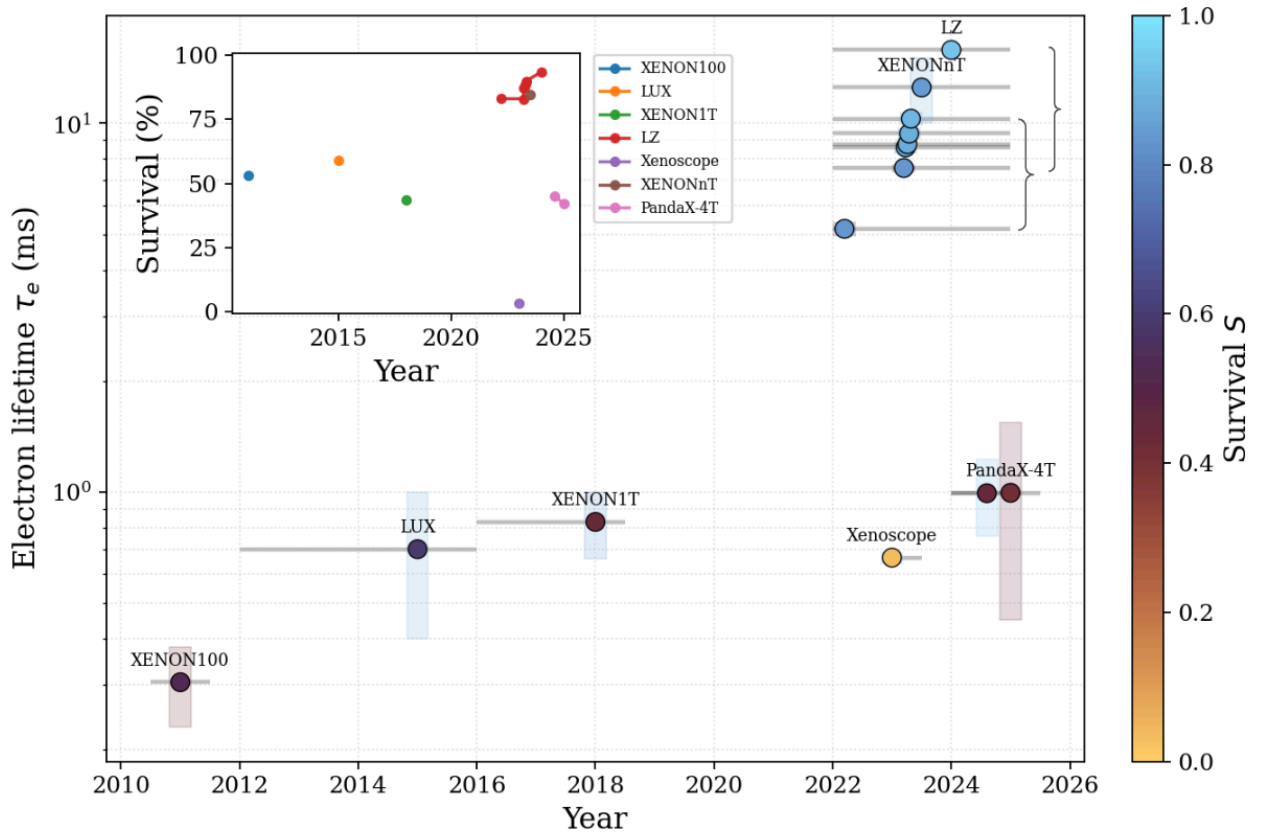


Figure 6.10: Historical electron lifetimes and implied charge survival in dual-phase xenon TPCs. Points show reported τ_e (log-scale) with translucent boxes indicating the span during operation (for LZ, statistical error on the lifetime measurement are shown instead). Marker colour encodes the survival $S = \exp(-t_d^{max}/\tau_e)$ and the inset explicitly shows the operational survival fractions for the various experiments. Early detectors (XENON100, LUX, XENON1T) achieved sub- ms to ~ 1 ms lifetimes, corresponding to $S \sim 40 - 60\%$ at their geometries, while current large instruments (XENONnT, LZ) reach $\tau_e \sim 10 - 16$ ms, yielding $S \sim 85 - 95\%$ for $h \simeq 1.5$ m at $\mathcal{O}(10^2)$ V cm $^{-1}$. Long-drift R&D (e.g. Xenoscope, $h = 2.6$ m) illustrates the survival penalty at fixed τ_e . For XLZD drifts of 3.0 – 3.86 m, the design goal is $S \gtrsim 90\%$, which requires $\tau_e \gtrsim 18 - 26$ ms for $E = 97 - 310$ V cm $^{-1}$ (Table 6.3), motivating continued gains in purification and HV stability.

LCE or its spatial uniformity. In very tall geometries the average distance to the PMT planes increases, raising absorption/scatter losses and introducing stronger depth (z) dependence. In very shallow, wide geometries the vertical path is short, but radial transport dominates: events produced near-wall experience more reflections on PTFE, and the angular acceptance of the top/bottom arrays varies more strongly with radius, producing larger radial non-uniformity unless compensated by higher coverage.

Photodetector coverage scales with geometry: the instrumented area of the PMT planes grows as d^2 , while the active mass grows as hd^2 . Pushing shallower/wider increases the required PMT count per unit mass (to maintain uniformity), which in turn raises aggregate dark noise and radioactivity from the PMTs: historically among the largest single-component contributors to the external γ budget in LXe TPCs, even after aggressive screening [58]. Going taller/narrower reduces PMTs per unit mass, but at the cost of lower LCE and stronger z -non-uniformity. In practice, a balanced cylinder thus minimises the coverage penalty while keeping optical performance in the regime demonstrated by current experiments.

Finally, PTFE reflectors are essential ($\geq 95\%$ VUV reflectivity in LXe [58]), but large wall area increases exposure to radon-progeny plate-out and surface charge accumulation, both of which can erode fiducial volume or disturb fields over time (§4). For a cylindrical TPC of diameter d and height h , the surface-to-volume ratio scales as $S/V = 4/d + 2/h$; for fixed active mass this grows at either extreme (very tall or very shallow), and is minimised near a balanced aspect ratio, reducing PTFE-related background/stability risks.

High-voltage headroom and long-term stability

Delivering and maintaining high cathode voltages remains one of the principal engineering constraints for dual-phase xenon TPCs. Given XLZD's scale (assuming $a \approx 1$), drift fields of $100 - 400 \text{ V/cm}$ translate to cathode biases of $\sim 100 - 130 \text{ kV}$, with additional headroom required for safe operation and conditioning. Taller TPCs would thus translate to even more difficult HV requirements as the cathode bias would have to scale with the increased height of the TPC. Shorter TPCs would require larger electrode grids, instead compromising on field uniformity due to electrostatic deflection (§6.2.3) and potentially higher surface fields as a result (subject to appropriate tensioning).

Moreover, experience across generations shows that no detector has reached its nominal HV design goal; the operational ceiling is instead limited by the emergence of faint light from microscopic emitters, electron emission at high-field edges, or outright breakdown. This pattern is summarised in Fig. 6.11, which compares design targets with the voltages actually sustained in stable running.

A further complication is long-term stability. Only in R&D experiments like Xenoscope [111] and XeBrA [214] have cathode biases up to -75 kV been achieved in LXe, with higher ($\sim 105 \text{ kV}$) having been demonstrated in LAr tests [152]⁷ but with run times not exceeding $\sim 1 \text{ hr}$ during these campaigns before light emission was observed; though this definitely does not mean sustaining such high voltages is not possible, it does identify a clear challenge as a feat that has not been explicitly overcome in the past.

LZ itself provides another example: its cathode held -32 kV stably for more than a year, but over time localised light emission emerged and forced re-biasing to a lower potential. This story is no stranger to any of the experiments mentioned so far, demonstrating that “HV ceilings” are not fixed, but time-dependent: microscopic surface evolution, conditioning history, and material degradation can reduce the breakdown threshold over multi-year operation even if stability is achieved initially. Future designs must therefore aim not only to deliver higher initial voltages but to sustain them reliably throughout the experiment's lifetime; in this regard, shallower TPCs are favoured. In general, these arguments motivate extensive R&D into grid conditioning and production, as simply achieving the nominal cathode bias for a chosen drift field is insufficient. Instead, being able to reach and hold a cathode voltage well above the operating requirement provides tolerance against gradual degradation and flexibility in adapting to evolving conditions. Such headroom is essential to maximise stable runtime and, consequently, total physics exposure.

⁷There is evidence to show that the LAr and LXe breakdown thresholds and, hence, mechanisms may be quite similar. As a result (see [81] figures 6.44 and 6.45 along with the accompanying discussion), electrode conditioning/surface finish could play more of a part in breakdown than other factors like ramp speed (typically in the range of $100 - 200 \text{ V/s}$) or pressure ($1.5 - 2.2 \text{ bar}$, well in the range of operation of most dual-phase LXe experiments operating in/near the LXe saturation point A.2) [215].

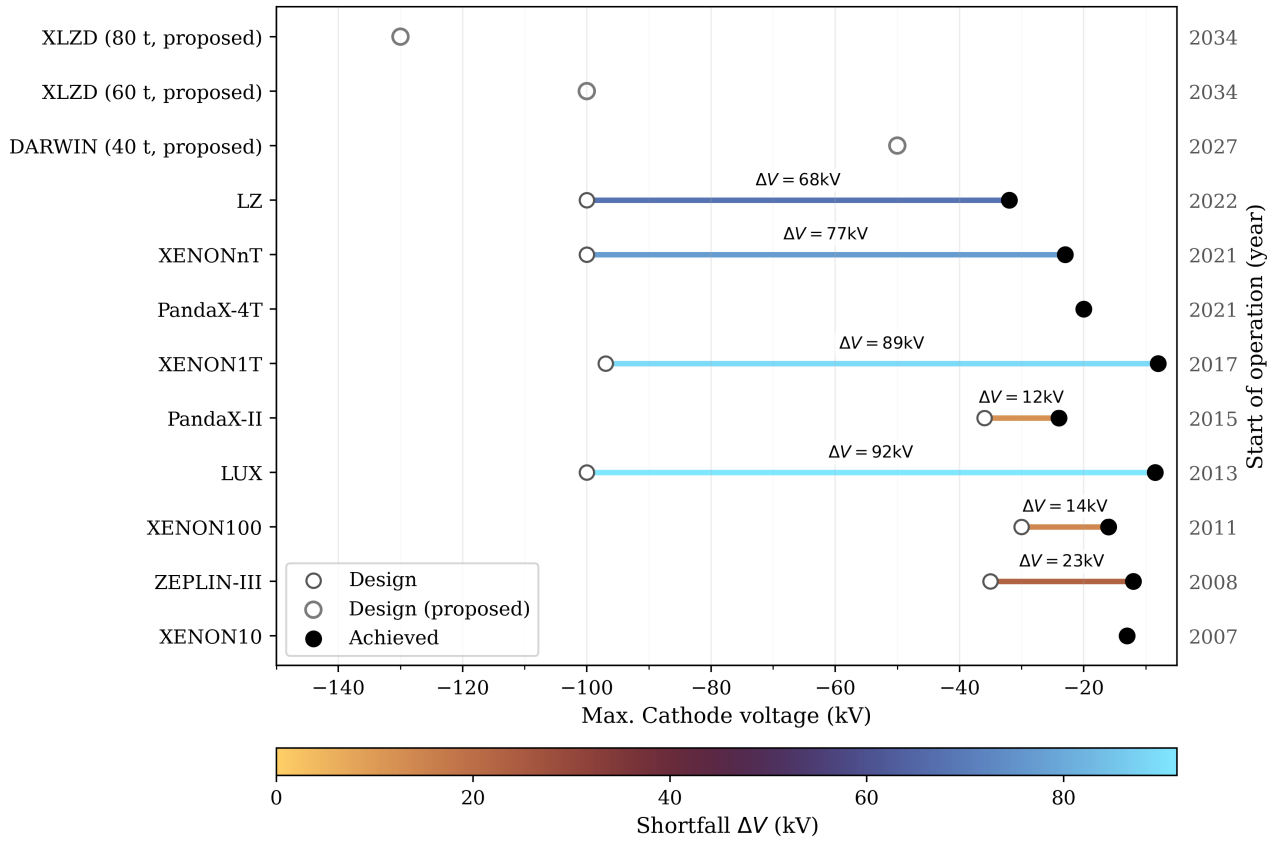


Figure 6.11: Design (open) vs achieved (filled) cathode voltages in LXe TPCs, ordered by start year; connector colour encodes shortfall $|\Delta V|$ (kV). Future experiments (XLZD and Darwin [186]) are shown as hollow markers. Values (other than LZ and XLZD (this work)) compiled from ZEPLIN-III [209, 210], XENON10 [211], XENON100 [176, 177], LUX [54, 126], PandaX-II [212], XENON1T [119], PandaX-4T [51], XENONnT [155, 213].

6.2.6 Summary of field-motivated requirements

Through §6.2 we laid out the foundational performance and engineering constraints that drive the HV design of a next-generation TPC. Table 6.4 distils these into concrete operating targets and headroom margins that we carry forward to §6.3.1, where we optimise the skin and cryostat geometry with long-term stability in mind.

6.3 Implications on Skin & Cryostat Design

The “skin” is the optically isolated xenon layer between the TPC field cage and the inner cryostat, first fully instrumented in LZ⁸. For XLZD, an instrumented skin is essential: surface-origin backgrounds - γ rays from cryostat materials, neutrons from radiative capture, and radon progeny - populate this outer xenon and would otherwise force overly conservative fiducial cuts in a programme capped at ~ 80 t of xenon. The skin therefore forms a core element of the anti-coincidence veto strategy (with the OD), providing the most direct tag of near-wall interactions while preserving fiducial mass.

Preliminary XLZD simulations (Fig. 6.12) summarise the relevant channels. For neutrons, rejection combines prompt signals from quenched elastic/inelastic scatters in the skin with delayed “ γ -splash” following captures in the OD or

⁸As discussed in §4.8 and [58].

Table 6.4: Baseline high-voltage requirements used in this work.

Parameter	Requirement	Notes / references
Drift field	90–400 V/cm	Covers low-leakage regime while preserving charge yield and manageable diffusion; upper bound matches headroom studies (see Sec. §6.3.1/Fig. 6.11).
Extraction field (LXe)	4–6.1 kV/cm	Targets $EEE \gtrsim 80\text{--}90\%$ based on current/previous experiments' trends; cf. §6.2.2.
Electroluminescence field (GXe)	≥ 8 kV/cm	Above EL threshold $\sim 4p$ kV/cm at $p \simeq 1.8$ bar; robust plateau $\sim 9\text{--}11$ kV/cm; e.g. [144, 195].
Aspect ratio (TPC)	Near 1:1	Reduces peak fields/sag and simplifies optics, HV trade-offs (§6.2.5).
Max surface fields	≤ 50 kV/cm	Limit at wires/edges to suppress emission/breakdown; set by wire pitch/diameter and local geometry; cf. [81, 152, 214, 215].
Max HV (cathode)	100 kV (60 t); 133 kV (80 t)	Consistent with $E_{\text{drift}} \sim 300\text{--}360$ V/cm over 3–3.9 m; contextualised by achieved HV survey (Fig. 6.11).
HV headroom	$\sim +20$ kV	Sized to reach ~ 400 V/cm for both 60, 80 t masses and tolerate ageing/conditioning drift; see §6.3.1.
Minimum skin thickness	$\gtrsim 3$ cm	Veto performance / self-shielding requirement; cf. §6.3.
Grid transparency	Anode 92%, cathode 96%, gate 97%	Trade-off with wire pitch/diameter controlling near-electrode uniformity; cf. [58, 67, 81], Fig. 5.8.

on structural materials; together these achieve the design target of $\gtrsim 95\%$ rejection of radiogenic neutrons. For γ rays, the critical lines are ^{208}Tl at 2.615 MeV and ^{214}Bi at 2.447 MeV. In LXe their photoelectric mean free path is metres (negligible traditional self-shielding), whereas the Compton scattering length is $\mathcal{O}(10\text{ cm})$ [216]. The TPC, with keV -scale threshold, efficiently tags Compton vertices and degrades γ energy; the skin, being only a few cm thick, contributes more modestly. Consistently, simulations show the side skin must be $\gtrsim 5$ cm to reduce the cryostat- γ energy deposition in the TPC to an acceptable fraction of the top flux (where no skin exists), with only weak improvement beyond this scale. The skin alone tags $\sim 70\%$ of ^{208}Tl backgrounds at a 100 keV threshold, and OD coincidence lifts the rejection above 80% .

The takeaway is twofold. First, XLZD requires an instrumented skin to control near-wall γ /neutron backgrounds without sacrificing fiducial mass - especially at XLZD's scale, with $\gtrsim 8\times$ the surface area of current-generation detectors. Xenon allocated to the skin can, in principle, be “traded” for xenon in the TPC (where the threshold is far lower), but at $r \approx 1.5$ m each additional centimetre of skin thickness carries a substantial cost: not primarily from radioactivity, but from foregone active/fiducial volume and hence potential lost exposure. This trade-off must be managed dynamically as HV configurations, materials choices, and physics-run plans evolve. Second, once a few centimetres are provided for instrumentation and basic shielding, preliminary simulations of veto performance have shown only weak dependence on further thickness; the dominant design driver then becomes the skin's role as an electrostatic standoff. Several centimetres of xenon are needed to keep surface fields on the cage and near the cryostat below breakdown with tolerance to construction variations. The next subsection (§6.3.1) develops a preliminary high-voltage design based on an LZ-like field cage scaled to XLZD; §6.3.2 then optimises the skin geometry under those standoff constraints.

6.3.1 Baseline Field Cage and High-Voltage Design

The optimisation of the XLZD cryostat and skin geometry is predicated on first establishing a robust baseline design for the TPC field cage. As laid out in § 6.2, the choice of HV configuration is strategically guided by physics requirements:

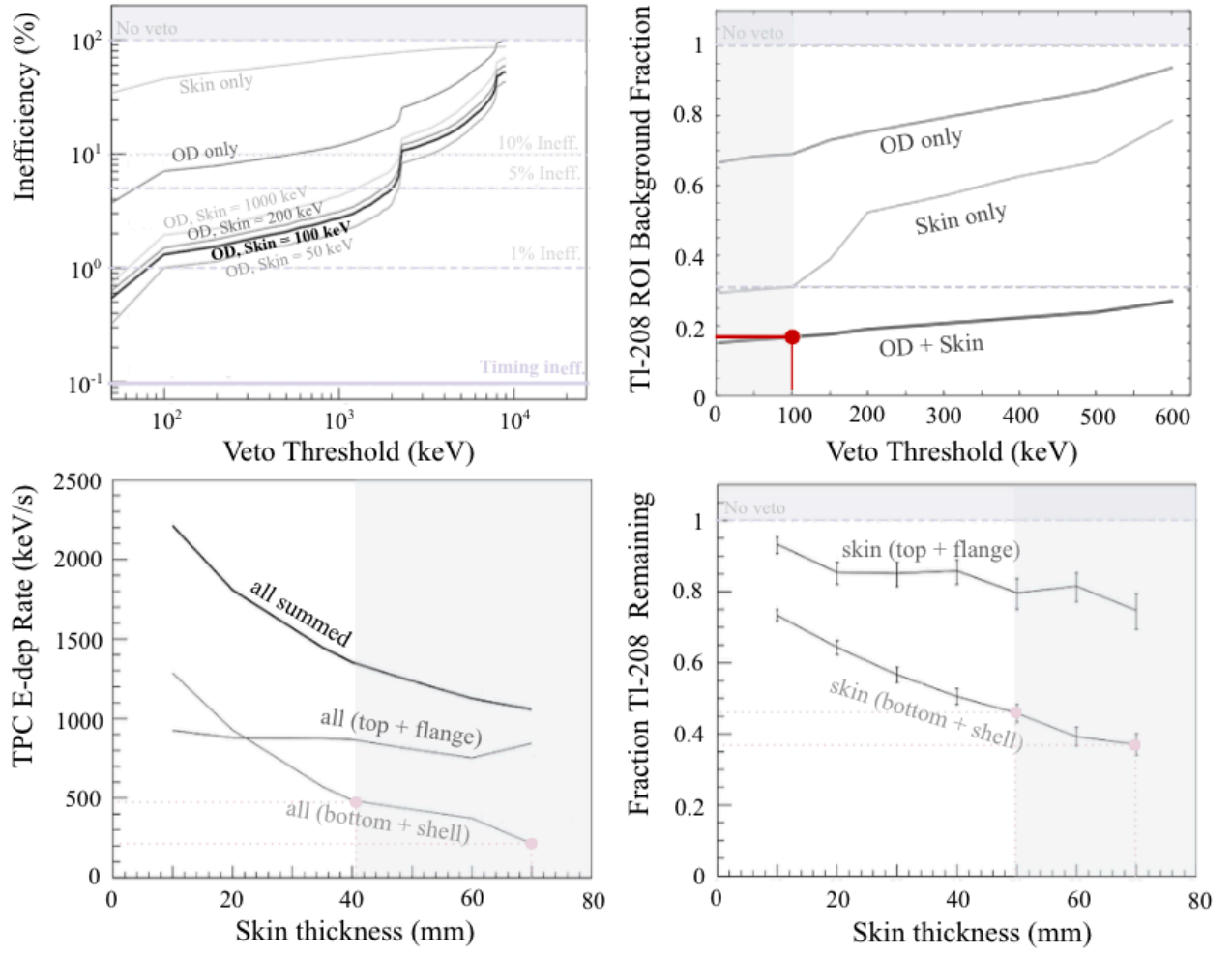


Figure 6.12: Simulated performance of the xenon skin in XLZD. (**Top left:**) Neutron veto inefficiency vs threshold for skin, OD, and combined operation. (**Top right:**) Surviving fraction of ^{208}Tl events in the $0\nu\beta\beta$ ROI vs skin/OD threshold. The target of 100 keV threshold is shown, and simulations assume LZ-like cryostat material backgrounds. (**Bottom left:**) Energy-deposition rate in the TPC from cryostat γ flux vs side-skin thickness. (**Bottom right:**) Surviving fraction of ^{208}Tl γ events vs skin thickness, showing only weak dependence beyond several cm. Together, these results establish that XLZD requires an instrumented skin, but that its thickness is optimised primarily by high-voltage standoff rather than incremental veto performance. Figures modified from [53] and preliminary studies conducted by the xenon futures group (see paper for further details on assumptions).

maximising electron transport efficiency and optical response, improving discrimination, and preserving fiducial mass. From these considerations, nominal field targets were identified: a drift field of $\sim 200\text{--}350$ V/cm, extraction fields of $\sim 4\text{--}6$ kV/cm in liquid xenon, and electroluminescence fields above ~ 8 kV/cm in the gas phase. These values balance discrimination power with stability, while keeping operational voltages within realistic engineering tolerances.

To translate these physics requirements into an electrostatic design, detailed simulations were performed in COMSOL MULTIPHYSICS using a two-dimensional, axisymmetric model. This is shown in Fig. 6.13 PTFE panels isolate the active xenon from the surrounding skin, while woven-mesh electrodes (cathode, gate, anode) establish the drift and extraction fields. The resistor ladder biasing the field-shaping rings (FSRs) was explicitly implemented, ensuring a graded potential distribution along the cage wall. Correct assignment of dielectric constants was essential to capture realistic boundary conditions: these are in line with the parameters used in field modelling for LZ as outlined in table 4.6. The values used were cross-checked against the most recent direct measurements in literature and those adopted

by other experiments for their analyses.

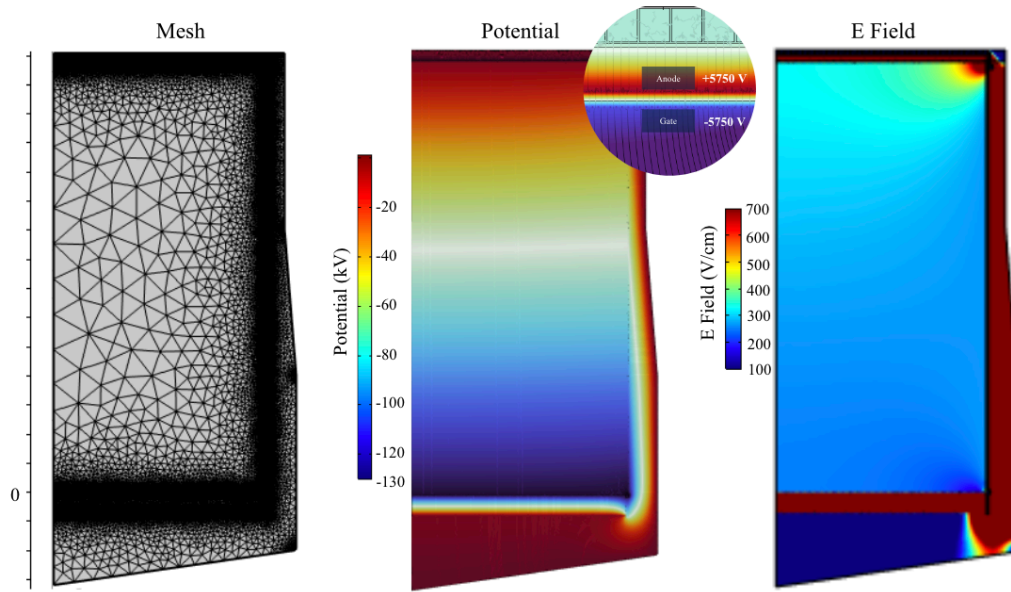


Figure 6.13: Baseline COMSOL electrostatic model for XLZD. **(Left)** Finite-element mesh, with finer resolution around electrodes and geometric edges. **(Centre)** Potential map of the TPC, showing smooth grading across the drift region; inset highlights electrode biasing at the anode and the gate. **(Right)** Magnitude of the electric field, demonstrating bulk uniformity and enhanced fields near the cathode and grid structures. This design is used for simulating both 60 t and 80 t cases.

Meshing was adapted to the electrostatics problem: coarser in the central drift region, where fields are highly uniform, and increasingly refined near regions of strong curvature or field concentration — for example around the cathode ring, near wire planes, and at the extraction region (Fig. 6.14). This adaptive approach ensures that sharp gradients are resolved without excessive computational load. In COMSOL, this kind of mesh refinement is intrinsic as a user-setting and does not require much manual intervention as was the case with FENICS.

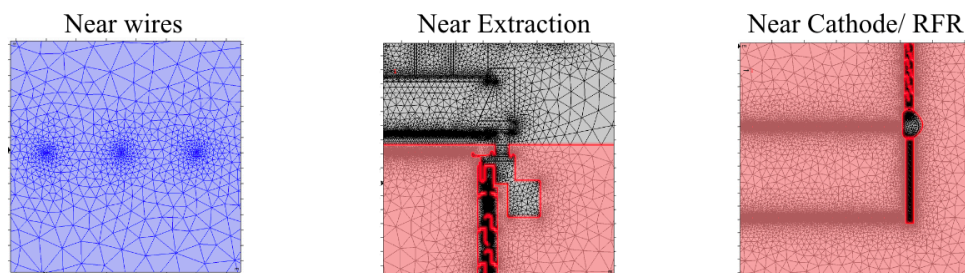


Figure 6.14: Examples of adaptive mesh refinement in the XLZD COMSOL model. Finer elements are used near high-curvature or high-field regions — **(Left)** near the wire planes, **(Centre)** the extraction region, and **(Right)** the cathode and RFR.

The central requirement of the baseline design is field uniformity: the resistor chain biasing the FSRs must enforce a uniform potential drop, ensuring vertical drift lines throughout the active volume. This both guarantees stable charge transport and minimises distortions at detector boundaries. Equally important is the suppression of near-boundary inhomogeneities, which otherwise generate charge-insensitive volumes where electrons are lost before reaching the gas

phase. Experience from LZ data and simulations highlights the regions most vulnerable to elevated or non-uniform fields:

- the inner PTFE wall surface (§4.2.1),
- the cathode and gate electrodes (§4.3),
- the cathode support ring-field cage interface, which sits at the corner between the drift region and the reverse-field region (RFR),
- and the gate–anode–cage interface, where liquid–gas field gradients must be carefully managed.

The latter two regions in particular are natural foci of breakdown risk. Sharp interfaces between materials, together with large potential gradients, can produce localised field enhancements. The preliminary field-optimisation studies conducted confirm the need for careful tuning: if the resistor ladder does not enforce a sufficiently smooth potential grading, equipotential lines can bend into the active volume, creating local “pockets” where electrons are diverted to PTFE surfaces or become trapped in potential wells.

The consequences can be significant: such distortions can bias $S2$ reconstruction, degrade fiducialisation, and generate pathological backgrounds — including isolated $S1$ or $S2$ signals, or false $S1$ – $S2$ coincidences arising from delayed electron release or increased charge loss. These effects have been documented in chapter 4 and also other dual-phase TPCs, and their mitigation requires proactive optimisation of the field cage and its interface with the skin. The first-pass optimised design achieves field values consistent with the targets outlined above. Table 6.5 summarises the representative results for the tuned resistor ladder configuration: These results demonstrate that the baseline design

Table 6.5: Summary of preliminary COMSOL field values for the baseline XLZD field cage design. Uncertainties reflect local variation across the fiducial volume.

Region	Field Value	Notes
Drift field	322.6 ± 6.6 V/cm	Uniform across $0.2 < z < 3.75$ m
Extraction (LXe)	4.72 ± 0.21 kV/cm	Consistent across surface
Electroluminescence (GXe)	9.17 ± 0.02 kV/cm	Above 8 kV/cm threshold
Reverse Field Region (RFR)	10.9 ± 1.0 kV/cm	Below 15 kV/cm limit

maintains the required uniformity in the drift field, with only minor variations with z and negligible dependence on radius. The extraction and electroluminescence fields comfortably exceed the thresholds for efficient electron emission and $S2$ production, while staying within stable operational margins.

Establishing this baseline is essential before moving to cryostat optimisation. The cryostat and skin geometry ultimately determine the radial clearance available around the field cage. If the cage itself were not properly graded, any reduction in skin thickness would exacerbate leakage of equipotential lines into the TPC volume. As illustrated in Fig. 6.15, the detailed field-cage geometry naturally produces localised scalloping at the PTFE boundary, while a misaligned taper at the cryostat wall can drive equipotential leakage into the drift region. Both effects highlight the sensitivity of the TPC–skin interface to electrostatic design choices. Conversely, with the baseline grading in place, we can now meaningfully assess how cryostat tapering and skin standoff impact both high-voltage safety margins and fiducialisation. The next subsection (§6.3.2) builds on this foundation, integrating the cryostat geometry into the electrostatic optimisation.

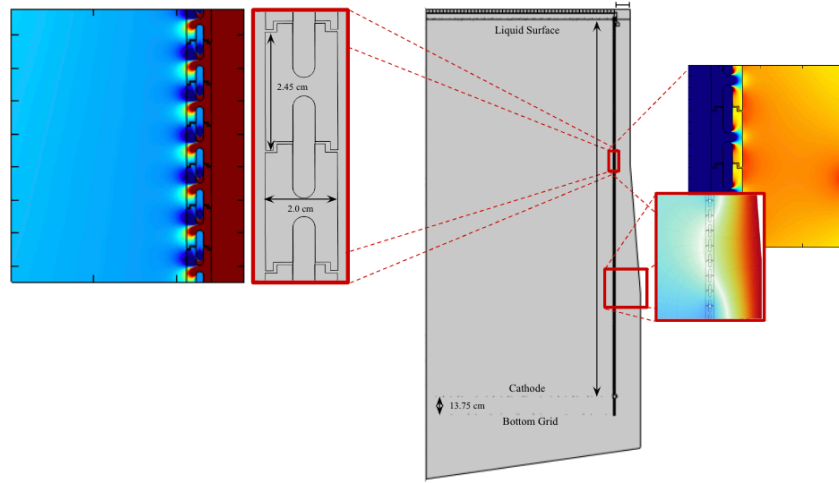


Figure 6.15: Field cage optimisation with explicit PTFE panel geometry. The detailed “tile” structure produces localised field scalloping (left), while a misaligned cryostat taper (right) can drive equipotential leakage into the active volume. Both effects motivate careful optimisation of the TPC–skin interface in the subsequent cryostat studies.

6.3.2 Field-Driven Optimisation of the Cryostat Geometry

Maximising the active LXe mass inside the TPC volume requires minimising the LXe volume within the skin; this is the optimisation process that sets the dimensions of the inner cryostat vessel wall. As discussed previously, any reduction in this skin thickness is constrained by γ /neutron veto efficiencies, which we saw starts to plateau after $\sim 4 - 5$ cm, and thus predominantly relies on electrostatic considerations. In particular, strong electric fields concentrate around the cathode structure at the base of the TPC where the potential-drop is the highest, and if the conductive cryostat wall is brought too close, the cathode’s surface field can exceed safe limits. Previous experiments, including LZ, imposed a conservative 50 kV/cm maximum field on any cathodic surfaces in LXe to avoid spurious electron emission or dielectric breakdown [214, 215]. Our design adopts this same 50 kV/cm criterion as a guideline. We therefore perform detailed electrostatic simulations (using the tuned 2D axially-symmetric COMSOL model described in §6.3.1) to determine the minimum radial skin thickness that keeps the cathode surface fields within this limit.

As shown in Fig. 6.16, the peak cathode surface field drops rapidly with increasing radial clearance. We find that a minimum clearance of about 8.5 cm at the cathode is required to keep the maximum field at or below ~ 50 kV/cm. In practice, we set 9.0 cm as the adopted skin thickness at the cathode plane taking into account machining and engineering tolerances. This 9 cm annular gap at the TPC bottom represents the baseline needed to satisfy the field constraint. Beyond that baseline, we then aim to reduce the skin volume elsewhere by introducing a tapered ICV profile above the cathode. Starting from the cathode elevation ($z = 0$ in our coordinate system), the inner cryostat wall is gradually brought closer to the TPC as one moves upward, thereby shrinking the skin region gradually over the bulk of the detector’s height. Electrostatic simulations indicated that from a purely field perspective the taper could begin immediately at the cathode plane without exceeding the 50 kV/cm limit (i.e. $y_L = 0$ was feasible). In fact, the highest surface fields are very localised right at the cathode ring, so once that region’s 9 cm standoff distance is set, the field profile allows a tighter cryostat spacing above. The only non-electrical constraint was mechanical: the high-voltage feedthrough assembly near the cathode requires some vertical clearance. In our design this necessitated a short

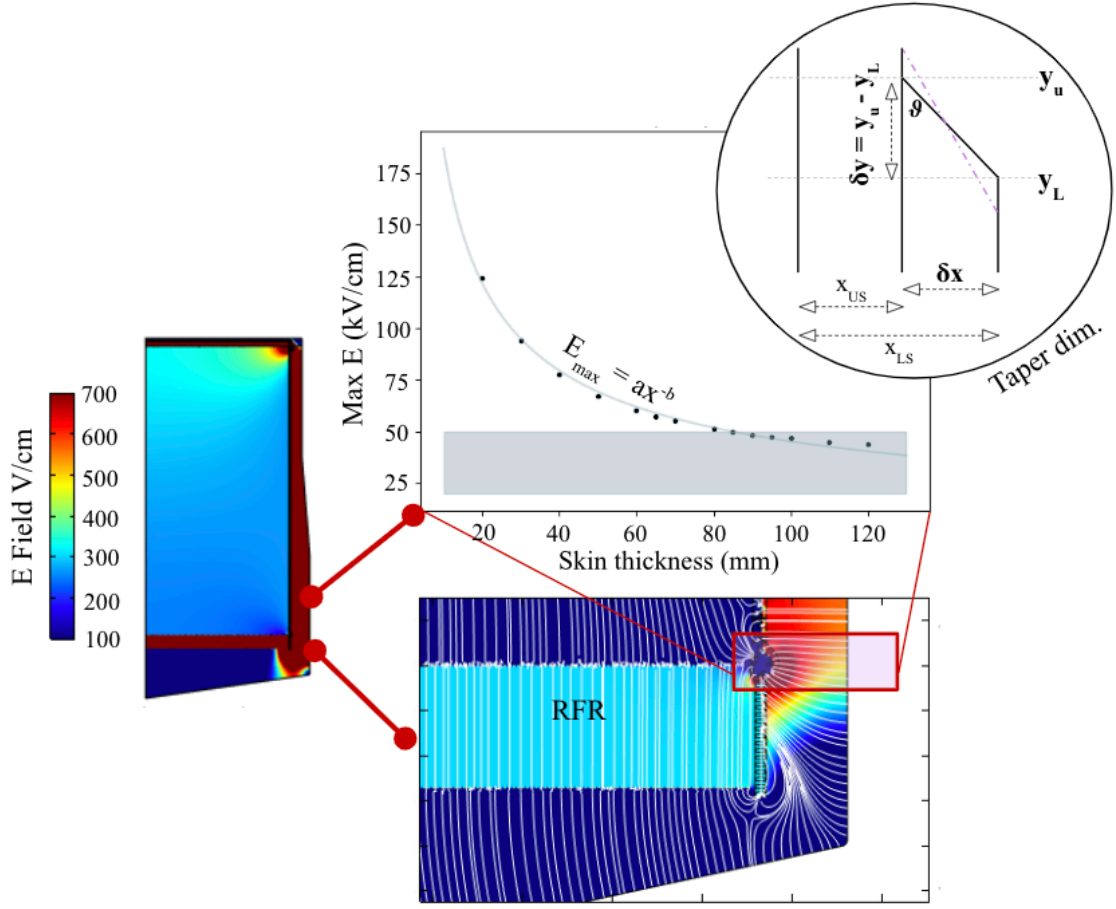


Figure 6.16: Electrostatic optimisation of the XLZD cryostat-skin clearance. **Left:** 2D axisymmetric field map showing peak fields concentrated at the cathode ring. **Centre:** power-law dependence of maximum surface field on side-skin thickness, fitted to $E_{max} = 775x^{-0.617}$; the shaded band indicates the safe operating region below 50 kV/cm. **Bottom inset:** zoom around the cathode showing field leakage into the TPC volume for insufficient clearance. **Top-right inset:** parameterisation of the tapered cryostat geometry, allowing the standoff to vary with height. Together these results motivate a minimum clearance of $\gtrsim 9$ cm at the cathode, tapering towards the top of the detector to reduce xenon consumption in the skin region.

cylindrical section of the cryostat (no taper) for approximately the first ~ 35 cm above the cathode to accommodate the feedthrough hardware. Above this point (roughly $y_L \approx 0.35$ m), the cryostat begins to taper inward. We choose a taper angle of $\sim 5^\circ$, which brings the radial gap from 9.0 cm at y_L down to a minimum of 3.5 cm over a vertical span of about 60 cm. Beyond a height of ~ 0.94 m, the inner wall remains at that smaller radius (a uniform ~ 3.5 cm skin) up to the top of the active region. This geometry achieves a substantial reduction in dead xenon volume while maintaining safe fields and a good veto efficiency.

Crucially, we verify that this aggressive taper does not introduce problematic field distortions or “leakage” of field lines out of the TPC volume. The worst-case scenario we considered was with the thinnest skin region (3.5 cm) and with conductive elements (photomultiplier tubes, PMTs) mounted on the cryostat wall, since any grounded objects protruding into the skin could locally enhance fields. We added a conservative model of the side skin PMTs in the simulation (approximating the array of 2-inch Hamamatsu R12699 [68] PMT bodies as a continuous grounded ring of 1.48 cm radial thickness on the ICV inner wall). Even under this worst-case configuration, the maximum field anywhere in the liquid was found to remain below 50 kV/cm, and no significant field penetration beyond the TPC’s

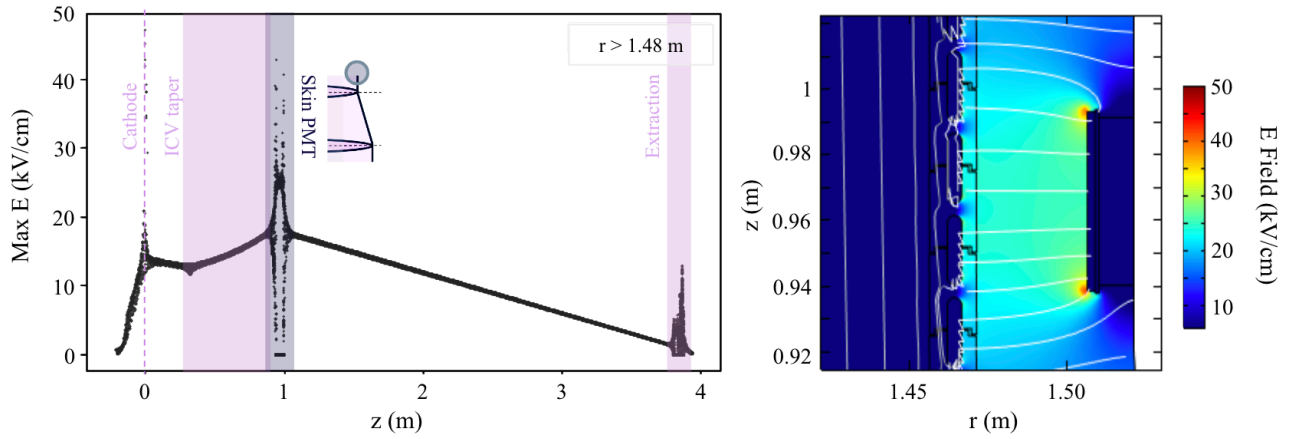


Figure 6.17: Left: The full field profile (magnitude only) as a function of the z within the skin region. The highest fields are evident in the regions near the cathode (cathodic field) and where the PMTs are instrumented (anodic) due to sharp corners and reduced radial distance between the PTFE wall and the PMT surface set to ground. **Right:** Simulation setup in COMSOL showing an example of the fields in a region of the skin where a PMT has been placed.

PTFE wall was observed. The highest fields in the system appeared at two locations: near the cathode (by design, $\sim 50 \text{ kV/cm}$ on the cathode support ring) and immediately around the PMT edges on the skin wall. Although the PMT bodies are anodic with respect to the LXe and therefore not electron-emissive, PMTs are not designed for strong external fields. Following LZ practice and dedicated R&D on Hamamatsu devices, we maintain a skin–PMT standoff of $\sim 3.5 \text{ cm}$, corresponding to a local exposure at the PMT surface to only a few kV/cm ; such conditions have been shown to be benign for stable operation [58, 68, 217] but could still benefit from further R&D. To further minimise risk, shielding or recessed mounting is preferred where compatible with optics and cabling, but the simulations indicate that even unshielded surfaces remain $< 50 \text{ kV/cm}$ and confined to the skin. Fig. 6.17 illustrates the resulting field configuration: the left panel shows the electric-field magnitude along the skin height, with peaks at the cathode and at the skin–PMT band; the right panel presents a radial field map with streamlines, confirming field containment by the PTFE wall and the absence of leakage into the TPC. As shown, all fields remain within the safe range (even with the PMTs grounded rather than biased at their nominal operation potential of $\sim -1 \text{ kV}$), and the TPC’s active volume is well-contained by the field cage with no field lines “leaking” out past the field cage. These simulation outcomes confirm that we can safely instrument the minimal skin region with PMTs for veto purposes, although we note that empirical tests in liquid xenon will be important to ensure that the PMT performance is not degraded by the surrounding field.

The field-driven cryostat optimisation described above yields a design that significantly boosts the detector’s overall efficiency. The final version is shown in Fig. 6.18. By tapering the cryostat inward, the volume of LXe in the skin is dramatically reduced, even with the much higher operational HV requirements of the cathode. In fact, compared to a hypothetical design with a constant 9 cm skin thickness throughout, the tapered geometry saves on the order of $\sim 1.65 \text{ m}^3$ of liquid xenon (approximately 4.84 tonnes of LXe⁹). This recovered xenon can be reallocated to the active TPC volume - either enabling a larger fiducial radius within the same cryostat, or simply reducing the total LXe inventory for a given fiducial mass. In our final 80-tonne TPC layout, the inner cryostat diameter at the level of the top electrode is about 5 cm smaller (on each side) than it would have been without the taper. Yet the

⁹Interestingly, if the HV feedthrough was not a constraint and the taper could be placed on the cathode plane, the total LXe mass saved would have been $\sim 5.68 \text{ t}$, roughly the fiducial mass of LZ currently.

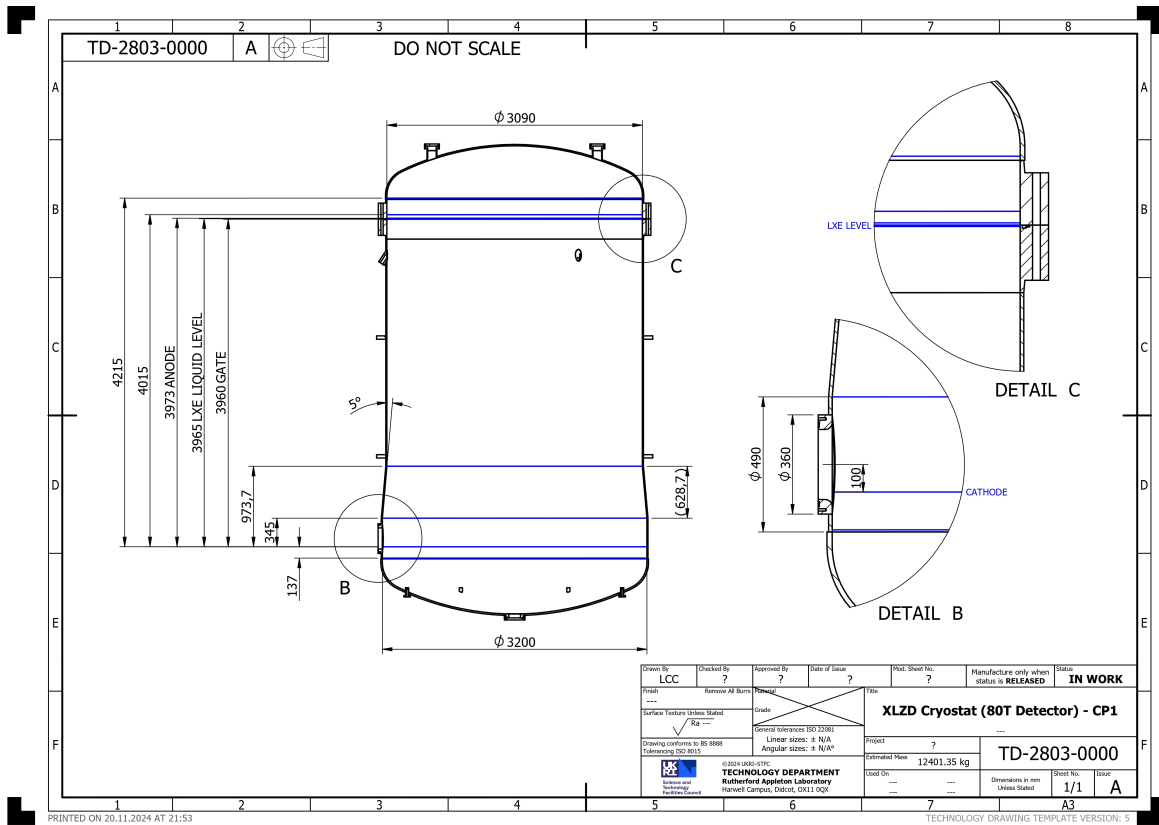


Figure 6.18: Engineering drawing of the preliminary XLZD ICV geometry, showing the tapered side-wall design 5° optimised for high-voltage standoff at the cathode. This design represents a first-pass mechanical realisation of the field-optimised cryostat profile. Drawing provided by L. Cooper.

cathode region still enjoys the required 9 cm clearance for safe high-voltage operation. In summary, by leveraging electrostatic simulations to inform the cryostat shape, we arrived at a configuration that minimises dead volume (from a pure geometric design, no-charge accumulation perspective) while preserving field uniformity and stability. This field-driven design will allow the detector to achieve a higher active-to-total mass ratio and improved physics reach without compromising on high-voltage safety margins.

6.4 The Road Ahead

XLZD now stands squarely in the design phase. The task before us is not a simple scale-up but a coordinated selection among credible architectures: high-voltage delivery and grid geometry, field-cage and reflector strategy, extraction and interface control, cryostat and skin topology, calibration deployment, materials and cleanliness—each traded against transport, reconstruction, and background requirements. Several progressive options sit alongside conservative baselines; what matters is whether a candidate delivers controllable fields, stable charge transport, robust calibration access, and a buildable path to low thresholds. Across the collaboration, engineering prototypes, field/optics simulations, background budgets, and systems-integration work are converging toward choices that can harden into hardware. Near-term decision points include working voltages and grid-deflection tolerances, extraction targets at the chosen gap and temperature, and the veto configuration that best supports physics-driven fiducialisation. These are design choices, and physics choices.

Against that backdrop, the results in these pages provide a through-line from microphysics to instrument design. A coherent transport picture—drift velocity, diffusion, and their field dependences—sets expectations for spatial and temporal resolution. Field reconstruction in LZ quantified non-uniformities and clarified how PTFE charging and geometry imprint on energy scale and fiducial volume. Updates to electroluminescence-gain modelling and an ionisation-only analysis outlined workable routes to sub-keV operation. Collectively, these translate qualitative desiderata into quantitative bounds: tolerable field curvature before bias dominates; grid and gap combinations that achieve extraction and gain at practical voltages; and how veto and cryostat choices interact with calibration and background rejection. The intended impact is pragmatic: fewer commissioning surprises, a faster path from first light to stable calibrations, and analyses that rely on demonstrated, not assumed, uniformity.

The immediate programme is correspondingly clear. For LZ, completion of the ^8B and S2-only analyses, field-aware fiducialisation with quantified azimuthal systematics, and strengthened low-energy neutrino measurements will stress-test response in the regime most relevant to next-generation design; parallel efforts in XENONnT and PandaX-4T provide complementary leverage. For XLZD, convergence on grid geometry and HV operating points, validation of extraction and EL gain at cryogenic conditions, and an agreed skin/outer-veto topology compatible with fiducial definitions will mark decisive progress toward a constructible, schedule-credible and risk-aware detector.

A focused microphysics agenda will tighten tolerances further. Electron momentum transfer at low fields, surface-charge dynamics on dielectrics and metals, interface stability, and impurity- and temperature-dependences of gain are all accessible to current or planned campaigns and each reduces design uncertainty—particularly for achieving stable operation at the highest envisaged voltages. The loop is healthy: data refine models; models close design space; design choices motivate new measurements.

It is an energising moment for dark-matter searches. With growing exposures, improved modelling, and disciplined design, the field is positioned for a decisive inference: either a statistically robust excess consistent across channels and calibrations, or strengthened exclusions across the benchmark spin-independent/spin-dependent WIMP–nucleon parameter space targeted by dual-phase xenon detectors. Either outcome is clarifying. In the former case, transport- and field-aware calibration will determine how quickly properties can be unfolded; in the latter, the same rigour keeps limits durable as we press towards the neutrino-limited regime.

The story that began with electrons in a field now shapes a detector intended to reveal what has so far remained unseen. As decisions firm and results land, the emphasis shifts from verdicts to measurement: characterising any signal if present, and compressing the viable space with statistical authority if not. The lamp is ready; the dark is where it belongs.

Appendices

*We shall not cease from exploration,
And the end of all our exploring
Will be to arrive where we started
And know the place for the first time.*

— T.S. Eliot



Single Electron Electroluminescence Yield Dependences

A.1 Scope & Motivation

THIS APPENDIX pieces together the theoretical framework behind a “quick-reference” toolkit for estimating the intrinsic electroluminescence (EL) yield of a single, already-extracted electron (SE) in xenon gas that is in equilibrium with its own liquid i.e. in saturated xenon vapour. This formalism is then extended to $Xe - H_2$ admixtures, supported by recent results from the HydroX experiment [218].

In a dual-phase TPC, the vapour pressure is dictated passively by the liquid temperature, so that the gas density and therefore the mean free path and excitation probability are fixed once the cryostat is cold¹. Above a threshold reduced field² the photon yield (LY in photons per electron) follows a simple linear law, parameterised by two empirically determined constants a (for example $\sim 151 \text{ photons } e^{-1} \text{ kV}^{-1}$) and b ($\simeq -147 \text{ photons } e^{-1} \text{ cm}^{-1} \text{ bar}^{-1}$ as in Aprile *et al.* [195]), which features part of the discussion in this section.

$$LY(E_g, h_g, P_g) = \left(a \frac{E_g}{P_g} + b \right) h_g P_g, \quad [E_g = \text{kV cm}^{-1}, h_g = \text{cm}, P_g = \text{bar}]. \quad (\text{A.1})$$

Equation A.1 should then hold for any pressure P_g , field E_g or gas gap h_g , provided that the xenon gas is supersaturated. As a result, the tables and heat maps provided in this section should be able to predict the raw number of VUV photons created by a single electron in any xenon TPC that employs a gaseous proportional-scintillation region. This relationship is also readily extended to provide an approximate value for *ADC* counts per single-electron pulse,

$$\text{ADC}_{\text{SE}} = LY \times \underbrace{\text{CE}}_{\text{dynode collection}} \times \underbrace{LCE}_{\text{geometry}} \times \underbrace{DPE \text{ Corr}}_{\text{double photoelectron}} \times \underbrace{QE}_{\text{quantum efficiency}} \times \underbrace{G_{\text{elec}}}_{\text{electronics gain}}.$$

This is defined and discussed in full detail in equation A.14. Such estimates are invaluable for first-pass peak-finding, S2-template building and fine-tuning event-reconstruction thresholds in existing or future xenon TPCs. They also provide a quick cross-check when optimising fields and geometry: once the gap and extraction region are fixed, raising E_g or lowering P_g translates linearly into the SE gain, and therefore into the ultimate energy and position resolution achievable after all other corrections (electron-lifetime, diffusion, optical transport) are applied. In this appendix we

¹Here we define “cold” as the final temperature of the operational TPC, at $\sim 174 \text{ K}$ or above the LXe-GXe saturation point.

²The field per unit pressure in *bar*.

do not model those detector-specific corrections themselves; photon detection efficiency, charge extraction probability and mesh transparency are treated and discussed instead in Chapters 3 and 6. Consequently, the numerical values quoted here should be regarded as first-order estimates with an accuracy of the order of $\sim \pm 15\%$, reflecting the spread of modern EL measurements.

A.2 The Standard Linear Gain Model

A.2.1 Electron energy distribution in a uniform field

For a weakly ionised gas, the steady-state electron distribution $f(\varepsilon)$ obeys a two-term Boltzmann equation [219, 220]

$$eE_g \frac{\partial f}{\partial \varepsilon} = N \sum_j \sigma_j(\varepsilon) v(\varepsilon) \mathcal{L}_j[f], \quad (\text{A.2})$$

with the gas number density expressed as $N = P_g/k_B T$ as an explicit function of temperature in K as per the ideal gas law, $\sigma_j(\varepsilon)$ the cross-section for collision channel j (elastic, excitation, ionisation, etc.) and $v(\varepsilon) = \sqrt{2\varepsilon/m_e}$. Finally, $\mathcal{L}_j$ subtracts electrons that lose energy $\Delta\varepsilon_j$ and adds those that scatter in from higher energies.

Below the 12 eV Xe ionisation threshold, the only important inelastic loss is the first atomic excitation at 8.3 eV [221]; elastic scattering therefore dominates, and a Chapman-Enskog expansion to first order in E_g gives [222]

$$\begin{aligned} f(\varepsilon) &\simeq f_M(\varepsilon; T) \left[1 + \frac{eE_g \lambda_{mfp}}{2k_B T} \left(\frac{\varepsilon}{k_B T} - \frac{3}{2} \right) \right], \\ f_M(\varepsilon; T) &= \frac{2}{\pi} \frac{\varepsilon^{1/2}}{(k_B T)^{3/2}} \exp\left(-\frac{\varepsilon}{k_B T}\right), \quad \int_0^\infty f_M(\varepsilon; T) d\varepsilon = 1, \end{aligned} \quad (\text{A.3})$$

where $\lambda_{mfp} = 1/N\sigma_{el}$. In this expression, f_M is simply the equilibrium Maxwell-Boltzmann energy-distribution function for electrons at the gas temperature T , while the bracketed term represents a small, field-induced perturbation to the thermal Maxwellian core valid in the regime where the mean energy gain between collisions is still $\lesssim \mathcal{O}(k_B T)$. Hence, the mean energy gain between collisions can be written.

$$\langle \Delta\varepsilon \rangle = \frac{eE_g \lambda_{mfp}}{2} \propto \frac{E_g}{N} \equiv \frac{E_g}{P_g} k_B T. \quad (\text{A.4})$$

This translates directly to the number of photons produced per single electron in a given interaction.

A.2.2 Excitation rate

The excitation coefficient (photons produced per *cm* transited by an electron) is then given by

$$k_{exc} = N_{Xe} \int_{\varepsilon_{th}}^\infty \sigma_{exc}(\varepsilon) v(\varepsilon) f(\varepsilon) d\varepsilon. \quad (\text{A.5})$$

From equation A.3 and propagating only a first-order expansion, the linear gain model can be reproduced subject to the assumption that only electrons with $\varepsilon > \varepsilon_{th}$ can contribute and thus, the excess probability is proportional to $\Delta\varepsilon$. The form of the coefficient can then be written as [72]

$$k_{exc}(E_g, P_g, T) = \alpha E_g - (\beta P_g + \gamma). \quad (\text{A.6})$$

It should be noted here that this form assumes that the density of saturated vapour is well described by a linear function of pressure $\rho(p) = a_0 + a_1 P$, which has been shown to be a good approximation to at least 10 bar [72, 223]. For completion, we also quote the averages of swarm-analysis fits compiled by Chepel & Araujo (2013) [72]³:

- the excitation coefficient $\alpha = (1.34 \pm 0.10) \times 10^2 \text{ photons } e^{-1} \text{ cm}^{-1} \text{ kV}^{-1}$
- the reduced field threshold $\beta = -177 \text{ cm}^{-1} \text{ bar}^{-1}$
- a small constant offset $\gamma = 45.7 \text{ cm}^{-1}$

A.2.3 Gap integration

For a uniform anode-cathode gap of physical thickness $h_g \text{ cm}$:

$$LY(E_g, h_g, P_g, T) = k_{exc} h_g. \quad (\text{A.7})$$

By applying the expression for k_{exc} in equation A.6, it is found that

$$LY = \left(a \frac{E_g}{P_g} + b \right) h_g P_g, \quad (\text{A.8})$$

where an equivalence between Chepel & Araujo [72] and Aprile et. al. [195] may be expressed as $a \equiv \alpha$ and $b = -\beta - \gamma/P_g$. The values of these fit coefficients will be discussed in §A.3.

A.2.4 Theoretical temperature dependence

The Clausius-Clapeyron relation [224] specifies the temperature dependence of vapour pressure at a discontinuous phase transition between two phases of a substance; this is where we start. For a dual phase TPC, the gas pocket is in equilibrium with the liquid; hence $P_g = P_{sat}(T)$.

$$\frac{dP_{sat}}{dT} = \frac{L}{T \Delta v} \quad (\text{A.9})$$

, where L is the molar latent heat, and $\Delta v (\simeq RT/P$ if the vapour behaves ideally) is the molar volume change of the phase transition. Integrating under the (fairly good) approximation that L is a constant over a narrow temperature interval yields $\ln(P_{sat}) = -\frac{L}{RT} + \text{const}$, which can be written instead, in terms of $\log_{10}(P_{sat})$. This introduces a small empirical offset C , which compensates for the latent-heat ($\sim \mathcal{O}(4\%)$ fluctuations) and non-ideality changes that occur over a wider ($\sim 160 - 200 \text{ K}$) range. The result is the three-term Antoine equation describing the saturated-vapour curve to $\pm 0.3\%$ by the Michels & Wassenaar fit [225] tabulated in the NIST WebBook [226]⁴,

$$\log_{10}(P_{sat}) [\text{bar}] = A - \frac{B}{T - C}, \quad A = 3.80675, B = 577.66, C = 13.0. \quad (\text{A.10})$$

Applying this condition to equation A.8 gives an explicit T -dependent gain.

$$LY = \left(\frac{a E_g}{10^{A - \frac{B}{T - C}}} + b \right) 10^{A - \frac{B}{T - C}} h_g. \quad (\text{A.11})$$

³See specifically table 4 of the reference for more details.

⁴For ultra-high precision, e.g. REFPROP's $\pm 0.02\%$ accuracy [226], a Clapeyron-type ‘‘Wagner equation’’ with eight terms is used instead.

As P_{sat} only varies by 12% between 165 K and 190 K , equation A.11 reproduces most cryogenic measurements to within 15%. This is discussed further and explicitly visualised for various dual-phase experiments in § A.2. For completion it should also be noted that for unsaturated or warm gas tests (Monteiro (2007) at 2 bar , 293 K [227]), P_g and T should be kept independent (not related to the Antoine equation), and retaining the γ/P_g term in equation A.6 captures the relationship with light yield more completely.

A.3 Photon Yield

A.3.1 Model Results & Discussion

To put the linear electroluminescence-gain law on the strongest quantitative footing, every pure-xenon EL measurement published from 1973 to 2024 was collected and recast in reduced variables,

$$x = \frac{E_g}{P_g} [kV \text{ cm}^{-1} \text{ bar}^{-1}], \quad y = \frac{LY}{h_g P_g} [\text{photons } e^{-1} \text{ cm}^{-1} \text{ bar}^{-1}] \quad (\text{A.12})$$

so that data with different gaps, pressures, or operational conditions lie on a common plane. Studies with information on the three key operating parameters (E_g , P_g , h_g), including operational temperature were chosen.

Cryogenic points ($T \lesssim 185 \text{ K}$) come from xenon vapour in equilibrium with liquid: exactly the regime relevant to dual-phase TPCs. Room-temperature points ($T \simeq 290 \pm 5 \text{ K}$) cover 1 – 10 bar GPSC (gas proportional scintillation chamber) measurements and Monte-Carlo/Boltzmann calculations [132]. Treating the two sets separately avoids conflating the known density dependence of the EL slope with genuine experimental scatter. We then fit the linear law in two ways:

- *Fit A* is completely temperature-agnostic: each point uses its reported (E_g , P_g).
- *Fit B* enforces the saturated-vapour relation $P_g = P_{sat}(T)$ for all cryogenic points.

Comparing the two fits quantifies both the intrinsic spread of the cryogenic data and the systematic shift that appears when room-temperature results are folded in. The fitted coefficients are discussed below; Fig. A.1 summarises every data set on a single reduced-field plane and table A.1 quantifies the fits.

Table A.1: Linear-gain coefficients obtained from the global fits and criteria discussed in the text. All errors are statistical 1σ from the weighted least-squares regression. A 5% “digitisation” uncertainty is added in quadrature when the original paper quotes only line fits.

Subset	a [photons $e^{-1} \text{ kV}^{-1}$]	b [photons $e^{-1} \text{ cm}^{-1} \text{ bar}^{-1}$]
Cryo-only	140 ± 6.5	-146 ± 9.6
Room-Temp (RT) only	111.0 ± 12.7	-95.8 ± 9.7
Fit A (Cryo + RT)	122 ± 8.9	-115 ± 9.8
Fit B (Sat-vap only)	144.0 ± 7.0	-136.0 ± 11.0

The “cryo-only” regression returns an amplification parameter $a_{cryo} = 140 \pm 15 \text{ photons } e^{-1} \text{ kV}^{-1}$. For the room-temperature data sets the slope collapses to $a_{RT} = 111 \pm 13 \text{ photons } e^{-1} \text{ kV}^{-1}$. This is the canonical density effect first noted by Monteiro (2007)[227]; at 293 K the gas density is roughly twice the saturated-vapour density at

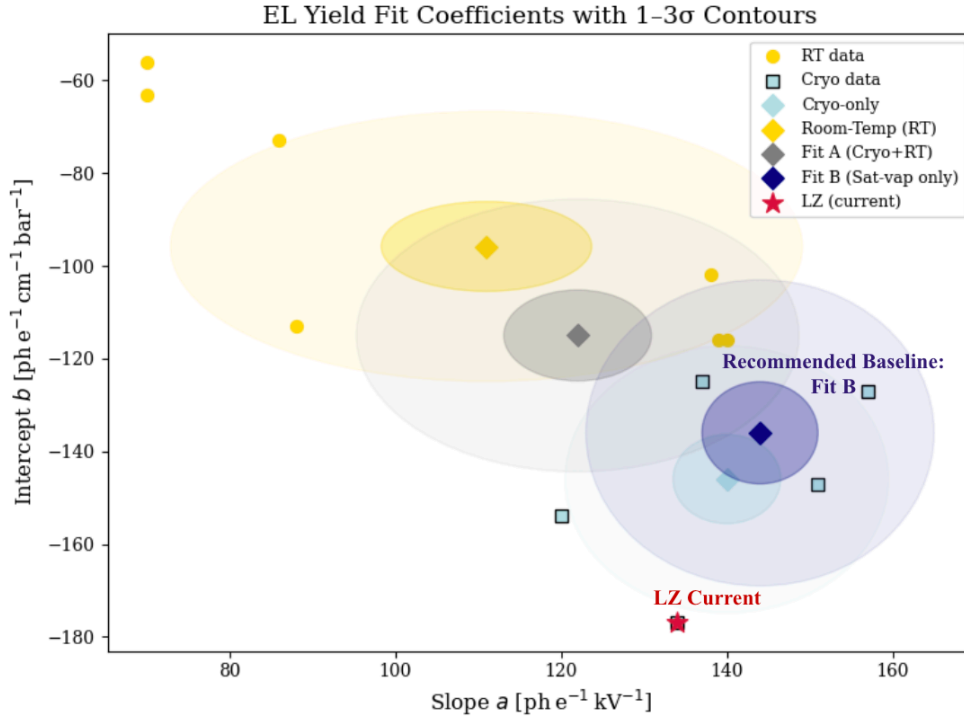


Figure A.1: Comparison of electroluminescence yield fit coefficients. Slope a versus intercept b for a variety of published EL-yield parameterisations. Light blue squares and gold circles denote individual cryogenic-vapour and room-temperature measurements, respectively. The large diamonds mark our four “global” linear fits (Cryo-only, RT-only, combined Cryo+RT, and saturated-vapour), with shaded 1 and 3σ ellipses drawn to scale in a and b . The red star indicates the LZ detector’s current simulations assumption. This plot highlights both the inter-study scatter in EL coefficients and the relative precision/similarity between each global fit.

175 K, so electrons gain less energy between collisions and excite fewer xenon dimers per centimetre. This quantitative difference is already visible in the earliest measurements (Parsons (1973) [228]) and remains consistent with the most recent room-temperature GPSC data of Fonseca (2021) [229].

Fit B (Fig. A.2) keeps only points demonstrably on the saturated xenon vapour curve and yields $(a, b) = (144 \pm 7, -136 \pm 11)$. However, there are a few excursions to take note of. The Fonseca (2021) [229] fit lies noticeably farther from the Antoine saturation curve because it represents a weighted average over several data sets taken at different liquid-level (and hence gas-gap) configurations. Small variations in liquid level directly change the effective gas pressure in the extraction region, so combining runs with 1 cm, 3.5 cm, and intermediate gaps produces a mean point that does not coincide exactly with the single-valued equilibrium curve. In contrast, each of the larger, dual-phase detectors (XENON100, XENON1T and XENONnT) was operated with a fixed, well-measured gas height and actively regulated pressure system, which should in principle follow the Antoine relation more closely. Their modest offsets from the curve likely stem from practical considerations; slight temperature gradients between the liquid and gas volumes, deliberate over- or under-pressurisation to optimise electron extraction (most likely) and prevent micro-condensation in the high-field region. These engineering choices shift the apparent saturation point by a few tenths of a bar, explaining why their markers lie just above or below the ideal vapour-pressure curve.

As modern dual-phase TPCs always operate on (or near) saturated vapour (cf. Fig. A.2), it is justified that Fit B should

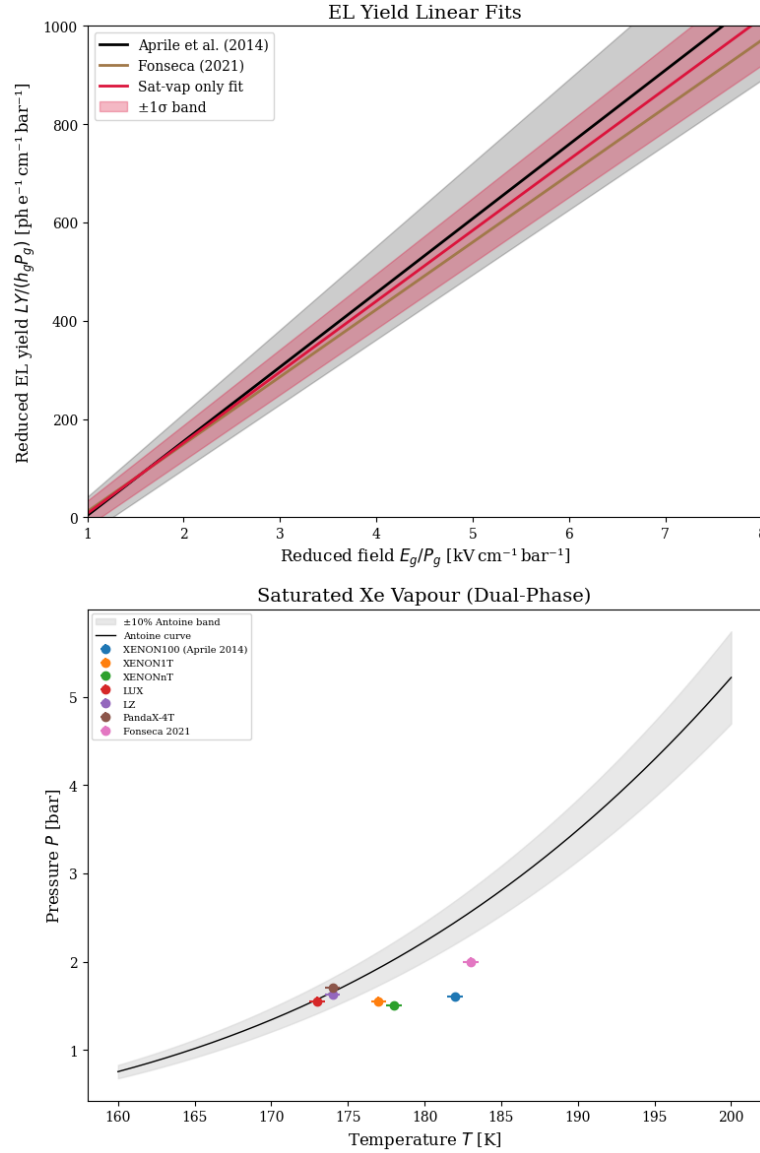


Figure A.2: (Top) Reduced EL-yield as a function of reduced field E_g/P_g , comparing literature fits (Chepel & Araújo 2013 [72]; Aprile *et al.* 2014 [195]; Fonseca 2021 [229]) and the saturated-vapour “Fit B” with its $\pm 1\sigma$ band. **(Bottom)** Xenon vapour saturation pressure vs. temperature from the Antoine equation ($\pm 10\%$), with operating points of major dual-phase detectors overlaid.

be the recommended baseline for first-order estimates of the resulting EL yields from these experiments.

Finally a note must be made to directly address the Chepel–Araújo (2013) [72] review, which adopts $(a, b) = (137, -177 - \frac{45.7}{P_g})$. This slope was extracted from pre-2000 data with lower light-collection efficiency, hence resulting in a more negative intercept due to averaging several warm-gas lines (particularly with pre-2000 slopes biased towards slopes with $a \sim 70 - 80$ [228, 230, 231]). LZ simulation packages still default to this pair. Using the Fit B values could raise the predicted single-electron gain by $\approx 20\%$ (Fig. A.3). The implications of this has not been tested yet but would likely lead to the re-tuning of various S2-yield-related simulation variables that have been calculated empirically in combination to match data. In essence, the impact on current LZ analyses should be minimal due to the degeneracy and highly-correlated nature of the corrections made downstream to the EL yield assumptions, but they should allow

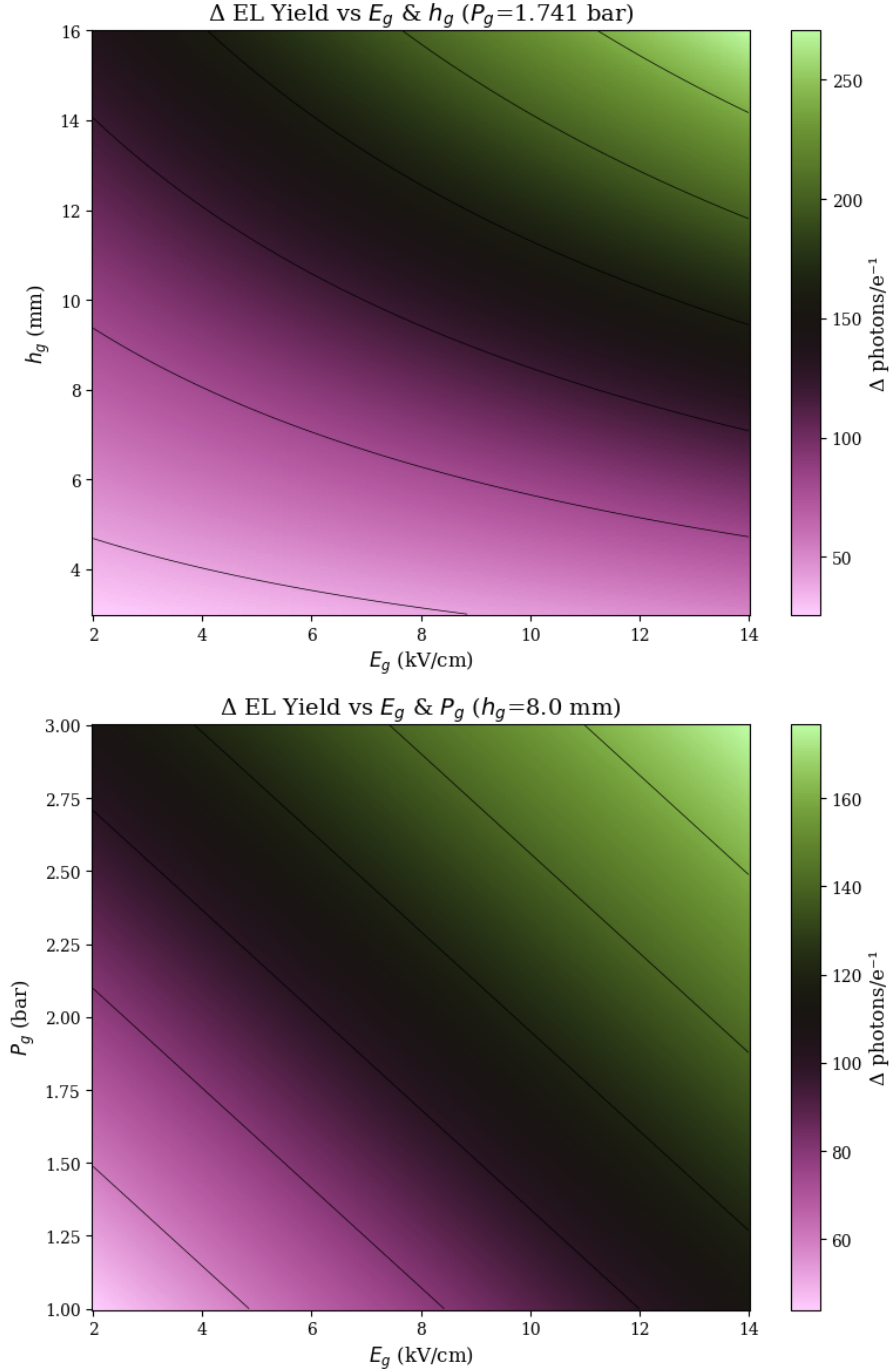


Figure A.3: Heat-map of the minimum difference in electroluminescence yield $\Delta LY = LY_{\text{Fit B}} - LY_{\text{CA}}$ (photons per electron), shown as **(Top)** a function of gas field E_g and gap h_g at fixed $P_g = 1.741$ bar, and **(Bottom)** a function of E_g and pressure P_g at fixed $h_g = 8$ mm. Contour lines mark equal-difference levels. This illustrates how deviations between the two parametrisations grow with increasing field, gap, or pressure using LZ's operational parameters as a reference.

for more accurate measurements of physical variables and quantities if corrected going forward, which could improve our understanding of S2 signals in TPCs like LZ.

Uncertainties & Potential Biases

- Pressure-temperature relationship

The Antoine relation (equation A.10) used in Fit B is shown to $\pm 10\%$ below 190 K in Fig. A.2. The figure also overlays the corresponding operating values for six “modern” dual-phase TPC-based detectors (XENON100, XENON1T, XENONnT, PandaX-4T, LUX, LZ), some of which lie inside that band, some which lie close but not quite within. Refitting with those points moves (A, B, C) by $< 1\%$, translating to $< 1\%$ bias on (a, b) .

- Low-field curvature

All linear laws overshoot below $E_g/P_g \lesssim 1\text{ kV cm}^{-1}\text{ bar}^{-1}$ [232]⁵. That region is never used for operation in dark matter searches (low extraction efficiency and EL yield, but if a detector chooses a very low anode-cathode field (e.g. 3 kV cm^{-1} at 1.6 bar), a correction of the yield of $\approx -5\%$ would be required.

- High-field multiplication

Above $E_g/P_g \gtrsim 6$ avalanche gain starts to inflate the apparent slope; none of the fits include those points. Megaton-scale detectors that contemplate 14 kV anode-gate potential differences must model the transition explicitly.

- Gap-height extrapolation

All data have $3 < h_g < 8\text{ mm}$. Going to slightly larger, cm -scale EL gaps (NEXT [233], DARWIN [234]) is safe only if the meshes maintain similar optical transparency. Otherwise b will shift.

- Temperature sensitivity

Below 185 K the saturated-vapour density changes by only $0.3\% \text{ K}^{-1}$. Even a 3 K control variation shifts the single-electron gain by $< 1\%$: much smaller than the $\pm 5\%$ optical-collection uncertainty in most analyses. Temperature therefore enters primarily via its influence on vapour pressure, not via additional microscopic scattering effects.

Adopting $(a, b) = (140, -146)$ with a $\sim 10\%$ systematic envelope captures the saturated-vapour cryogenic EL data available from 1976 $\rightarrow$ 2024 as illustrated in Fig. A.1. Using older room-temperature parameters (Chepel–Araújo [72] or Akimov [230]) could under-predict an S2 photon budget by 20 – 30%, directly biasing energy and position reconstruction.

⁵The study cited here is for predominantly Krypton but includes discussions of Xenon for comparison.

A.3.2 From Photons to ADC Counts

The intrinsic quantity delivered by the EL model is the number of VUV photons produced per extracted electron,

$$N_\gamma \equiv LY(E_g, h_g, P, f) \quad [\text{photons/e-}], \quad (\text{A.13})$$

but the experiment records a digitised area in ADC counts. The chain of efficiencies between the excimer yield and the digitiser can be factorised as

$$\text{ADC}_{\text{SE}} = LY \times \underbrace{\text{CE}}_{\text{dynode collection}} \times \underbrace{\text{LCE}}_{\text{geometry}} \times \underbrace{\text{DPE Corr}}_{\text{double photoelectron}} \times \underbrace{\text{QE}}_{\text{quantum efficiency}} \times \underbrace{G_{\text{elec}}}_{\text{electronics gain}}. \quad (\text{A.14})$$

- The photon detection efficiency is defined as $PDE = LCE \times QE$. This is sometimes referred to as the g_1 value, quantitatively capturing geometric light collection and optics, mesh transparency and the photocathode quantum efficiency.
- The dynode collection efficiency (CE) is the probability that a photoelectron released from the cathode actually reaches the first dynode of the PMT.
- The double photoelectron effect or DPE accounts for the $\sim 20 - 30\%$ chance that a 175 nm photon ejects two electrons from a bialkali photocathode.
- G_{elec} converts photoelectrons into ADC area (e.g. 0.50 ADC/PE for the LZ digitiser [235]).

Putting in representative LZ numbers and the pure-Xe yield at $\sim 6.75 \text{ kV cm}^{-1}$ (from Fit B in table A.1)

$$\begin{aligned} N_\gamma &= 610 \text{ ph/e-}, \\ \text{ADC}_{\text{SE}} &= N_\gamma \times (PDE) \times (CE) \times (DPE \text{ Corr}) \times (G_{\text{elec}}) \\ &= 610 \times (0.12) \times (0.90) \times (1 + 0.30) \times (0.50) \\ &\approx 43 \text{ ADC counts/e-}, \end{aligned} \quad (\text{A.15})$$

2σ away from the $49 \pm 3 \text{ ADC counts}$ observed for single electrons in LZ commissioning data [235], but still reasonable given this *very* quick calculation.

As $N_\gamma \propto LY$, the same formula can also immediately predict how the digitised SE pulse area scales with field, gap or even H_2 admixture fraction f to first-order for low f (see §A.4). It is also noted that any of the associated uncertainties will propagate linearly: a $\pm 10\%$ relative error on the photon yield or on PDE translates to the same $\pm 10\%$ on the expected ADC area. Consequently, once LY is fixed by the fit in § A.4, the equations in § A.5 provide a direct, first-pass SE-template normalisation for any future Xe or $Xe - H_2$ TPC. The mechanisms via which H_2 quenches the S2 signal, the fit procedure and associated uncertainties are next discussed.

A.4 The Effect of Hydrogen-Doping on Microscopic Scattering and EL Yield

When a small hydrogen molar fraction $f = N_{H_2}/(N_{H_2} + N_{Xe}) \ll 1$ is added to xenon gas, several microscopic interaction channels are introduced that alter the electron swarm and thus the electroluminescence yield [236–238]. In this section, a theoretical framework is suggested, extending the well-established pure-xenon case, to deal with admixtures of gases, particularly xenon and hydrogen. In dual-phase time projection chambers, even a sub-percent admixture of H_2 can measurably reduce S2 light through (i) increased elastic scattering (shortening mean free path), (ii) additional low-energy inelastic (rotational/vibrational) losses (cooling the high-energy tail), and (iii) VUV self-absorption of the 172 nm excimer photons by H_2 . This appendix provides a self-contained, first-principles derivation of how to incorporate these effects into the familiar linear EL “gain” law discussed in the previous section, culminating in explicit definitions and rough estimates of new mixture parameters K_a , K_b , κ . This discussion will be broken down into two parts:

- §A.4.1 *First-Order Mixture Theory*: This is an extension to the Boltzmann-equation analysis of pure Xe to a $Xe - H_2$ mixture, where we will derive the perturbed electron energy distribution to $\mathcal{O}(f)$, then substitute into the excitation-rate integral to obtain a linearised excitation coefficient $k_{\text{exc}}(f)$.
- §A.4.1 *Estimating K_a , K_b , κ* : We will provide explicit integral definitions of K_a (slope reduction) and K_b (threshold shift), followed by numerical, order-of-magnitude estimates based on published cross-sections. This will be used to draw conclusions on the validity of this first-order theory, and to what extent (and how) the approximation appears to deviate from observations.

A.4.1 First-Order Mixture Theory

Pure-Xenon Benchmark and Notation

In pure xenon, the stationary, isotropic Boltzmann equation for the single-electron energy distribution $f_0(\varepsilon)$ under a uniform reduced electric field E_g is written as [132, 239],

$$eE_g \frac{\partial f_0(\varepsilon)}{\partial \varepsilon} = N_{Xe} \left[\sigma_{\text{el}}^{Xe}(\varepsilon) \mathcal{L}_{\text{el}}[f_0] + \sigma_{\text{exc}}^{Xe}(\varepsilon) \mathcal{L}_{\text{exc}}[f_0] \right], \quad (\text{A.16})$$

where each of the terms are defined as follows:

- e is the elementary charge; E_g (in $kV \text{ cm}^{-1}$) is the reduced electric field across the gas gap.
- $N_{Xe} = P_g/(k_B T)$ is the xenon number density (per cm^3) at pressure P_g and temperature T .
- $\sigma_{\text{el}}^{Xe}(\varepsilon)$ is the momentum-transfer (elastic) cross section for electrons colliding with xenon atoms [239, 240].
- $\sigma_{\text{exc}}^{Xe}(\varepsilon)$ is the electronic-excitation cross-section for Xe (threshold $\sim 8 \text{ eV}$).
- $\mathcal{L}_{\text{el}}$ and $\mathcal{L}_{\text{exc}}$ are the collision operators (Fokker-Planck or Boltzmann-integral forms) for elastic and excitation processes, respectively [132].

By solving equation (A.16) (with Magboltz or Biagi's formalism), one obtains $f_0(\varepsilon)$. The pure-Xe EL excitation coefficient $k_{\text{exc}}^{(0)}$ (*photons e⁻¹ cm⁻¹ bar⁻¹*) is then defined by integrating the product $\sigma_{\text{exc}}^{Xe} v(\varepsilon) f_0(\varepsilon)$ over energy:

$$k_{\text{exc}}^{(0)} = N_{Xe} \int_0^\infty \sigma_{\text{exc}}^{Xe}(\varepsilon) v(\varepsilon) f_0(\varepsilon) d\varepsilon. \quad (\text{A.17})$$

Empirically, across many GPSC (gas proportional scintillation counter) and dual-phase TPC measurements (see table A.1),

$$k_{\text{exc}}^{(0)} = \alpha E_g - \beta P_g - \gamma, \quad \begin{cases} \alpha \approx 122 \text{ photons } e^{-1} \text{ kV}^{-1}, \\ \beta \approx -115 \text{ photons } e^{-1} \text{ cm}^{-1} \text{ bar}^{-1}, \\ \gamma \approx 0 \text{ cm}^{-1} \text{ (small residual intercept)}. \end{cases} \quad (\text{A.18})$$

Consequently, the macroscopic single-electron light yield in a gas layer of thickness h_g is

$$LY^{(0)} = k_{\text{exc}}^{(0)}(h_g) = [\alpha E_g - \beta P_g - \gamma] h_g. \quad (\text{A.19})$$

In the limit $\gamma \rightarrow 0$ i.e. in the case of an “ideal fit”, the yield goes to zero when $\alpha E_g = \beta P_g$; this is what we expect in this regime, where slope reduction and threshold shift are highly (anti) correlated[241].

Extending to a $Xe - H_2$ Mixture

In §A.3, the relevant coefficients for a pure-xenon system are discussed. These are now well-established from both measurement and simulation. On the other hand, new coefficients are needed to provide a complete description of the H_2 admixture and these are less precisely known or understood; beyond simulations, no dedicated experimental measurement or theoretical framework characterising the differences exists. One aim of this appendix is to attempt some preliminary quantification and validation of these effects using data from the HydroX experiment [218].

We start by introducing a small H_2 fraction $f = N_{H_2}/(N_{H_2} + N_{Xe}) \ll 1$. Throughout, $N \approx N_{Xe}(1 + f) \approx N_{Xe}$ to $\mathcal{O}(f)$, so we can keep only linear corrections in f . The Boltzmann equation for the isotropic distribution $f(\varepsilon; f)$ in the mixture becomes

$$eE_g \frac{\partial f(\varepsilon; f)}{\partial \varepsilon} = N \left[(\sigma_{\text{el}}^{Xe} + f(\sigma_{\text{el}}^{H_2} - \sigma_{\text{el}}^{Xe})) \mathcal{L}_{\text{el}}[f] + \sigma_{\text{exc}}^{Xe} \mathcal{L}_{\text{exc}}[f] + f \sigma_{\text{rot,vib}}^{H_2} \mathcal{L}_{\text{rot,vib}}[f] \right], \quad (\text{A.20})$$

where,

- $\sigma_{\text{el}}^{H_2}(\varepsilon)$ is the H_2 momentum-transfer cross section. In the 10–15 eV energy region (relevant for Xe excitation), $\sigma_{\text{el}}^{H_2}$ often exceeds σ_{el}^{Xe} by a factor $\sim 10 - 20$ [132, 236].
- $\sigma_{\text{rot,vib}}^{H_2}(\varepsilon)$ is the combined rotational and vibrational excitation cross section of H_2 , with threshold losses in the $\Delta\varepsilon \approx 0.015 - 0.5 \text{ eV}$ range [242]. These inelastic collisions “cool” the swarm at low energies.
- $\mathcal{L}_{\text{rot,vib}}$ is the collision operator that removes electrons from energy ε to $\varepsilon - \Delta\varepsilon$.

This distribution can be expanded in powers of f :

$$f(\varepsilon; f) = f_0(\varepsilon) + f f_1(\varepsilon) + \mathcal{O}(f^2), \quad (\text{A.21})$$

where $f_0(\varepsilon)$ satisfies the pure-Xe Boltzmann equation (A.16). Substituting into (A.20) and collecting orders:

- $\mathcal{O}(f^0)$ recovers the pure-Xe equation

$$eE_g \partial f_0 / \partial \varepsilon = N_{Xe} [\sigma_{el}^{Xe} \mathcal{L}_{el}[f_0] + \sigma_{exc}^{Xe} \mathcal{L}_{exc}[f_0]].$$

- $\mathcal{O}(f^1)$ yields a linear equation for $f_1(\varepsilon)$:

$$eE_g \frac{\partial f_1}{\partial \varepsilon} = N \sigma_{el}^{Xe} \mathcal{L}_{el}[f_1] + N \sigma_{exc}^{Xe} \mathcal{L}_{exc}[f_1] \quad (\text{A.22})$$

$$+ N [\sigma_{el}^{H_2} - \sigma_{el}^{Xe}] \mathcal{L}_{el}[f_0] + N \sigma_{rot,vib}^{H_2} \mathcal{L}_{rot,vib}[f_0]. \quad (\text{A.23})$$

Physically, the third term on the right is a source term reflecting that, in the mixture, elastic scattering is now governed by $\sigma_{el}^{H_2}$ instead of σ_{el}^{Xe} (with weight f). The fourth term is a new inelastic “cooling” channel from H_2 rotational and vibrational excitations, again at $\mathcal{O}(f)$.

As $f_0(\varepsilon)$ is known (from the pure-Xe solution), each of the source terms on the right of (A.23) is a known function of ε . By then solving the Chapman–Enskog hierarchy, the first-order correction $f_1(\varepsilon)$ takes the approximate form [236, 242]:

$$f(\varepsilon; f) \approx f_0(\varepsilon) \left[1 + \chi_0 \frac{E_g}{N} (1 - K_e f) \right] + \mathcal{O}(f^2). \quad (\text{A.24})$$

In this expression:

- $\chi_0 \equiv \frac{e\lambda_{mfp}}{2k_B T}$ is a small, dimensionless field-coupling parameter (proportional to the ratio of energy-gain per collision to thermal energy). The quantity λ_{mfp} is the characteristic mean free path for energy-transfer collisions in pure Xe.
- K_e is the ratio of momentum-transfer integrals in the 10 – 15 eV region:

$$K_e = \frac{\int_{10 \text{ eV}}^{15 \text{ eV}} \sigma_{el}^{H_2}(\varepsilon) [\mathcal{L}_{el} f_0(\varepsilon)] d\varepsilon}{\int_{10 \text{ eV}}^{15 \text{ eV}} \sigma_{el}^{Xe}(\varepsilon) [\mathcal{L}_{el} f_0(\varepsilon)] d\varepsilon}. \quad (\text{A.25})$$

With $\sigma_{el}^{H_2} \approx 10 \times \sigma_{el}^{Xe}$ around 10 – 15 eV [236, 239], we find numerically $K_e \sim 1020$. The factor $(1 - K_e f)$ in (A.24) indicates that the high-energy tail of the electron distribution is suppressed in proportion to f .

- The $\sigma_{rot,vib}^{H_2}$ -term does not explicitly appear in (A.24), but its effect is implicitly encoded in a slightly shifted normalisation and in the definition of K_e (through modified energy flux). More precisely, one can show that the low-energy losses to H_2 rotational/vibrational excitations “cool” the Maxwellian-like core of f_0 , thereby raising the effective threshold for Xe electronic excitation. We will see how that enters as K_b .

First-Order Excitation Coefficients

To find the perturbed EL excitation coefficient $k_{exc}(f)$, we can substitute (A.24) into the electron-impact Xe-excitation integral:

$$k_{exc}(f) = N \int_0^\infty \sigma_{exc}^{Xe}(\varepsilon) v(\varepsilon) f(\varepsilon; f) d\varepsilon. \quad (\text{A.26})$$

Expanding to first order in f yields:

$$\begin{aligned} k_{exc}(f) &= N \int \sigma_{exc}^{Xe} v [f_0 + f f_1] d\varepsilon + \mathcal{O}(f^2) \\ &= \underbrace{N \int \sigma_{exc}^{Xe} v f_0 d\varepsilon}_{k_{exc}^{(0)}} + f N \int \sigma_{exc}^{Xe} v f_1 d\varepsilon + \mathcal{O}(f^2). \end{aligned} \quad (\text{A.27})$$

By definition, the first term is the pure-Xe coefficient $k_{exc}^{(0)}$, which we know is equivalent to $\alpha E_g - \beta P_g - \gamma$. To evaluate the second term, note that $f_1(\varepsilon) \approx \chi_0 (E_g/N) (1 - K_e)$ is approximately proportional to $f_0(\varepsilon)$ itself (up to a slowly varying factor). Therefore,

$$\int_0^\infty \sigma_{exc}^{Xe}(\varepsilon) v(\varepsilon) f_1(\varepsilon) d\varepsilon \approx \chi_0 \frac{E_g}{N} (1 - K_e) \int_0^\infty \sigma_{exc}^{Xe}(\varepsilon) v(\varepsilon) f_0(\varepsilon) d\varepsilon = \chi_0 \frac{E_g}{N} (1 - K_e) \frac{k_{exc}^{(0)}}{N}. \quad (\text{A.28})$$

Since $k_{exc}^{(0)} = \alpha E_g - \beta P_g - \gamma$, the ratio $[k_{exc}^{(0)}/N]$ is known. The key point here is that the H_2 elastic scattering enhancement factor K_e reduces the effective αE_g term. Meanwhile, the rotational/vibrational term in (A.23) produces a net downward shift in the mean energy, effectively requiring a larger field to reach the 8 eV threshold. One can show (Chapman–Enskog) that this threshold “lift” enters as an additive term $K_b f P_g$ in the subtracted part of the excitation coefficient. Combining both effects:

$$k_{exc}(f) = [\alpha (1 - K_a f)] E_g - [\beta + K_b f] P_g - \gamma + \mathcal{O}(f^2), \quad (\text{A.29})$$

, where we have set $K_a = K_e$.

Physical interpretation:

- The term $\alpha (1 - K_a f) E_g$ indicates that H_2 elastic scattering increases the collision frequency, so electrons gain less energy between collisions. The factor $(1 - K_a f)$ shows the *fractional reduction* of the pure-Xe gain slope α per unit fraction f .
- The term $(\beta + K_b f, P_g)$ shows that H_2 rotational/vibrational inelastic collisions produce many small energy losses (on the order of ~ 0.1 eV each), shifting the mean electron energy downward. To overcome the 8 eV Xe excitation threshold, a slightly larger field is needed. Equivalently, the “threshold term” βP_g is increased by $K_b f P_g$.
- The constant γ is typically small or zero in a perfect linear fit.

Finally, to account for VUV self-absorption by H_2 , we can also include a survival factor

$$S(f) = \exp[-\kappa f h_g], \quad \kappa = N_{H_2} \sigma_{ph}^{H_2}(172 \text{ nm}), \quad (\text{A.30})$$

so that the *observed* single-electron photon yield becomes

$$LY(f) = k_{exc}(f) (h_g) \exp[-\kappa f h_g]. \quad (\text{A.31})$$

Here $h_g P_g$ is the column density in the gas gap. Thus,

$$LY(f) \approx [\alpha (1 - K_a f) E_g - (\beta + K_b f) P_g - \gamma] h_g \exp[-\kappa f h_g]. \quad (\text{A.32})$$

As $\kappa f h_g \ll 1$ for $f \lesssim 1\%$ and $h_g \sim 1 \text{ cm}$ at $1 - 2 \text{ bar}$, the VUV self-absorption factor should typically be a few percent at most, but may become non-negligible at higher f . Unfortunately most hydrogen cross-sections are either not measured well or not measured in the energy ranges or for the wavelengths we are interested in (example [243]) leaving large uncertainties in the potential values of K_a (EL slope gain), K_b (effective threshold), κ (attenuation of observed light). For now, we will have to rely on fit results to give us a gauge of what values these parameters might take and then assess if they seem reasonable given literature and a few back-of-the-envelope estimates.

A.4.2 Experimental Results: HydroX

To validate the above model, we compare its predictions to single-electron EL yield measurements from the HydroX apparatus at SLAC: a dedicated study of xenon gas with H_2 admixtures.

The discussion in this section pertains to two dedicated runs operating at 191 K and 194 K ⁶, respectively; in each, the “cathodic” plate was held at $+1 \text{ kV}$, while anode mesh was held at potentials of $+6, +7, +8 \text{ kV}$. With an 8 mm gas gap, this corresponds to uniform fields of $E_g = 6.25, 7.50, 8.75 \text{ kV cm}^{-1}$. The experiment allows for measurements of the S2 pulse area in $V\mu\text{s}$ rather than an absolute photon count. As the aim is to reach an estimate for the relative photon yields per electron in such a detector, these raw yields are converted to the normalised fraction $LY(f)/LY(0)$ in the following study. This directly measures S2 suppression at each (f, E_g) point, ready to be compared to simulations. GARFIELD++ simulations were then conducted for every combination of field and H_2 fraction $f = 0 - 1\%$, tracking $\mathcal{O}(200)$ electrons per point. The code employs MAGBOLTZ V13.0 cross-sections and, in this configuration, assumes (i) a perfectly uniform gap field, (ii) fixed thermodynamic state, and (iii) “cooling-only” H_2 physics (no VUV self-absorption or quenching is simulated) [132]. This has important implications for our understanding of the S2 suppression-inducing mechanisms at play due to the presence of H_2 , particularly giving us a glimpse into the interplay of these mechanisms with the H_2 fraction and the electric field, as we will see later.

Before confronting the measurements with Garfield++ or with the Chapman–Enskog expansion, we first test whether a model-independent exponential ansatz reproduces the data. For each electroluminescence field E_g we fit the normalised electroluminescence yield

$$\mathcal{S}(f, E_g) = \frac{LY(f, E_g)}{LY(0, E_g)} \quad (\text{A.33})$$

to the two-parameter surface

$$\mathcal{S}(f, E_g) = \exp[-(k_0 + k_1(E_g - E_0))f]. \quad (\text{A.34})$$

Here f denotes the H_2 molar fraction (% units), and the reference field is fixed at $E_0 = 7 \text{ kV cm}^{-1}$ (an arbitrary field choice). The resulting coefficients are

$$k_0 = 1.364 \pm 0.031 \text{ per } \% H_2, \quad k_1 = 0.274 \pm 0.022 \text{ per } \% H_2 \text{ per } \text{kV cm}^{-1}, \quad (\text{A.35})$$

⁶We combine both as it was found that the effect of temperature variation was $< 1\%$ in the field & pressure regime investigated.

the former quantifying the baseline suppression at 7 kV cm^{-1} , the latter, k_1 , representing the linear field-slope of the suppression. Residuals remain mostly confined to ± 0.15 (fractional units; see Fig. A.4), demonstrating that equation A.34 captures the essential (f, E_g) dependence of the HydroX data⁷.

This is not just a fortuitous coincidence, however. If we start again with the first-order Chapman–Enskog prediction (equation A.31):

$$LY(f, E_g) \approx [1 - K_a(E_g)f] LY(0, E_g) \exp[-\kappa f h_g], \quad (\text{A.36})$$

which, when expanded to leading order in f , yields an overall exponential with effective coefficient

$$k_{eff}(E_g) \simeq K_a(E_g) + \kappa h_g. \quad (\text{A.37})$$

Hence,

$$k_0 \longrightarrow K_a(E_0) + \kappa h_g, \quad k_1 \longrightarrow [dK_a/dE_g]_{E_0}. \quad (\text{A.38})$$

The fitted $k_1 < 0$ foreshadows the negative field-dependence $dK_a/dE_g \approx 0.03$ per kV cm^{-1} extracted explicitly later. Likewise, $k_0 \sim 1.36$ is consistent with $K_a(E_0) \approx 0.2$ per % and $\kappa h_g \approx 1$, lending physical meaning to both empirical parameters. The exponential surface, therefore encodes the combined effects of H_2 -induced elastic scattering and photon attenuation, and it provides a quantitative bridge to the more detailed Chapman–Enskog analysis developed in previous sections.

This “extra quenching” can be quantitatively visualised too. In Fig. A.5, the normalised EL yield maps are shown for both data and simulations. A difference map is then constructed to directly observe Q_{extra} , isolating the additional suppression produced by photon-loss mechanisms and higher-order collisions.

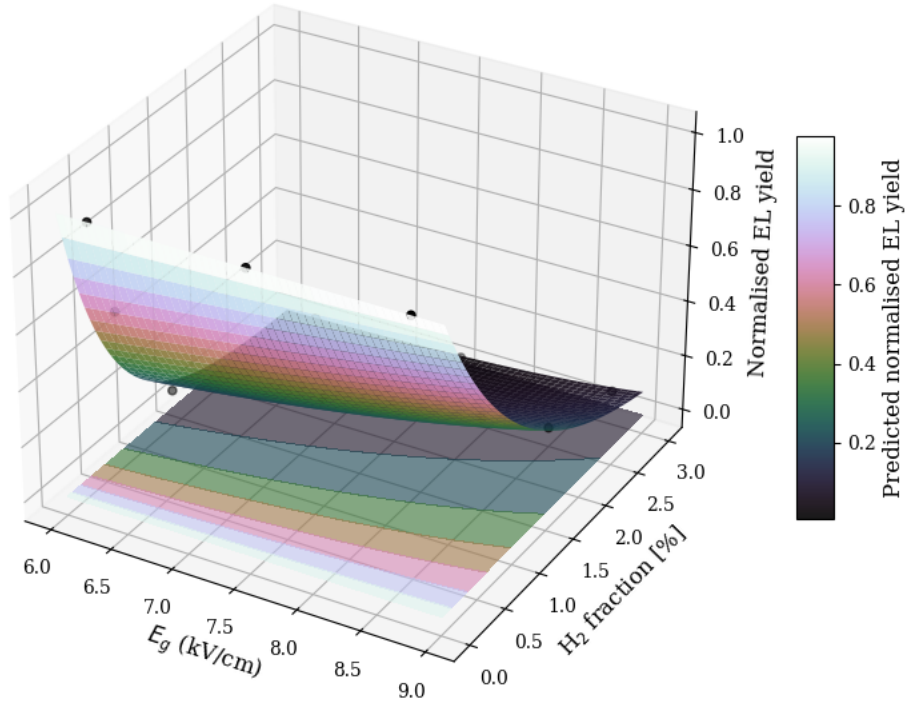
$$Q_{extra}(f, E_g) = \mathcal{S}_{data} - \mathcal{S}_{sim} = 1 - \frac{\mathcal{R}(f, E_g)}{\mathcal{R}(0, E_g)}, \quad (\text{A.39})$$

where $R = \frac{\mathcal{S}_{data}}{\mathcal{S}_{sim}}$.

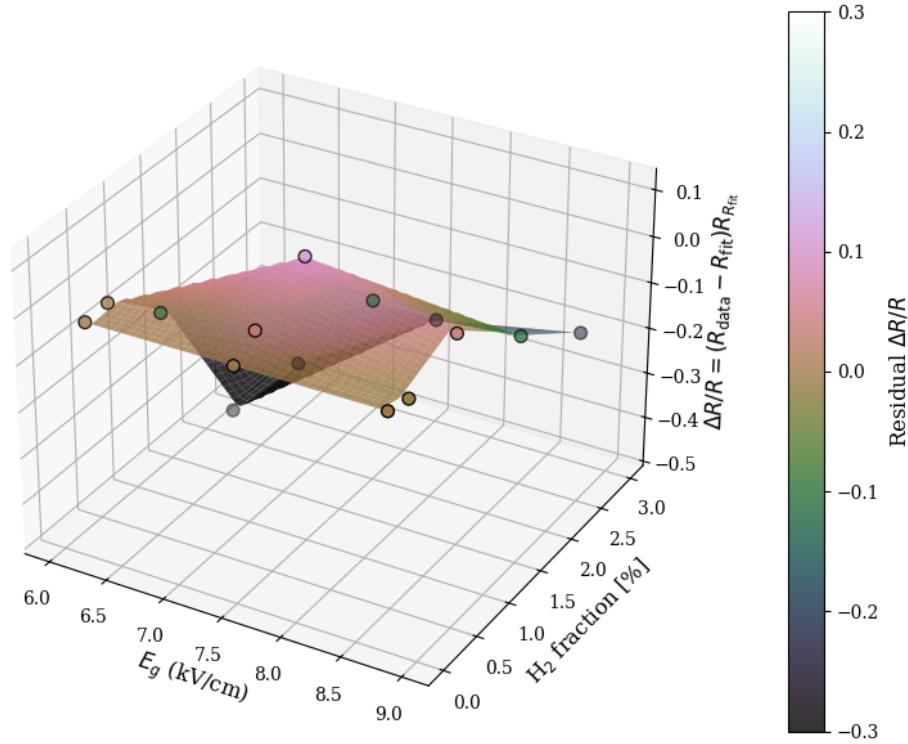
Over the (E_g, f) plane, the additional-quenching surface Q_{extra} exhibits four clear behaviours. First, for hydrogen fractions up to 1% the deficit rises essentially linearly with f , the slope⁸ increasing from $\sim 0.16 f$ at $E_g = 6.25 \text{ kV cm}^{-1}$ to $\sim 0.19 f$ at $E_g = 7.50 \text{ kV cm}^{-1}$ (Fig. A.6); this is exactly the first-order Chapman–Enskog expectation in which the elastic-scattering term $K_a f$ and the self-absorption term $\kappa h_g f$ add coherently. Secondly, once the admixture exceeds 1% the contours bend upward, indicating processes whose rates grow faster than f . Two such mechanisms are well established in noble-gas literature: (i) resonant re-absorption of $172 \text{ nm } Xe_2$ excimer photons, whose optical depth scales with f^2 when hydrogen introduces additional absorption centres, and (ii) collisional quenching of the Xe_2^* state via $H_2 - H_2$ and $H_2 - Xe$ energy-transfer channels, whose frequency is proportional to the square of the impurity density [72, 241]. Thirdly, at fixed fraction the extra deficit increases with field up to 7.5 kV cm^{-1} and

⁷At least within the domain of fields and H_2 fractions measured.

⁸Starting with the small-fraction fit to the data/simulation ratio, $R(f, E_g) = c(E_g) - m(E_g)f$, and combining with the definition of the extra-quench surface yields $Q_{extra} = -(m/c)f$.



(a) Best-fit exponential surface $\mathcal{S}(f, E_g) = \exp[(k_0 + k_1(E_g E_0))f]$ superimposed on the normalised HydroX EL-yield data.



(b) Fractional residual map $(S_{data} - S_{fit})/S_{fit}$ for the same parametrisation, showing most points within ± 0.15 of the surface.

Figure A.4: An exponential trend is immediately apparent in the 191 K S2 suppression fraction data. Shown here is a fit characterising the relationship between the relative EL yield, H_2 fraction and E field configuration.

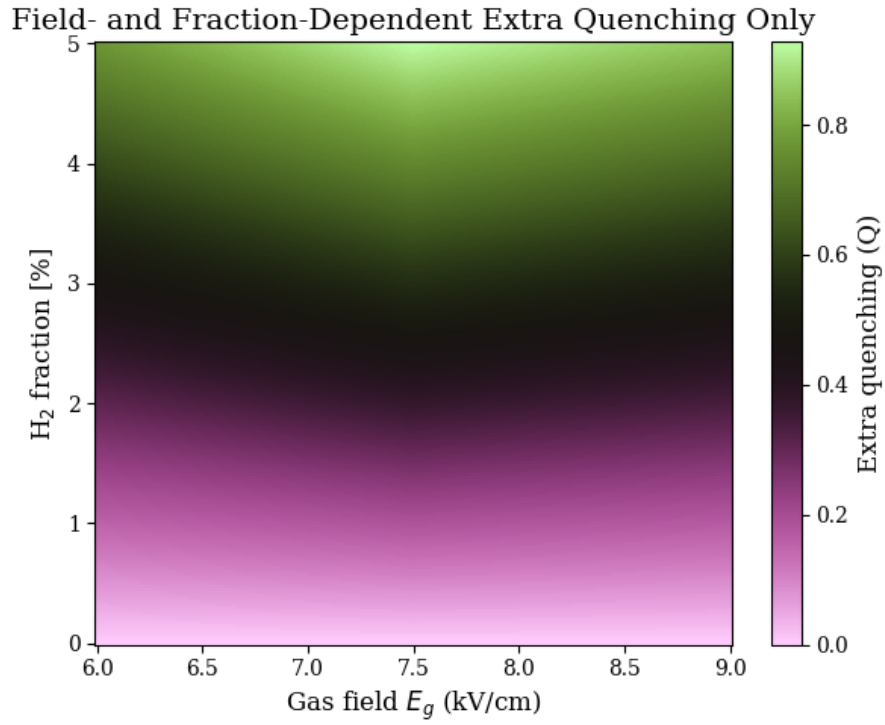


Figure A.5: Extra-quenching map $Q_{extra}(f, E_g)$, defined as the yield deficit that remains after subtracting the GARFIELD++ cooling-only prediction. Colours represent the additional S2 suppression as a function of H_2 fraction and electroluminescence field.

then saturates; the rise reflects the waning influence of cooling at higher mean electron energies, after which photon-loss terms dominate and their own field dependence flattens. Finally, both maps are normalised to unity at $f = 0$, confirming that the colour scale isolates hydrogen-specific physics rather than instrumental gain. The surface reaches a maximum $Q_{extra} \simeq 0.90$ at $E_g = 7.5 \text{ kV cm}^{-1}$, $f \approx 5\%$, implying that up to $\sim 90\%$ of the yield loss in that regime is attributable to photon self-absorption, Xe_2 quenching, or $H_2 - H_2$ scattering rather than to elastic cooling.

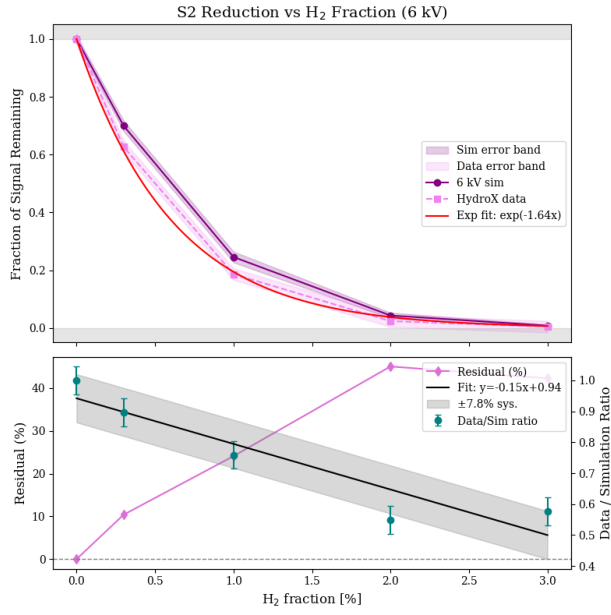
Global α , β , κ , K_a Fits

Having established that elastic cooling alone cannot explain the observed S2 suppression, we now perform a global four-parameter fit that combines the pure-Xe constants α, β with the hydrogen coefficients K_a and κ . The fifth parameter, the cooling term K_b , was not retained; when introduced the likelihood surface becomes nearly flat and the minimiser fails to converge. This numerical instability reflects a genuine degeneracy: below $f = 1\%$, the Chapman–Enskog cooling term $K_b f$ and the photon-loss exponent $\kappa f h_g$ are algebraically similar. Additional data at lower fields and fractions would be required to separate these.

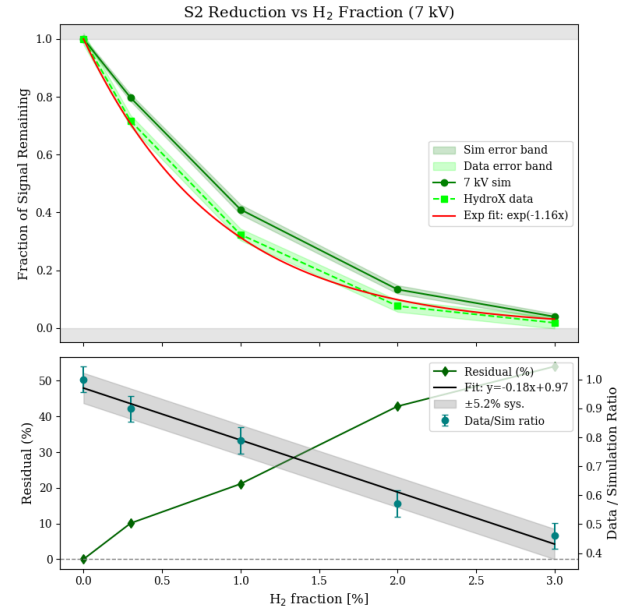
Due to HydroX having only taken preliminary data at this point, we will use scaled simulations yields (according to the discussions previously and the parameters in Fig. A.6), to map the cooling-only simulations calculations to the data curves. This forms the basis of our models without needing to use the data directly, also leaving both 191 K and 194 K runs data for validation. The fit strategy is then as follows:

- **Pure-Xe anchor** (α, β)

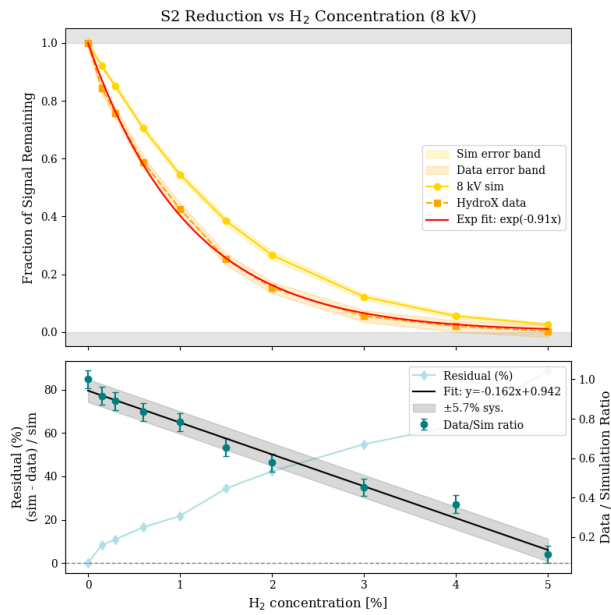
The $f = 0$ yields for each field are fitted with $LY(0) = (\alpha E_g - \beta P_g) h_g$ as in §A.2.3 and equation A.8. This



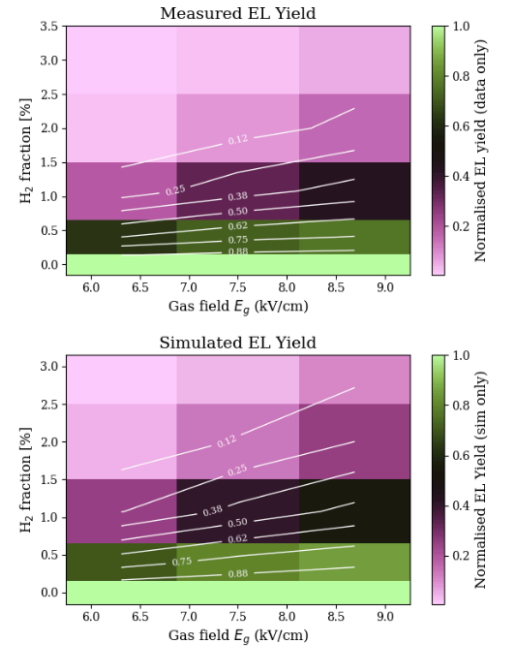
(a) 6 kV anode.



(b) 7 kV anode.



(c) 8 kV anode.



(d) Simulated and measured normalised EL yield map.

Figure A.6: Exponential-fit summary: (a)–(c) Normalised S2-yield reduction $LY(f)/LY(0)$ versus H_2 fraction for electroluminescence fields 6.25, 7.50, 8.75 $kV\ cm^{-1}$ (upper panels), together with the fractional residuals relative to the exponential fit (lower panels). Data points are compared with the GARFIELD++ cooling-only prediction (shaded band representing the standard error of the mean photon count ($\approx 2 - 3\%$)); solid curves show the best-fit surface. (d) Two-dimensional maps of measured (upper) and simulated (lower) normalised yields on the (E_g, f) grid; white contours mark equal suppression levels. All yields are referenced to the corresponding pure-Xe point, so colour encodes the additional S2 loss induced by hydrogen.

yields

$$\begin{aligned}\alpha &= 61.6 \pm 2.4 \text{ phot } e^{-1} \text{ kV}^{-1}, \\ \beta &= 69.9 \pm 3.0 \text{ e}^{-1} \text{ cm}^{-1} \text{ bar}^{-1}.\end{aligned}\tag{A.40}$$

- **H_2 coefficients**

With α , β fixed, all $f > 0$ points are fitted to

$$LY(f) \approx [\alpha (1 - K_a f) E_g - \beta P_g] h_g \exp[-\kappa f h_g].\tag{A.41}$$

- **Linear interpolation in E_g**

The three fitted values of K_a and κ (for each field) are interpolated linearly (this is an assumption we will have to make at the moment due to lack of statistics and justified due to the small field interval),

$$\begin{aligned}K_a(E_g) &= 0.50 - 0.035 E_g, \\ \kappa(E_g) &= 2.31 - 0.19 E_g,\end{aligned}\tag{A.42}$$

providing a continuous surface for arbitrary field.

Table A.2 collects the first-order hydrogen coefficients extracted at each drift-field setting. Quoted errors are 1σ statistical uncertainties propagated from the photon-counting bands in Fig. A.6. These HydroX coefficients are lower than the canonical “pure-Xe” numbers by $\geq 50\%$ (table A.1), placing them even below the room-temperature fit made at 1 bar and 293 K. The exact reason for this is unclear, but could be due to HydroX operating at an intermediate thermodynamic point (~ 191 K, ~ 2.1 bar) and also could point to presence of impurities in the detector⁹.

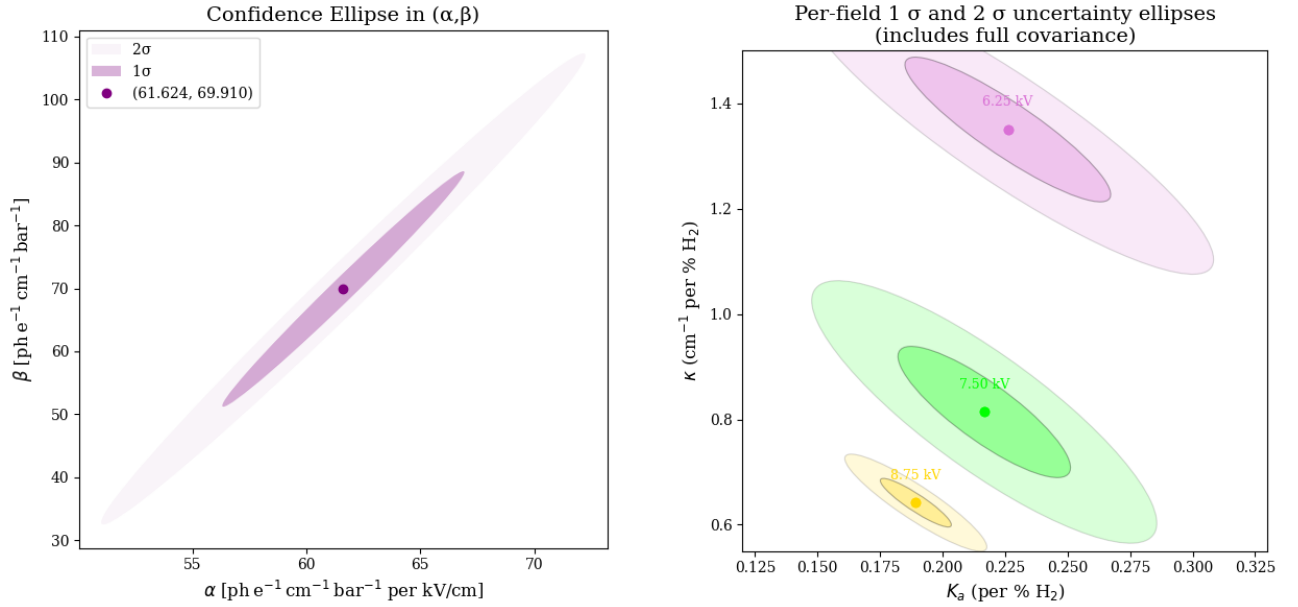
Table A.2: Best-fit Chapman–Enskog coefficients and their correlations. The pure-Xe slope/threshold pair (α, β) is obtained from the $f = 0$ anchor points; the H_2 coefficients (K_a, κ) are fitted separately for each drift field. Quoted uncertainties are 1σ statistical errors propagated from the full covariance matrices.

Pure-Xe fit			
Parameter	Value $\pm$ stat. error	Unit	$\rho(\alpha, \beta)$
α	61.624 ± 5.310	$\text{ph e}^{-1} \text{ kV}^{-1}$	+0.991
β	69.910 ± 18.693	$\text{ph e}^{-1} \text{ cm}^{-1} \text{ bar}^{-1}$	
First-order H ₂ coefficients by field			
E_g [kV cm ⁻¹]	K_a [per % H ₂]	κ [cm ⁻¹ per % H ₂]	$\rho(K_a, \kappa)$
6.25	0.226 ± 0.041	1.350 ± 0.137	-0.90
7.50	0.217 ± 0.034	0.814 ± 0.125	-0.85
8.75	0.189 ± 0.014	0.642 ± 0.046	-0.91

It is also important to note that the per-field 2×2 covariance matrices exhibit a strong anti-correlation between K_a

⁹Perhaps most likely due to the significant magnitude of the suppression, especially as there are studies that confirm that very small impurity concentrations can have significant impact on the yield parameter. See Fig. 6 of [241] for example, between the pure-Xe run and 0.1% CO_2 run, α decreased from $\sim 132 \text{ phot } e^{-1} \text{ kV}^{-1}$ to $\sim 50 \text{ phot } e^{-1} \text{ kV}^{-1}$. Others have also been studied, like CH_4 [244], showing similar. It seems logical that trace concentrations of such impurities (maybe more likely O_2 , H_2O , N_2 as well) could reproduce the decrease in yield paired with the slightly higher temperatures of operation.

and κ ($\rho \approx -0.85 : -0.90$). Fig. A.7 visualises this through 1σ and 2σ ellipses whose long axes are tilted along the direction $K_a + \kappa h_g = \text{const.}$ Importantly, that very combination, responsible for the leading exponential factor in equation A.41 is still determined to better than $\sim 8\%$, despite the elongation.



(a) Joint 1σ and 2σ confidence region for the pure-Xe coefficients (α, β), obtained from the $f = 0$ anchor points. These are fairly different to the coefficients found in table A.1, showing the impact of adding H_2 even in small fractions cannot be treated independently to the pure-Xe component.

(b) 1σ (dark) and 2σ (light) error ellipses in the (K_a, κ) plane for each drift field. The pronounced tilt ($\rho \approx -0.9$) shows that an upward fluctuation in K_a must be compensated by a downward fluctuation in κ to keep the model anchored to the data.

Figure A.7: Degeneracies in the fit values for the four-parameters.

Fig. A.8 overlays the fitted curves on the normalised data for all three drift-fields; the shaded bands are $\pm 1\sigma$ from the full covariance and the data points have uncertainties inherited and propagated from simulation data errors (photon statistics $\sim 4\%$) along with the data-simulations scaling. All HydroX points lie comfortably within the 95% confidence envelope, indicating that the two-parameter model reproduces the data to within a few percent over the full range of fields and hydrogen fractions.

To stress-test the parametrisation, K_a and κ are linearly interpolated onto a dense grid spanning $E_g : (5-10 \text{ kV cm}^{-1})$ (equation A.42) and compared with every measurement (taking both 191 K and 194 K data) in the nine-panel map of Fig. A.9. Every point with $f \geq 1\%$ lies within $\pm 5\%$. In the intermediate range $0.30 - 1\%$ the residuals stay between 13% and 4%. Only one sparsely populated bin ($f = 0.15\%$ at 6.7 kV cm^{-1}) exhibits a larger excursion (-29%). Across three fields and five pressures, the first-order Chapman–Enskog description therefore reproduces the data to present precision. With more data, these measurements can be further formalised and confirmed.

The key next steps are therefore (i) measuring $f < 0.1\%$ and $E_g < 5 \text{ kV cm}^{-1}$ to isolate a possible K_b term, and (ii) upgrading GARFIELD++ cross-sections to include H_2 momentum transfer and other mixing terms. Together these

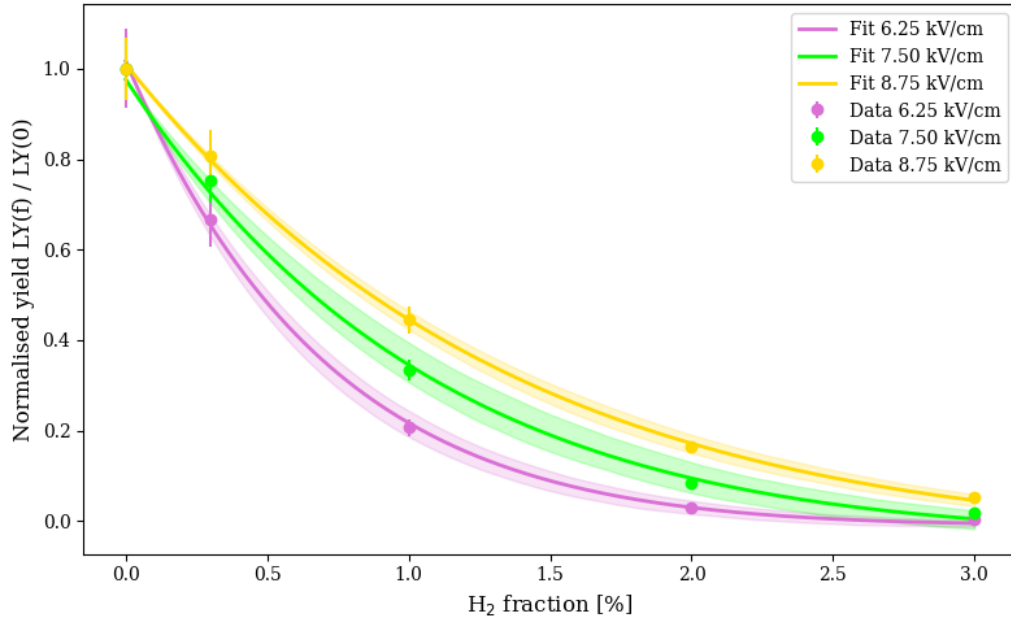


Figure A.8: Normalised single-electron yield versus H_2 fraction for the three HydroX drift fields. Markers show the data, solid curves the best-fit Chapman–Enskog model (equation A.41); shaded bands are the propagated $\pm 1\sigma$ uncertainties from the (K_a, κ) covariance at each field.

will complete the first-order parameter set $\{K_a, K_b, \kappa\}$ and supply detectors with a turnkey model for H_2 -doped operation. Even in its present form the $\{\alpha, \beta, K_a, \kappa\}$ set already predicts the single-electron EL yield to first order across the HydroX operational phase-space, offering an immediate baseline for refining event-reconstruction algorithms, especially the identification and energy-calibration of small S2 signals.

A.5 Outlook

The work in this appendix closes a fifty-year loop on xenon electroluminescence.

- A single, cryogenic gain law

Across data sets from 1976 $\rightarrow$ 2023 the proportional-scintillation yield follows,

$$LY = \left((144 \pm 7.0) \frac{E_g}{P_g} - (136 \pm 11) \right) h_g P_g, \quad (\text{A.43})$$

i.e. the Fit B coefficients corresponding to when the gas is saturated vapour (170 – 185 K). This is visualised in Fig. A.10. Room-temperature slopes can be up to $\approx 2\times$ smaller; using them would under-predict single-electron gains by 30 – 40% in any dual-phase TPC. For single phase experiments like HydroX, the “cryo-only fit” coefficients in table A.1 (without requiring a saturated vapour), should be a better approximation but one should note the higher temperatures might result in fit parameters which deviate away from the “cryo-only” fits and more towards the “room-temperature” fits.

- Explicit temperature study for dual phase experiments

Imposing the Antoine curve in the fit trims the residual scatter and shows that a ± 0.5 K control band shifts the EL yield by $< 1\%$. Future detectors can treat $P_{sat}(T)$ as an intrinsic parameter, not a nuisance.

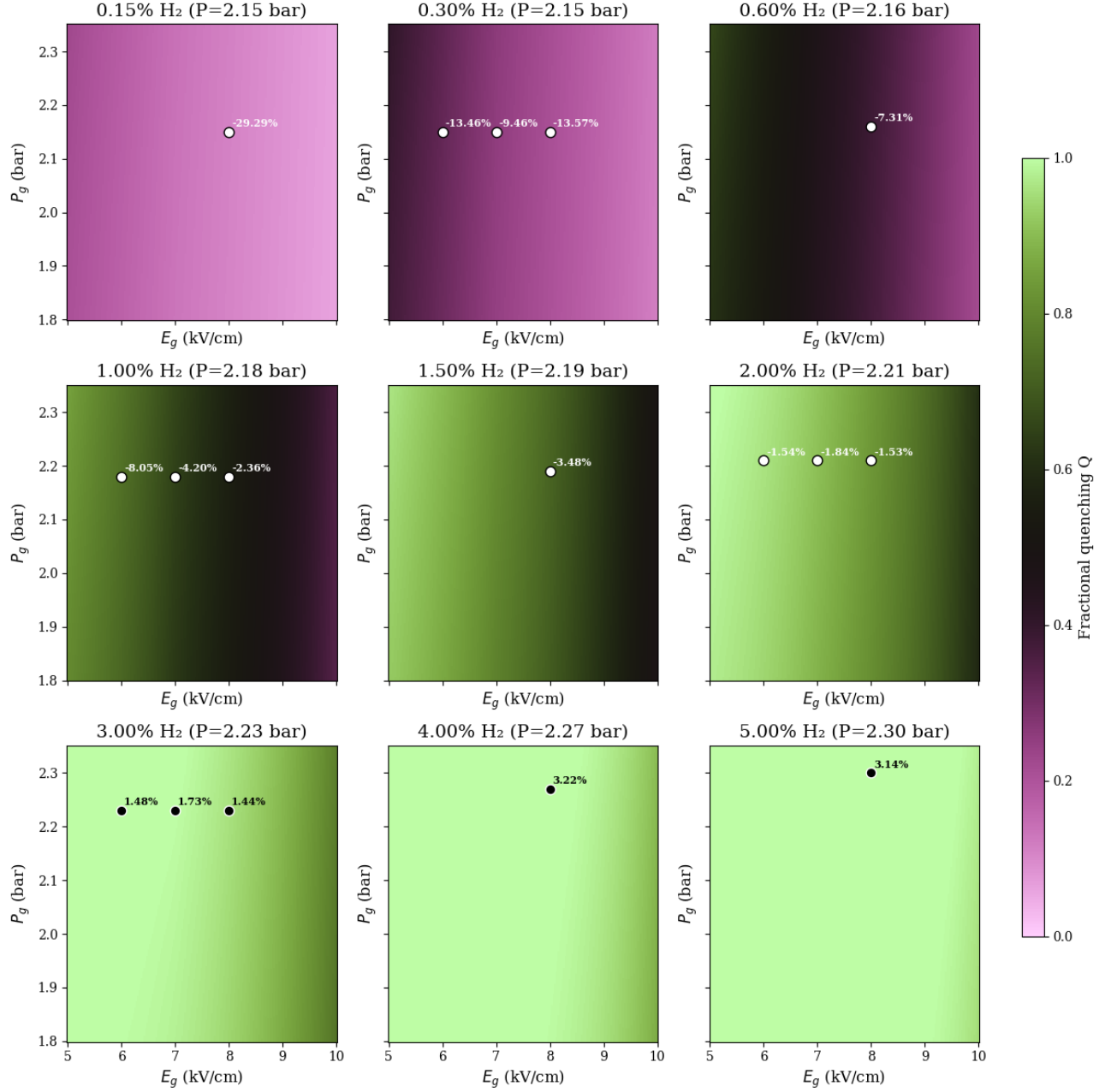


Figure A.9: The final model for $\text{Xe} - \text{H}_2$ admixtures. Each panel displays the model-predicted fractional quench $Q_{\text{model}}(E_g, P_g; f)$ for a fixed H_2 fraction (panel title). The colour scale runs from $Q_{\text{model}} = 0$ (no quenching, pale pink) to $Q_{\text{model}} = 1$ (full quenching, deep green). White circles mark the HydroX measurements at that fraction; the over-printed number is the percentage deviation $\Delta = 100 (Q_{\text{model}} - Q_{\text{data}}) / Q_{\text{data}}$. All points with $f \geq 1\%$ lie inside $|\Delta| < 5\%$; the largest excursion, -29% , occurs at the sparsely sampled $f = 0.15\%$ bin.

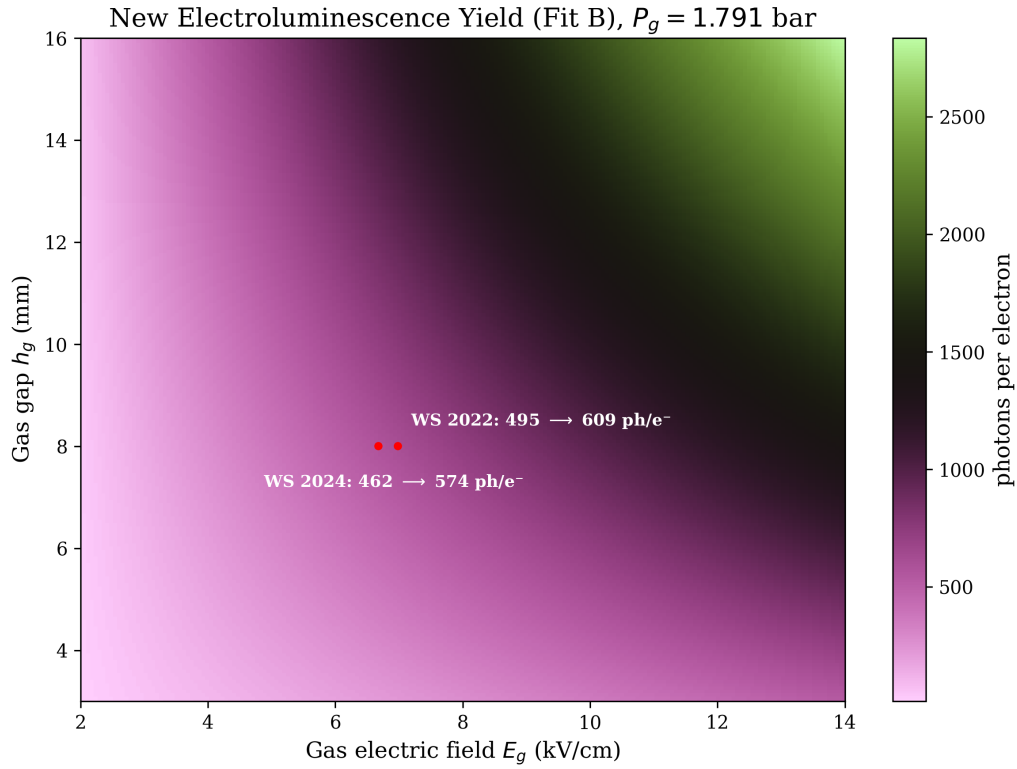


Figure A.10: Projected electroluminescence photon yield per extracted electron, computed from the saturated–vapour Fit B at $P_g = 1.791 \text{ bar}$, as a function of gas field E_g and gas-gap thickness h_g . The colour scale (and overlaid contours) show the total photons per electron produced in the gap. Red points mark the WS 2022 and WS 2024 configurations, illustrating the difference in the predicted EL yield between the Chepel-Araujo fit $\rightarrow$ Fit B.

- Consistency with “industry standards”

Aprile *et. al.* [195] and Chepel–Araújo’s [72] review bracket the new best-fit (Fig. A.11): for example, both deviate by only $\pm 5\%$ around the new slope measurement. Adopting the updated pair therefore preserves continuity while removing a long-standing 10 – 15% ambiguity between collaborations. Furthermore, NEST global fit yields also show closer agreement to Fig. A.10, for example the equivalent for NEST prediction for SR1 is 631 ph/e^- .

- For the first time we provide a quantitative, first-order description of electroluminescence in $Xe - H_2$ mixtures, anchored to new HydroX (SLAC) single-electron data rather than legacy pure-Xe fits. The compact parameter set $\{\alpha = 61.624 \pm 5.310, \beta = 69.910 \pm 18.693, K_a(E_g), \kappa(E_g)\}$ now predicts S2 yield to $\pm 5\%$ across 69 kV cm^{-1} and up to 3% hydrogen and can be used as a baseline to improve our understanding of the quenching mechanisms in such admixtures, as well as improving event/ signal reconstruction in the short-term.

$$LY(f) \approx [\alpha (1 - K_a f) E_g - \beta P_g] h_g \exp[-\kappa f h_g]. \quad (\text{A.44})$$

There are also a few important practical implications of these results, particularly for the design of any new detectors and particularly for pure-Xe designs. These are as follows:

- For a fixed gate-anode potential difference equation A.11 provides a direct viewport into the photon-budget of any given experiment: $+1 \text{ kV cm}^{-1} \text{ bar}^{-1}$ enhances yields by $\approx 140 \text{ photons e}^{-1} \text{ mm}^{-1}$, regardless of the TPC size.

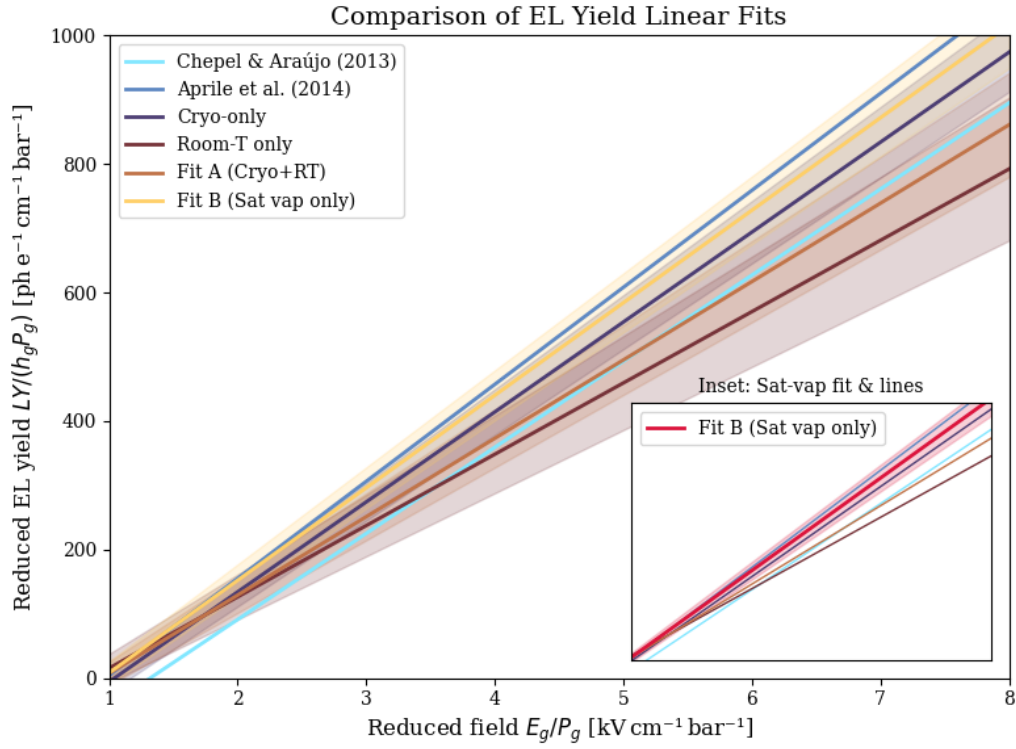


Figure A.11: Reduced EL yield as a function of reduced electric field. Solid lines are linear regressions from Chepel & Araújo (2013) [72] (as per LZ’s parameterisation)(bright blue), Aprile et al. (2014) [195] (XENON100) (teal), cryogenic-only (navy), room-temperature-only (dark brown), Fit A combining both regimes (light brown), and Fit B from saturated-vapor data (yellow). Shaded regions indicate the 1σ standard error intervals for the Aprile et al., cryo-only, room-temperature, Fit A, and Fit B datasets. Fit B is the suggested best fit parameterisation for cryogenic dual-phase xenon experiments. For clarity, an inset has been provided showing only Fit B with its uncertainty band (red) and all other mean fit parametrisations for comparison: it is clear that the room-temperature data tends to bias the fits to a lower slope coefficient ‘a’.

- The new (a, b) can be hard-coded as the default S2 model in S2 simulation softwares like BACCARAT, NEST, etc. without extra temperature flags: only H_2 or N_2 admixtures require the extensions of § A.4.
- Even a 2 cm EL gap in a DARWIN-class detector remains in the linear regime if mesh transparency is $\geq 90\%$. Extrapolating the slope adds only $\pm 4\%$ uncertainty at full height.

In short, the cryogenic fit provided here is the updated gain law which should be used as a baseline for present and next-generation xenon experiments. Adopting it will remove a significant systematic from S2-based energy and position reconstruction, while also anchoring all mixture studies that follow.

Little by little, one travels far.

— J. R. R. Tolkien, *Lord of the Rings*

B

Powell's Method

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OPTIMISATION TECHNIQUES lie at the heart of many problems in physics, particularly where model parameters must be inferred indirectly through their imprint on experimental observables. In this work, a central challenge emerges from the need to simultaneously vary multiple free parameters describing the effective surface charge distribution on the inner PTFE wall, with the aim of reproducing the experimentally observed wall shape using electric-field simulations. This inverse problem is intrinsically degenerate: distinct configurations of charge patches can give rise to similar degrees of agreement when compared to data, obscuring a unique solution and demanding an optimisation strategy capable of navigating a correlated and weakly constrained parameter space. While a range of optimisation strategies may be applied in such settings¹ - including simplex-based methods such as Nelder-Mead [152], as well as stochastic sampling algorithms such as Metropolis-Hastings [81] - the focus here is placed on Powell's direction-set method. Empirically, this approach was found to exhibit a higher probability of reliable convergence, with reduced computational cost and to identify physically reasonable representative solutions within the family of charge configurations compatible with the observed data. Accordingly, this appendix provides a brief overview of Powell's direction-set method in the context of the electric-field studies of Chapter 4, along with a short discussion of its practical usage in this analysis.

¹Alternative optimisation strategies have been employed in closely related studies (see citations in text) addressing the same problem, where their implementation and behaviour are discussed in detail; these are referenced here for completeness.

B.1 The Algorithm

In the electric-field studies presented in Chapter 4, the optimisation problem is formulated as the determination of an effective surface charge distribution on the inner PTFE wall that reproduces the experimentally measured wall position as a function of drift coordinate, $r_{\text{data}}(z)$. The surface charge is parameterised in terms of a set of patch-charge coefficients,

$$\boldsymbol{\theta} \equiv \{q_1, q_2, \dots, q_N\}, \quad (\text{B.1})$$

each corresponding to a localised charge element applied as a Neumann boundary condition in the field simulation. For a given choice of $\boldsymbol{\theta}$, the electric field is recomputed and used to infer a simulated wall position $r_{\text{sim}}(z; \boldsymbol{\theta})$.

The optimisation task is therefore to identify the set of patch charges that minimises the discrepancy between the measured and simulated wall profiles. This discrepancy is quantified using a chi-squared statistic,

$$\chi^2(\boldsymbol{\theta}) = \sum_i \frac{[r_{\text{data}}(z_i) - r_{\text{sim}}(z_i; \boldsymbol{\theta})]^2}{\sigma_r^2(z_i)}, \quad (\text{B.2})$$

where $\sigma_r(z_i)$ denotes the uncertainty on the reconstructed wall position at drift coordinate z_i . Minimisation of χ^2 therefore corresponds to a maximum-likelihood estimate under the assumption of Gaussian errors.

Powell's direction-set method addresses this problem through a sequence of one-dimensional line minimisations in the space of patch-charge coefficients, without requiring gradient information. A detailed description of the full method is given in Powell's original paper [245]. Starting from an initial parameter vector $\boldsymbol{\theta}_0$, the objective function is minimised successively along a set of search directions $\{\mathbf{d}_1, \dots, \mathbf{d}_N\}$,

$$\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k + \alpha_k \mathbf{d}_k, \quad \alpha_k = \arg \min_{\alpha} \chi^2(\boldsymbol{\theta}_k + \alpha \mathbf{d}_k), \quad (\text{B.3})$$

with the initial directions typically aligned with the individual patch-charge axes.

After completing a full cycle of line minimisations, the algorithm evaluates the net displacement in parameter space,

$$\Delta \boldsymbol{\theta} = \boldsymbol{\theta}_{\text{final}} - \boldsymbol{\theta}_{\text{initial}}, \quad (\text{B.4})$$

which captures the cumulative direction along which the greatest reduction in χ^2 was achieved. This displacement is promoted to a new search direction and replaces one of the existing directions in the set, allowing subsequent iterations to proceed along correlated combinations of patch charges that most efficiently reduce the wall-shape mismatch. In this way, the method adaptively reshapes its search directions to follow the valleys of the objective-function landscape, rather than repeatedly probing along fixed parameter axes.

In practice, the optimisation described above is implemented using the Powell algorithm as provided by the

`scipy.optimize.minimize`

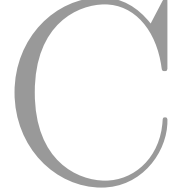
routine within the SciPy optimisation framework [246]. The χ^2 function defined in Eq. (B.2) is supplied directly as the scalar objective function, with no gradient information provided. The optimiser therefore relies solely on repeated

evaluations of $\chi^2(\boldsymbol{\theta})$ to guide the search through parameter space and identify a best-fit charge configuration.

This behaviour is particularly advantageous in the present application, where the mapping between surface-charge configurations and the reconstructed wall profile is intrinsically degenerate. Distinct patch-charge distributions can yield comparably good agreement with the measured $r(z)$, giving rise to extended, weakly constrained directions in parameter space. Powell's method does not resolve this degeneracy, but instead converges to a representative solution within the family of charge configurations compatible with the data. A more detailed examination of these degeneracies, together with their impact on the inferred charge distributions and associated uncertainties, is presented in Chapter 4.

Think about the deflections. The offense can't score every play. They're just trying to get a good shot. If I can deflect a pass, even if it doesn't cause a turnover, it will throw their timing off half-a-second. That half-a-second might mess up their shot.

— Draymond Green



Grid Deflection in Dual-Phase TPCs

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WHEN THE EXTRACTION REGION high-voltage is active, an electrostatic pressure is exerted on the gate and anode woven electrodes. Positioned within the liquid and gaseous phases of the xenon near the top of the chamber respectively (as shown in Fig. C.1, this dielectric creates two distinct field regions, defined by the relatively flat liquid-gas interface which is measured to a precision of $10 \mu m$ by the level sensors and regulated by the weir reservoir [58]. Due to the dielectric contrast between the two phases, the electric field in the liquid (E_l) is lower than

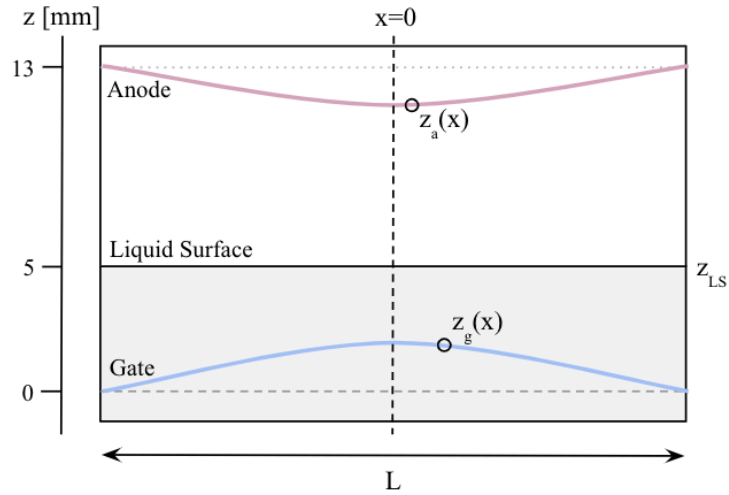


Figure C.1: Illustration of the deflection of the gate and anode electrodes with $z_a^{max} = 13 \text{ mm}$ and $z_g^{min} = 0 \text{ mm}$.

that in the gas phase (E_g). The field strengths in both regions are typically carefully optimised in the design phase of any experiment as we have touched on previously. Specifically, E_l is set to ensure efficient electron extraction by overcoming the potential barrier at the interface (§6.2.2), while E_g is chosen to maximise electroluminescence yield for effective signal detection. Given that the required field strengths typically range between $5\text{--}10 \text{ kV/cm}$, corresponding to an extraction efficiency of $> 85\%$, the system operates in an electrostatically dominated regime; namely, though

gravitational, mechanical and buoyant forces contribute to the complete description of the system, any deflection or sag observed in the electrodes is predominantly driven by electrostatic forces and can be well-explained by electrostatics alone. This appendix aims to present a theoretically-derived model for deflection as a function of field.

Field homogeneity is critical for accurate event reconstruction and improved signal to background discrimination. Deviations from the expected uniform gate-anode gap, whether due to field-induced deformation or warping can hence have significant consequences. In the extraction region, spatial field non-uniformities may manifest as a non-trivial xy -dependence in the extraction efficiency and electroluminescence yield with the potential to distort and degrade the S2 signal resolution. While minor variations in S2 yield across the detector can be calibrated and corrected, significant grid deflection poses a greater challenge. High-energy depositions, such as those from neutrinoless double beta decay ($Q_{\beta\beta} = 2.45783 \pm 0.0037 \text{ MeV}$), are expected to produce large-amplitude S2 signals that are particularly sensitive to variations in the extraction field due to the potential risk of saturation. In contrast, lower-energy nuclear recoils from WIMP interactions ($\mathcal{O}(10\text{s}) \text{ keV}$), though less likely to cause DAQ saturation still rely on a well-characterised extraction field for accurate reconstruction due to potential deflection-induced spatial non-uniformities in S2 amplification. Hence, deflection can impact both high- and low-energy searches. These effects necessitate precise measurements in LZ to ensure optimal detector performance and mitigate or correctly account for systematic uncertainties in rare event searches.

Finally, even slight deflection in the extraction region can elevate the local surface fields on the grid wires, potentially triggering unwanted electron emission or electrical breakdown and thereby contributing to spurious background signals (§6.2.3). Such deflection may also alter the effective drift distance used in drift velocity or diffusion measurements (chapter 3), introducing further systematic uncertainties. While deflection does not directly modify the intrinsic properties of electron drift or diffusion, the resulting electric field non-uniformities can indirectly impact the measured transport parameters by altering local conditions. A thorough understanding of these effects is therefore essential, not only for mitigating background risks and ensuring reliable drift velocity and diffusion measurements, but also for achieving precise event reconstruction and informing critical design decisions for future TPCs.

C.1 Modelling Grid Deflection

Building on the simplified framework for the physics of a displaced parallel-wire system in a drift tube, it is reasonable to expect that an approximate set of equations can be analytically derived to predict the expected deflection within acceptable tolerances for a given electric field or voltage configuration. In the following treatment, the interplay between deflection-induced field modifications and the resulting feedback loop, where an increased field further amplifies the deflection, is explicitly considered.

C.1.1 The Catenary Solution

The simplest approach to this problem treats the electrostatic deflection of a wire as the equilibrium condition between the restoring force due to tension and the electrostatic force exerted by the applied potential difference. In this treatment, the wire is assumed to be isolated, with its deformation governed by the balance between the Coulomb force pulling it towards the opposing grid and the tensile force resisting this displacement.

For a wire oriented along the x -direction, the force per unit length f_l is given by the well-known relation:

$$f_l = -\tau_x \frac{\partial^2 z}{\partial x^2}. \quad (\text{C.1})$$

This equation describes the balance between the wire's tension τ_x and its deflection $z(x)$, where the second derivative represents the local curvature of the wire. The negative sign indicates that the restoring force opposes the displacement, acting to minimise curvature and restore equilibrium. In the context of electrostatic deflection, this restoring force is counteracted by the electrostatic attraction from the applied voltage, which deforms the wire and alters the local electric field E .

$$f_l = \frac{1}{2} \epsilon (E_{top}^2 - E_{bottom}^2) p. \quad (\text{C.2})$$

Solving Equation C.1 and applying boundary conditions $x = \pm L/2$, for L the full diameter of the wire and p the pitch, yields a parabolic deflection relation.

$$z(x) = \frac{f_l}{2\tau_x} \left(\frac{L^2}{4} - x^2 \right). \quad (\text{C.3})$$

The maximum deflection occurs at $x = 0$. For a mesh grid, the effective force per wire is distributed across both x - and y -direction wires, effectively halving the per-wire force. Incorporating this and substituting Equation C.2, the maximum deflection for a given grid i is:

$$z_i = \frac{1}{32\tau_i} \epsilon_i (E_{i,top}^2 - E_{i,bottom}^2) p_i L^2. \quad (\text{C.4})$$

While this first-order derivation provides a reasonable estimate of deflection, it does not fully capture higher-order effects arising from coupling between tensile forces and Coulomb interactions, which may lead to subtle adjustments in the equilibrium shape.

C.1.2 The Euler-Lagrange Method

The parallel wire approximation in the catenary model offers a simplified picture by treating each wire in the woven mesh as an independent tensioned strand, allowing for straightforward analytical solutions to electrostatic deflection as seen previously. However, this approach neglects mechanical interactions between neighbouring wires, which can redistribute tension and reduce overall sag. A natural extension is a membrane model, which treats the grid as a continuous, tensioned surface where forces are more evenly distributed. While this framework accounts for global tension effects, it overestimates the stiffness of the mesh by assuming that individual wires do not deform independently at all. The Euler-Lagrange approach surpasses all of these models by minimising the total system energy, simultaneously incorporating electrostatic forces, wire tension, and elastic energy in a globally coupled framework. Unlike the catenary model, it accounts for wire interactions; and unlike the membrane model, it retains the local flexibility of individual wires, treating the full electromechanical system in a self-consistent manner. This makes the Euler-Lagrange approach the most physically complete and accurate method for predicting grid deformation under realistic experimental conditions.

Consider a uniform 2D mesh approximated as a system of parallel wires extending along the x and y directions (Fig. 4.13). To describe the equilibrium configuration of this system, we seek to determine the action, which is obtained by constructing the Lagrangian $\mathcal{L}$ that governs the behaviour of the system. The Lagrangian encapsulates the competing contributions of the system's energy, including the elastic energy $U_{elastic}$ associated with the pre-tensioning of the wires and the electrostatic energy U_{elec} arising from the capacitance between the stainless steel mesh surfaces. The equilibrium shape of the mesh is then found by minimising the action functional, whose stationary points are determined by the Euler-Lagrange equations. These equations provide a self-consistent description of the mesh deformation, ensuring that the electrostatic forces and mechanical constraints are properly accounted for in the system's response.

We begin by defining the Lagrangian. Since the system is in quasi-equilibrium and does not involve kinetic energy contributions K , the Lagrangian is entirely determined by the potential energy V .

$$\begin{aligned}\mathcal{L} &= T - V \\ &= -(U_{elastic} + U_{elec}).\end{aligned}\tag{C.5}$$

For a stainless steel mesh, that is pre-tensioned to a force τ , each wire segment with an initial unstressed length δl_0 stores elastic potential energy. The elastic energy per segment $U_{elastic}^0$ in the absence of an applied field is given by:

$$\begin{aligned}U_{elec}^0 &= \frac{1}{2} \frac{A \delta l_0}{Y} \sigma^2 \\ &= \frac{1}{2} \frac{\delta l_0}{AY} \tau^2\end{aligned}\tag{C.6}$$

, where $\tau = \sigma A$, defines the tension as a product of A , the circular cross-sectional area of the wire and σ , the stress. Introducing the Young's Modulus Y , as the stress (σ) per unit strain ($s = \frac{\delta x}{\delta l_0}$), an expression for the pre-tensioned length, $\delta l_{pre} = \delta l_0 + \delta x$, of the wire may be derived.

$$\begin{aligned}\delta l_{pre} &= \delta l_0 + \sigma \frac{\delta l_0}{Y} \\ &= \delta l_0 \left(1 + \frac{\tau}{AY}\right).\end{aligned}\tag{C.7}$$

So far we have only tried to tackle the problem of the elastic potential energy in the wire in a zero-field environment. When an external voltage is applied, the wire will further deform. The new deformed length δl can be expressed in terms of the deformation gradient (the extended line segment),

$$\begin{aligned}\delta l &= \delta l_{pre} \left(1 + \left(\frac{dz}{dx}\right)^2\right)^{\frac{1}{2}} \\ &\simeq \delta l_{pre} \left(1 + \frac{1}{2} \left(\frac{dz}{dx}\right)^2\right).\end{aligned}\tag{C.8}$$

Here we have made the assumption ($\frac{dz}{dx} \ll 1$) that in the small deformations regime, where the length scale of the gate-anode separation is much smaller than the diameter of the electrode mesh, a first order expansion is sufficient to accurately describe the system without loss of accuracy. The elastic energy stored in the single wire segment is then calculated from the elastic energy density $u_{elastic} = \frac{1}{2} Y s^2$,

$$\delta U_{elastic} = \int_V u_{elastic} dV = \frac{1}{2} Y \left(\frac{\delta l - \delta l_0}{\delta l_0}\right)^2 A \delta l.\tag{C.9}$$

This can be re-written in terms of the pre-tensioned length segment δl_{pre} , over which we need to integrate to take into account the deformation of each complete wire length along any given direction.

$$\begin{aligned}\delta U_{elastic} &= \frac{AY\delta l_0}{2} \left[\frac{\tau}{AY} + \frac{1}{2} \left(1 + \frac{\tau}{AY} \right) \left(\frac{dz}{dx} \right)^2 \right]^2 \\ &= \frac{\tau}{2} \delta l_{pre} \left[\left(\frac{\tau}{AY} \right) \left(1 + \frac{\tau}{AY} \right)^{-1} + \left(\frac{dz}{dx} \right)^2 + \mathcal{O} \left(\frac{dz}{dx} \right)^4 \right].\end{aligned}\quad (C.10)$$

To determine the total elastic energy stored in the mesh, we integrate over its entire structure. A wire oriented along the x -direction at a given position y extends from $-x_0$ to x_0 , where $x_0 = \sqrt{R^2 - y^2}$. Summing over all wires, with N_i wires per unit length in both x and y directions, yields the total elastic energy expression.

$$U_{elastic} = U_0^x + U_0^y + \int_R \frac{\tau}{2} \left[N_x \left(\frac{dz}{dx} \right)^2 + N_y \left(\frac{dz}{dy} \right)^2 \right] dx dy. \quad (C.11)$$

Finally, by accounting for the combined deflection contributions from both the gate and the anode, and expressing the wire density as $N = 1/p$, where p represents the pitch of the mesh, we obtain the final expression for the elastic potential energy stored in the gate and anode wire meshes due to deformation of the grids:

$$\begin{aligned}U_{elastic} &= U_{0,g}^x + U_{0,g}^y + \int_R \left[\frac{\tau_g}{2} \left(\frac{1}{p_g^x} \left(\frac{dz_g}{dx} \right)^2 + \frac{1}{p_g^y} \left(\frac{dz_g}{dy} \right)^2 \right) \right] dx dy \\ &+ U_{0,a}^x + U_{0,a}^y + \int_R \left[\frac{\tau_a}{2} \left(\frac{1}{p_a^x} \left(\frac{dz_a}{dx} \right)^2 + \frac{1}{p_a^y} \left(\frac{dz_a}{dy} \right)^2 \right) \right] dx dy.\end{aligned}\quad (C.12)$$

Next, we must find an expression for the electrostatic energy stored in the system. Conventionally, this is done by integrating the local capacitance per unit area over the surface.

$$U_{elec} = \frac{1}{2} \int_R C_{eff}(x, y) V^2 dx dy. \quad (C.13)$$

As both the gate and anode grids are deflecting, the electrostatic energy must account for the position-dependent capacitance between the two deforming surfaces. Instead of treating either grid as a fixed reference, we must incorporate both $z_g(x, y)$ (gate height after deflection) $z_a(x, y)$ (anode height after deflection) explicitly. The capacitance per unit area now depends on the local separation between these surfaces and is further modified by the permittivities of the liquid and gaseous xenon regions. This defines the system's effective capacitance, C_{eff} , for a given potential difference V applied between the grids. Additionally, the liquid-gas interface at z_{LS} introduces two distinct dielectric regions, which can be modelled as two capacitors in series. The explicit dependence of capacitance on the grid deflections introduces a feedback loop, where increased deflection alters the local electric field, further influencing the grid deformations. This feedback mechanism is directly incorporated into our model.

$$U_{elec} = \frac{1}{2} \int_R \epsilon_{GXe} \frac{V^2}{(z_a - z_{LS}) + (z_{LS} - z_g)/\epsilon_{LXe}} dx dy \quad (C.14)$$

We are now ready to define the final Lagrangian of the system. Considering the symmetric case, as in LZ, where $N_x = N_y = N = 1/p$ and $p_x = p_y$ for both gate and anode grids:

$$\mathcal{L} = -\tau_a \left(\frac{1}{p_a} \left(\frac{\partial z_a}{\partial x} \right)^2 \right) - \tau_g \left(\frac{1}{p_g} \left(\frac{\partial z_g}{\partial x} \right)^2 \right) - \frac{1}{2} \epsilon_{GXe} \frac{V^2}{(z_a - z_{LS}) + (z_{LS} - z_g)/\epsilon_{LXe}}. \quad (C.15)$$

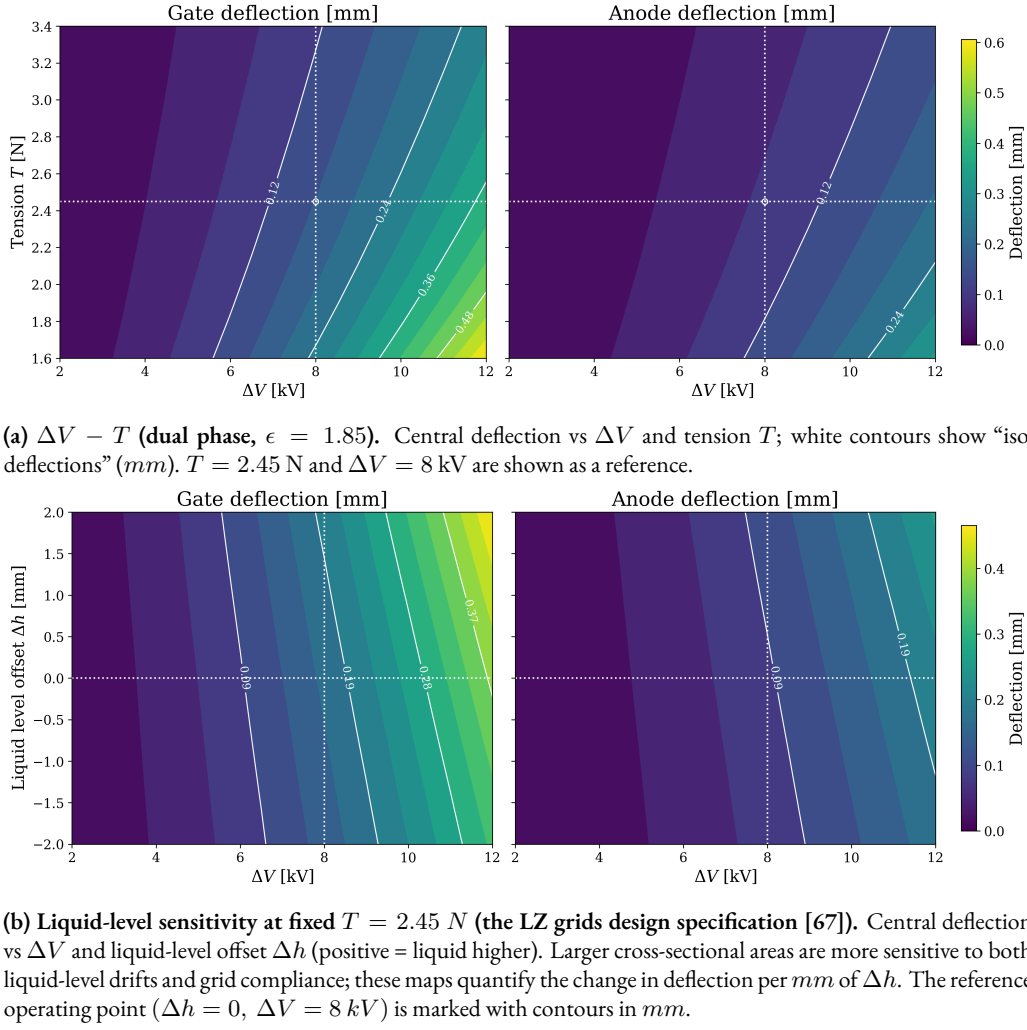


Figure C.2: NLDE predictions for gate (left) and anode (right) deflection.

The equilibrium condition is then found by solving the Euler-Lagrange equation,

$$\sum_i \partial_i \left(\frac{\partial \mathcal{L}}{\partial (\partial_i z_j)} \right) = \frac{\partial \mathcal{L}}{\partial z_j}, \quad (\text{C.16})$$

which, when applied to the Lagrangian in Equation C.15, results in a system of differential equations governing the deflections of the gate and anode. Due to the nonlinearity introduced by the electrostatic feedback, these equations must be solved numerically to obtain the equilibrium shape of the grids.

$$\frac{\tau_a}{p_a} \frac{\partial^2 z_a}{\partial x^2} = + \frac{1}{4} \frac{\epsilon_0 V^2}{((z_a - z_{LS}) + (z_{LS} - z_g)/\epsilon_{LXe})^2} \quad (\text{C.17})$$

$$\frac{\tau_g}{p_g} \frac{\partial^2 z_g}{\partial x^2} = - \frac{1}{4} \frac{\epsilon_0 V^2}{(\epsilon_{LXe}(z_a - z_{LS}) + (z_{LS} - z_g))^2}$$

The preliminary data from open-air tests during the design phase of the grids may be used to test the model. In this case, the system description is much more simple.

$$(\partial_x^2 + \partial_y^2)z = - \frac{\epsilon E^2 p}{2\tau} = \zeta \quad (\text{C.18})$$

, where ζ is a constant. Solving in cylindrical coordinates with the boundary condition $z(\pm R) = 0$ (no deflection where the grids are clamped down into the glue ring),

$$z = -\zeta(R^2 - \rho^2) \quad (\text{C.19})$$

, for ρ the radial coordinate of any given point on the grids. The model demonstrates a strong agreement with the measured data (§6.2.3, Fig. 6.5), achieving within 3.7% accuracy, and notably outperforming the catenary approximation (deviations averaging $\sim 11.5\%$). This analysis is therefore crucial not only for refining our understanding of electron transport within the LZ TPC—particularly in the context of error propagation - but also for improving our characterisation of the electric fields (Chapter 4), electroluminescence yields, and structural tolerances for deflection. These insights thus directly inform grid tensioning requirements (Fig. C.2) for future experiments even beyond XLZD.

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