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Neutrino Physics at a Research Reactor: Backgrounds and Analysis

A Dissertation Presented for the
Doctor of Philosophy
Degree
The University of Tennessee, Knoxville

Blaine Heffron

May 2023

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Acknowledgements

I would like to thank my advisor Alfredo Galindo-Uribarri for his assistance throughout my time at UT with both my Masters and PhD work. I would also like to thank Michael Mendenhall for the help he gave me with respect to the analysis of the PROSPECT data. I learned a tremendous amount from reading the code for his analysis and simulation packages. Many thanks to the PROSPECT collaboration for providing a rigorous education in the physics of neutrino detection, especially the main PIs: Nathaniel Bowden, Bryce Littlejon, Peter Mumm, Karsten Heeger, David Jaffe, and Russel Neilsen.

Thanks to David Glasgow for letting us borrow his Germanium detector and data acquisition equipment for the gamma background measurement at HFIR. Thank you for all of your assistance with getting the detector working and reading the data. Thanks to David Radford for his assistance in analyzing Germanium detector data and understanding their operation.

Thanks to my colleagues within our group at UT. Jeremy for his assistance with various items related to the PROSPECT analysis, Diego for providing scripts for IBD analysis, and Corey for helping build the Ge detector stand. Also thanks Diego and Jeremy for their help with the Ge measurements and building the water shield.

Thanks to my friends in Knoxville, especially Shane for some great chess games and Clara for many great conversations. Thanks to my girlfriend Gabrielle for her support during the writing and defending of my dissertation.

Thanks to my friends Drew, Trevor and Chris back home in Charleston for the many great times. Thanks Chris for the many great adventures and Jeremy for the great conversations.

Thanks to my family, especially my parents for always supporting me in my endeavors.

Abstract

The field of neutrino physics has a rich history and is currently the subject of much active research. The discovery of neutrino oscillations led to the conclusion that neutrinos have mass which was in contradiction to the Standard Model. Now researchers are investigating a number of open questions regarding neutrino properties such as their mass values or the existence of CP violation in the weak interaction. In order to answer these questions experimental and analytical techniques of neutrino detection are becoming more advanced, entering into an era of precision neutrino detection.

Nuclear reactors as a source of antineutrinos have played a historically important role in the field, and provide important knowledge at the interface of particle and nuclear physics. Recent and future planned experiments at reactors must deal with intense sources of gamma and neutron radiation while also discriminating neutrino events from cosmic rays. For this reason it is important to have a detailed understanding of the background radiation at the experiment site. This allows for effective shielding design for background mitigation and aids in understanding the requirements of analysis methods for background rejection. To that end, this dissertation provides the first high resolution spatial characterization of the gamma radiation field at the neutrino experiment hall at the High Flux Isotope Reactor (HFIR) in Oak Ridge, TN.

In the second part of the dissertation I discuss the PROSPECT experiment which measured the antineutrino flux at HFIR in 2018. This was the first high

precision measurement of the ^{235}U antineutrino energy spectrum. Sophisticated analysis techniques to select the antineutrino events were employed based on a detailed understanding of the detector response and the cosmic and reactor backgrounds present in the detector. Nowadays computational resources have grown to the point where it is feasible to utilize computationally expensive machine learning methods for such analysis tasks. This work includes an in depth comparison between classical analysis techniques and novel applications of machine learning, the latter of which are shown to improve the effective statistics of the experiment.

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Nomenclature

$\bar{\nu}$	Antineutrino
ν_e	Electron Neutrino
$\bar{\nu}_e$	Electron Antineutrino
ν_μ	Muon Neutrino
$\bar{\nu}_\mu$	Muon Antineutrino
ν_τ	Tau Neutrino
PROSPECT	Precision Reactor OSCillation SPECTrum
CC	Charged Current
CE ν NS	Coherent Elastic Neutrino-Nucleus Scattering
CL	confidence level
CNN	Convolution Neural Network
DAQ	Data acquisition
DAR	Decay at rest
DIF	Decay in flight
ENDF	Evaluated Nuclear Data File

ES	Elastic Scattering
FC	Feldman-Cousins
FEP	Fluorinated ethylene propylene
GCN	Graph Convolutional Network
GNN	Graph Neutral Network
HRIBF	Holifield Radioactive Ion Beam Facility
HV	High voltage
IBD	Inverse Beta-Decay
JEFF	Joint Evaluated Fusion and Fission
LBL	Long baseline
MSW	Mikheyev–Smirnov–Wolfenstein
MTAS	Module Total Absorption Spectrometer
mwe	Meters water equivalent
NC	Neutral Current
PLA	Polylactic acid
PMNS	Pontecorvo–Maki–Nakagawa–Sakata
PMT	Photomultiplier tube
RAA	Reactor Antineutrino Anomaly
ROI	Region of Interest
RS	Raster scan

SBL	Short baseline
SM	Standard Model
SNS	Spallation Neutron Source
TAS	Total Absorption Spectroscopy
vLBL	Very long baseline

Chapter 1

Historical Overview and Theoretical Background of Neutrino Oscillation Physics

1.1 General Introduction

Neutrino Physics has had a rich history over the past several decades, largely due to the neutrino being one of the most difficult of the Standard Model (SM) particles to detect. This is largely due to the fact that it is both electrically neutral and has a very small mass. Its only channels of interaction are via the weak interaction and gravity. Given the elusive nature of the neutrino, it is understandable that it is one of the least understood of the SM particles. Experiments are still ongoing in order to determine the masses of the three SM flavors of neutrinos, whether the neutrino is its own antiparticle (i.e a Majorana fermion), if CP violation occurs due to neutrino properties, and whether or not there are other flavors of neutrinos beyond the 3 SM ones.

Within the context of neutrino physics, nuclear reactors play an important role. Nuclear reactors are the largest source of man-made neutrinos and thus make a natural

candidate for the study of neutrino physics. Experiments done at reactors face a number of challenges unique to the reactor environment. Chapter 2 will go into detail regarding the reactor physics relevant to neutrino physics measurements along with experimental techniques utilized. Reactors contain significant amounts of background radiation due to their operation. These backgrounds largely are from neutrons and γ -rays both from the interactions within the core and secondary interactions of neutrons in structural materials throughout the building. Thus, in order to perform a successful neutrino experiment within a reactor, one must find ways to mitigate the backgrounds related to the reactor operation. This will be the main focus of chapter 3 wherein I will detail gamma measurements taken at HFIR so as to better understand the types of shielding required for neutrino experiments in that space.

Another factor to take into account when measuring neutrinos at a reactor are cosmic ray backgrounds. Because reactors are located on the surface of the Earth, the signals produced by cosmic rays can often pollute the neutrino signal, and are not feasible to shield from due to the highly penetrative nature of this type of background along with weight and space requirements of the facility. Thus, it is important for the neutrino detection system to utilize specific signatures of the neutrino interaction in order to distinguish signal from cosmic interactions. Chapter 5 will go into more detail about the signal filtering strategies used by the PROSPECT experiment to deal with cosmic backgrounds after chapter 4 which goes over the details of the PROSPECT experiment..

In addition to the conventional strategies for dealing with cosmic backgrounds outlined in chapter 4, chapter 6 will detail the usage of machine learning models to aid in signal detection which could be applied to any segmented neutrino detector. Machine learning has seen a large increase in popularity over the past couple of decades to the increasing availability of both computing power and software easing the implementation of such techniques. A number of neutrino experiments and other high energy physics experiments have already been leveraging the power of machine

learning, and the applications described in this dissertation can add to this growing list.

1.2 Historical context

The neutrino was first described in 1934 by Fermi in his theory of Beta Decay [1, 2, 3], in which the reaction

$$n^0 \rightarrow p^+ + e^- + \bar{\nu}_e \quad (1.1)$$

was postulated in order to explain the continuous spectrum of electron energies measured from beta decaying nuclei. It wasn't until 1956 when the first neutrino was detected using a source of anti-neutrinos from a nuclear reactor at Savanna River Site [4]. Now known as the Reines and Cowan experiment, the inverse beta decay (IBD) reaction

$$\bar{\nu}_e + p \rightarrow n + e^+ \quad (1.2)$$

was detected using a container of water to provide protons surrounded liquid scintillator complete with photomultiplier tubes to detect the annihilation gammas from the outgoing positron. The outgoing neutron was detected via neutron capture on cadmium, which was dissolved into the water using a cadmium chloride mixture. This pioneering experiment draws many parallels to modern day neutrino experiments which are in essence a refinement of this same experimental technique.

In the SM of particle physics, the neutrino is classified as a lepton and has 3 different types analogous to its heavier partner charged leptons - the electron, muon and tau particles. The muon neutrino (ν_μ) was first detected at Brookhaven in 1962 [5]. The existence of the tau neutrino (ν_τ) was implied after the tau particle's discovery in a series of experiments performed in 1974 by the SLAC-LBL group lead by Martin Perl [6] and was first detected in 2000 by the DONUT group [7].

Questions remained about this neutral particle, such as its rest mass. The first experiment to measure the neutrino's velocity in 1976 [8] used a comparison of muon

and neutrino velocities, finding that the neutrino velocity agreed to the speed of light in vacuum at a 95% confidence level. Experiments since, including the latest measurement by OPERA [9], confirm this finding measuring $(v - c)/c = (2.7 \pm 3.1(stat.)_{-3.3}^{+3.4}(sys.)) \times 10^{-6}$.

The first experimental evidence of a nonzero neutrino mass came back in 1968, when Davis et al. measured the solar neutrino flux finding a deficit relative to experimental calculations [10]. This result was confirmed in 1989 by the Kamiokande experiment [11], and later by the GALLEX [12] and SAGE [13] experiments. These results point to neutrino flavor oscillation, which can only be possible if the neutrino has a nonzero rest mass [14]. Pontecorvo first pointed out that neutrino oscillation between ν_e and $\bar{\nu}_e$ might be possible inspired by the observed neutral kaon-antikaon oscillation in 1957 [15, 16]. After the discovery of the muon, it was then theorized that oscillation between leptonic states could occur [17, 18]. In 1996, the LSND experiment claimed evidence of $\nu_\mu \rightarrow \nu_e$ oscillation [19], finding an oscillation probability of $0.31 + / - 0.05(stat.)_{-0.10}^{+0.11}(sys.)$. Since then a number of experiments have been carried out to measure the oscillation parameters that describe neutrino mixing. These will be described more in the following section detailing the neutrino mixing formalism 1.3.

1.3 Neutrino Oscillation Formalism

In this section the basic neutrino oscillation formalism is described. The relations between the theoretical neutrino properties and the degree of mixing are enumerated. This is accomplished using plane wave assumptions for the neutrino propagation. The idea that neutrinos can oscillate into different flavor states came about shortly after the muon lepton state was discovered [17, 16] and was first hinted at experimentally by Davis et al. due to a deficit in the measured solar neutrino flux [10]. This initiated several experiments to further explore the properties of the neutrino related to these oscillations.

The formal theory behind neutrino oscillations was developed in 1975-76 by Eliezer and Swift [20], Fritzsch and Minkowski [21] and Pontecorvo and Bilenky [22]. The theory behind neutrino oscillations is based on the idea that the flavor eigenstate of the neutrino which is produced in a weak interaction is composed of a superposition of mass eigenstates. What follows is a derivation of the neutrino oscillation amplitude assuming k mass eigenstates of the neutrino following the treatment described in [23], pages 247-9. Note that in the following derivation the speed of light, mass of the electron, reduced Planck's constant, and vacuum permittivity are set to 1.

The neutrino with flavor α and momentum $\vec{p}$ originating from a charged-current weak interaction can be represented by the flavor state

$$|\nu_\alpha\rangle = \sum_k U_{\alpha k}^* |\nu_k\rangle \quad \alpha \in \{e, \mu, \tau\} \quad (1.3)$$

where U , often referred to as the Pontecorvo-Maki-Nakagawa-Sakata mixing matrix, is unitary and complex. Note that if the number of mass states is greater than 3, this implies that there are $k - 3$ sterile neutrino states, called such because they do not interact via a leptonic interaction and must only interact via gravity and non-SM interactions.

We assume orthonormal massive neutrino states $\langle \nu_k | \nu_j \rangle = \delta_{kj}$ and orthonormal flavor states enforced by the unitary nature of U , $\langle \nu_\alpha | \nu_\beta \rangle = \delta_{\alpha\beta}$. The massive states are eigenstates of the Hamiltonian, thus propagate through vacuum as planewaves,

$$|\nu_k(t)\rangle = e^{-iE_k t} |\nu_k\rangle. \quad (1.4)$$

Thus, the time evolution of the flavor state at time t is

$$|\nu_\alpha(t)\rangle = \sum_k U_{\alpha k}^* e^{-iE_k t} |\nu_k\rangle. \quad (1.5)$$

From the unitary nature of U we can invert [1.3](#) to find the mass eigenstates in terms of U ,

$$|\nu_k\rangle = \sum_{\alpha} U_{\alpha k} |\nu_{\alpha}\rangle. \quad (1.6)$$

We can substitute [1.6](#) into [1.5](#) to get

$$|\nu_{\alpha}(t)\rangle = \sum_{\beta \in \{e, \mu, \tau\}} \left(\sum_k U_{\alpha k}^* e^{-iE_k t} U_{\beta k} \right) |\nu_{\beta}\rangle. \quad (1.7)$$

Thus the amplitude of a transition from flavor α at time $t = 0$ to β at time t is

$$A_{\nu_{\alpha} \rightarrow \nu_{\beta}}(t) = \sum_k U_{\alpha k}^* U_{\beta k} e^{-iE_k t}, \quad (1.8)$$

with probability

$$P_{\nu_{\alpha} \rightarrow \nu_{\beta}}(t) = |A_{\nu_{\alpha} \rightarrow \nu_{\beta}}(t)|^2 = \sum_{k,j} U_{\alpha k}^* U_{\beta k} U_{\alpha j} U_{\beta j}^* e^{-i(E_k - E_j)t}. \quad (1.9)$$

Neutrinos detected in experiments have a lower energy threshold of around 100 keV, and since the neutrino mass is less than 1 eV with the current lowest upper bounds set by the KATRIN experiment [\[24\]](#), it is a good approximation to treat the neutrino as traveling at the speed of light. Thus, the energy for mass state k can be approximated as $E_k \approx E + \frac{m_k^2}{2E}$, where $E = |\vec{p}|$. Therefor the energy difference between two mass states can be approximated as

$$E_k - E_j \approx \frac{\Delta m_{kj}^2}{2E}, \quad (1.10)$$

where $\Delta m_{kj}^2 \equiv m_k^2 - m_j^2$.

Substituting [1.10](#) into [1.9](#), and utilizing the fact that neutrinos propagate very close to the speed of light so that $t = L$ where L is the distance from the source to

the detector, we get

$$P_{\nu_\alpha \rightarrow \nu_\beta}(L, E) = \sum_{k,j} U_{\alpha k}^* U_{\beta k} U_{\alpha j} U_{\beta j}^* \exp\left(-i \frac{\Delta m_{kj}^2 L}{2E}\right). \quad (1.11)$$

Thus the phase of the oscillation depends on the squared-mass differences between mass states and the distance energy ratio L/E , while the amplitude of the oscillation is only dependent on the elements of the mixing matrix U . In practice it is useful to separate the real and imaginary components of this probability equation. By utilizing the unitarity of the matrix U , we find that

$$\begin{aligned} P_{\nu_\alpha \rightarrow \nu_\beta}(L, E) = & \delta_{\alpha\beta} - 4 \sum_{k>j} \Re[U_{\alpha k}^* U_{\beta k} U_{\alpha j} U_{\beta j}^*] \sin^2\left(\frac{\Delta m_{kj}^2 L}{4E}\right) \\ & + 2 \sum_{k>j} \Im[U_{\alpha k}^* U_{\beta k} U_{\alpha j} U_{\beta j}^*] \sin\left(\frac{\Delta m_{kj}^2 L}{2E}\right). \end{aligned} \quad (1.12)$$

In the following sections we will describe two neutrino mixing and then how to apply this formalism to an experimental measurement in order to extract bounds on mixing parameters.

1.3.1 Two Neutrino Mixing

In practice it is useful to simplify the oscillation formalism to two neutrinos in order to reduce the number of relevant parameters for an experiment. This works out because most experiments are only sensitive to mixing between two different neutrino flavors based on the L/E region probed. The argument for why this is a valid approximation for different experiments is provided in section 1.5 where the experimental data for solar and atmospheric experiments points to a mass splitting hierarchy where one of the mass squared differences is much larger than the other (see figure 1.2 for a visualization of this hierarchy in the three neutrino case).

Given two flavor states α, β corresponding to one of $e, \mu, \mu, \tau, e, \tau$ or a linear combination of two flavor states (e.g. $\nu_\beta = c_\mu \nu_\mu + c_\tau \nu_\tau$ where $c_\mu^2 + c_\tau^2 = 1$) and two mass states ν_1, ν_2 , we have an effective two-neutrino mixing matrix

$$U = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \quad (1.13)$$

where $0 \leq \theta \leq \pi/2$. The mass squared difference in the two neutrino case is $\Delta m^2 \equiv \Delta m_{21}^2 = m_2^2 - m_1^2$. We will define ν_1 as the lighter of the two neutrino masses so that Δm^2 is positive.

Substituting the unitary matrix from equation 1.13 into the equation for the oscillation probability $P_{\nu_\alpha \rightarrow \nu_\beta}$ in equation 1.11, we find that the two neutrino oscillation probability takes the form

$$\begin{aligned} P_{\nu_\alpha \rightarrow \nu_\beta}(L, E) &= \frac{1}{2} \sin^2 2\theta \left[1 - \cos \left(\frac{\Delta m^2 L}{2E} \right) \right] \\ &= \sin^2 2\theta \sin^2 \left(\frac{\Delta m^2 L}{4E} \right) \quad (\alpha \neq \beta), \end{aligned} \quad (1.14)$$

which yields the survival probability (due to unitarity)

$$P_{\nu_\alpha \rightarrow \nu_\alpha}(L, E) = 1 - \sin^2 2\theta \sin^2 \left(\frac{\Delta m^2 L}{4E} \right). \quad (1.15)$$

Converting from our natural units to units used in experiments (source-detector distances of meters [kilometers] and neutrino energies in MeV [GeV] for reactor [accelerator] experiments), we have

$$P_{\nu_\alpha \rightarrow \nu_\beta}(L, E) = \sin^2 2\theta \sin^2 \left(1.27 \frac{\Delta m^2 [\text{eV}^2] L [\text{m or km}]}{E [\text{MeV or GeV}]} \right) \quad (\alpha \neq \beta). \quad (1.16)$$

1.3.2 Averaged Transition Probability

In practice since detectors only have a finite spatial resolution and energy resolution and the source of the neutrinos has some width and some energy distribution, we must

average this transition probability over the standard deviation of the L/E ratio. Given a distribution $\phi(L/E)$ of the L/E ratio which takes all of these effects into account, we will measure an average transition probability of

$$\langle P_{\nu_\alpha \rightarrow \nu_\beta}(L, E) \rangle = \frac{1}{2} \sin^2 2\theta \left[1 - \left\langle \cos \left(\frac{\Delta m^2 L}{2E} \right) \right\rangle \right] \quad (\alpha \neq \beta), \quad (1.17)$$

where the average is found by integrating over the distribution. A realistic example can be found assuming a Gaussian distributed ϕ with standard deviation $\sigma_{L/E}$. This yields an average cosine function

$$\left\langle \cos \left(\frac{\Delta m^2 L}{2E} \right) \right\rangle = \cos \left(\frac{\Delta m^2}{2} \left\langle \frac{L}{E} \right\rangle \right) \exp \left[-\frac{1}{2} \left(\frac{\Delta m^2}{2} \sigma_{L/E} \right)^2 \right]. \quad (1.18)$$

Figure 1.1 plots the transition probability (dashed) as a function of $\frac{L}{E} \Delta m^2$ in [km]/[GeV] [eV²] and the averaged transition probability (solid) assuming a Gaussian L/E distribution with $\sigma_{L/E} = 0.2 \langle \frac{L}{E} \rangle$. This plot assumes $\sin^2 2\theta = 1$. This plot makes it clear that for $\frac{\Delta m^2 L}{2E} \ll 1$, the experiment is not sensitive to oscillations while for $\frac{\Delta m^2 L}{2E} \gg 1$, the experiment is only sensitive to the value of $\sin^2 2\theta$. The solid line most closely follows the dashed line at values of $\frac{\Delta m^2 L}{2E} \approx 1$, thus defining the sensitivity of a given experiment to Δm^2 . A table of different types of oscillation experiments and their corresponding sensitivities to mass squared differences can be found in table 1.1.

1.4 Neutrino Oscillation Experiments

Neutrino oscillation experiments can be grouped into 7 categories: solar, reactor long baseline (LBL), reactor short baseline (SBL), atmospheric, accelerator disappearance, and accelerator appearance. Solar experiments measure the neutrino flux from the sun, see 1.4.1. Atmospheric experiments measure the neutrino flux from cosmic ray interactions in the atmosphere, see 1.4.2. Reactor experiments measure antineutrinos

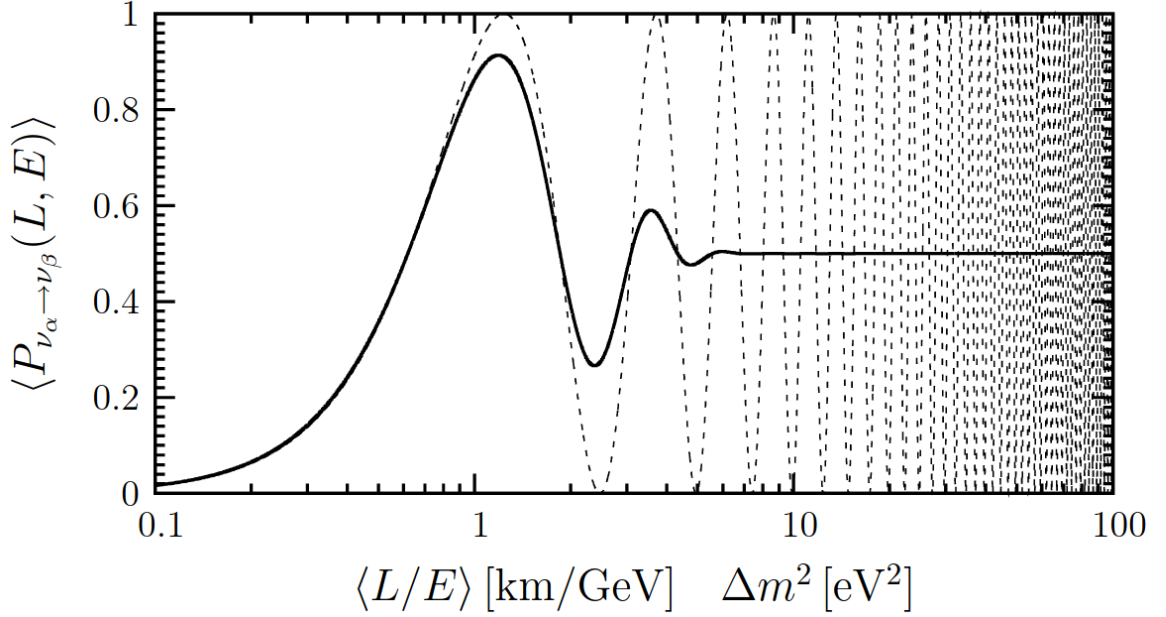


Figure 1.1: $\nu_\alpha \rightarrow \nu_\beta$ transition probability as a function of $\frac{L}{E}\Delta m^2$ assuming $\sin^2 2\theta = 1$. Dashed line is transition probability, solid is transition probability averaged over a Gaussian L/E distribution with $\sigma_{L/E} = 0.2\langle\frac{L}{E}\rangle$. Source: [23].

Table 1.1: Oscillation experiments and their typical source-detector lengths L and neutrino energies E and their corresponding Δm^2 sensitivities. Source: [23].

Experiment Type	L	E	Δm^2 sensitivity
Reactor SBL	10 m	1 MeV	0.1 eV ²
Accelerator SBL (Pion DIF)	1 km	$\gtrsim 1$ GeV	$\gtrsim 1\text{eV}^2$
Accelerator SBL (Muon DAR)	10 m	10 MeV	1 eV ²
Accelerator SBL (Beam Dump)	1 km	10 ² GeV	10 ² eV ²
Reactor LBL	1 km	1 MeV	10 ⁻³ eV ²
Accelerator LBL	10 ³ km	$\gtrsim 1$ GeV	$\gtrsim 10^{-3}\text{eV}^2$
ATM	20-10 ⁴ km	0.5 - 10 ² GeV	10 ⁻⁴ eV ²
Reactor VLB	10 ² km	1 MeV	10 ⁻⁵ eV ²
Accelerator VLB	10 ⁴ km	$\gtrsim 1$ GeV	$\gtrsim 10^{-4}\text{eV}^2$
SOL	10 ¹¹ km	0.2 - 15 MeV	10 ⁻¹² eV ²

from nuclear fission reactors at distances of meters (SBL, [1.4.5](#)), 1-10s of km (LBL, [1.4.6](#)) and 100s of km (vLBL, [1.4.6](#)). Accelerator experiments measure neutrinos from particle beam interactions on targets produced via particle accelerators. These can be grouped into short baseline ([1.4.3](#)) where the distance from source to detector is on the order of meters and long baseline ([1.4.4](#)) where the distance is on the order of kilometers.

1.4.1 Solar Neutrino Experiments

The first experiment to measure the solar neutrino flux was started in 1968 by Davis et. al [[10](#)] at the Homestake mine in South Dakota. The experiment utilized the inverse beta decay reaction



first suggested by Pontecorvo in 1946 [[25](#)] for detecting solar neutrinos. This experiment laid the groundwork for future experiments utilizing the inverse beta decay reaction such as PROSPECT which will be discussed in detail in chapter [4](#).

The Homestake experiment consisted of a single tank filled with 60,000 liter tank of tetrachloroethylene (C_2Cl_4). Every two months the Argon was extracted from the tank using a chemical extraction and the ^{37}Ar is counted using proportional counters. Due to this chemical extraction process this type of experiment is known as a radiochemical experiment. After correcting for the production of Ar due to cosmic background radiation and the decay half life of ^{37}Ar the IBD event rate was estimated at 0.047 ± 0.013 atoms/day. The lower energy threshold of the Chlorine IBD process is 0.814 MeV which means the Homestake experiment is mostly sensitive to neutrinos from the ^8B beta plus decay process.

The Gallium experiments GALLEX [26], GNO [27], and SAGE [13] are also radiochemical experiments that utilize the inverse beta decay reaction



which has a lower energy threshold of 0.233 MeV making it more sensitive to the pp reaction and electron capture ${}^7\text{Be}$ reaction which contribute to 54% and 27% of the predicted IBD event rate within the detector.

A third type of solar neutrino experiment is the water Cherenkov type detector. This type detects the Cherenkov radiation produced from the ultrarelativistic leptons traveling through the water which are byproducts of neutrino interactions in and around the detector. The Cherenkov light is produced with an energy spectrum

$$\frac{dN}{d\lambda dx} = 2\pi\alpha \left[1 - \left(\frac{1}{nv} \right)^2 \right] \lambda^{-2} \quad (1.21)$$

for a charged particle along a track coordinate x , velocity v and wavelength λ through a medium with index of refraction n , and fine structure constant α [28]. For a relativistic particle in water the Cherenkov radiation consists of about 340 photons/cm with wavelengths between 300 and 600 nm [23]. The radiation is produced with an opening cone half angle of $\cos(\theta) = 1/nv$ which yields $\theta \approx 41^\circ$ for water which has an index of refraction of 1.33 [29].

An array of photomultiplier tubes (PMTs) align the surfaces of the water tank and precise timing of the detection of the Cherenkov radiation allow for a reconstruction of the particle track of the relativistic particle. In order to achieve a precise enough reconstruction for neutrino identification a PMT coverage of at least 20% of the surface area of the tank is required.

There have been several water Cherenkov type experiments that have contributed to our knowledge of solar physics and supernova neutrinos which these experiments

are sensitive to. These include the Kamiokande [30], Kamiokande-II [31], Super-Kamiokande [32], and SNO [33, 34, 35] experiments.

The Kamiokande experiment was the first to utilize the water Cherenkov radiation for neutrino detection. It was originally designed to detect nucleon decays. In order to detect ^8B neutrinos with energies in the 10 MeV range, the backgrounds for the detector had to be reduced substantially. To achieve this, the detector was modified so that an inner volume of water was shielded by an outer volume of water. The inner volume consisted of a cylinder of height 13.1 m and diameter 14.4 m consisting of 2142 tons of purified water with 20% surface coverage utilizing 948 PMTs. This configuration was named Kamiokande-II. The reaction used to detect neutrinos was the elastic scattering (ES) reaction

$$\nu_e + e^- \rightarrow \nu_e + e^-, \quad (1.22)$$

with the kinetic energy of the electron being measured through the Cherenkov radiation.

Super-Kamiokande expanded on this by differentiating the detection of electron and muon neutrinos due to the difference in topology of the emitted Cherenkov light. Utilizing the same concept as Kamiokande-II, Super-Kamiokande expands its inner volume to a height of 42 m and a diameter of 39.3 m and increases the surface area covered to 40% using 11146 PMTs.

SNO was the first to detect tau neutrinos which is accomplished via their heavy water based Cherenkov detector. The first iteration of the SNO experiment consisted of a kiloton of 99.92% isotopically enriched D_2O which is contained within a 6 m radius spherical vessel. It detected neutrinos through three interaction channels - charged current (CC), neutral current (NC), and electric scattering (ES). The CC interaction involving inverse beta decay with deuterium is

$$\nu_e + d \rightarrow p + p + e^-. \quad (1.23)$$

This interaction has a low neutrino energy threshold of 1.442 MeV. The neutrino energy is well approximated by measuring the kinetic energy of the electron. Because of high backgrounds at such low energies, SNO only had sensitivity to electron energies down to 5.5 MeV corresponding to a neutrino energy of 6.9 MeV. This meant SNO was only sensitive to ^8B neutrinos. The ES interaction is the same used for water based detectors as in equation 1.22. SNO was also limited by their 5.5 MeV electron kinetic energy threshold for this reaction.

The NC interaction for neutrino with lepton flavor α

$$\nu_\alpha + d \rightarrow p + n + \nu_\alpha \quad (1.24)$$

and has a neutrino energy threshold of 2.224 MeV which means it is only sensitive to ^8B neutrinos. This interaction allows detection of all three known lepton flavors which allows for a model independent test of the total neutrino flux for each flavor coming from the sun. In the first phase the neutron was detected by its capture on deuteron which results in a single 6.25 MeV gamma.

The second phase of SNO improved their NC interaction detection by adding 2 tons of NaCl. This added the detection of the neutron via the neutron capture on ^{35}Cl

$$n + {}^{35}\text{Cl} \rightarrow {}^{36}\text{Cl}, \quad (1.25)$$

which yields 8.57 MeV of energy in the form of several gamma rays. The gamma rays in this process are emitted isotropically which produces topologically distinct signals compared to the Cherenkov radiation emitted from leptons, allowing a strong background rejection. Note that the usage of a neutron capture agent added to the detector is the same idea used by the PROSPECT detector for reactor $\bar{\nu}_e$ as will be discussed in detail in chapter 4.

The third phase of SNO utilized 3-He proportional counting tubes for detecting thermal neutrons within the D₂O. This allowed for increased efficiency for neutron detection.

1.4.2 Atmospheric Neutrino Experiments

Cosmic rays consist primarily of highly energetic protons and to a smaller extent heavier nuclei. A flux of these particles pervades the universe and their interactions with the Earth's atmosphere creates neutrinos. The primary production of atmospheric neutrinos is due to pions that are produced by cosmic ray interactions with nuclei in the atmosphere which will then decay via the reactions [23]

$$\pi^+ \rightarrow \mu^+ + \nu_\mu, \quad \pi^- \rightarrow \mu^- + \bar{\nu}_\mu. \quad (1.26)$$

Muons can also decay before reaching the ground resulting in electron neutrinos via the reactions

$$\mu^+ \rightarrow e^+ + \nu_e + \bar{\nu}_\mu, \quad \mu^- \rightarrow e^- + \bar{\nu}_e + \nu_\mu. \quad (1.27)$$

These neutrinos are produced with a wide range of energies varying from 100s of MeV to greater than TeV scale. Neutrinos within the range 100 MeV to 100 GeV are able to be detected by underground neutrino detectors.

The first experiments to detect atmospheric neutrinos were performed in the East Rand Proprietary Gold Mine in South Africa [36] and the Kolar Gold Field Mine in South India [37]. Both experiments had rock overburden greater than 8000 meters water equivalent (mwe). These experiments utilized liquid scintillator to detect muons formed from ν_μ interactions in the surrounding rock.

The Kamiokande experiment discussed in section 1.4.1 was able to detect ν_μ and ν_e atmospheric neutrinos via the detection of muons and electrons formed in the surrounding rock and within the detection volume [38]. The Irvine-Michigan-Brookhaven (IMB) detector [39, 40, 41, 42] utilized a similar design as Kamiokande.

8000 tons of water with a fiducial mass of 3300 tons in a 24 m x 18 m x 19 m tank was outfitted with 2048 PMTs. It operated with a 1570 mwe overburden. The MACRO experiment was another large area scintillator coverage experiment that operated under 3700 mwe overburden with dimensions 76.6 m x 12 m x 9.3 m [43].

The Soudan2 experiment [44] was an iron tracking calorimeter that operated in the Soudan Underground Mine State Park in northern Minnesota. It contained 963 tons of iron with a fiducial volume of 770 tons arranged in a honeycomb geometry. The detection of ionizing particles was accomplished via 1 m long, 1.5 cm diameter hytrel plastic tubes filled with a mixture of argon and CO₂ gas. A hexagonal lattice of 1.6 mm thick steel plates enclosed the tubes and an electric field was applied to force the drifting of charged particles up the tube to vertical anode wires at the tube ends which are read out by a cathode strip. Topological reconstruction was performed based on the tube location and the drift time which is proportional to the drift distance. The detector took data from April 1989 to June 2001 for a fiducial exposure of 5.90 kton-years. The Frejus [45] and NUSEX [46] experiments also tracked muon neutrinos using tracking-calorimeters.

The IceCube neutrino observatory is situated at the South Pole [47]. As of this publication it is the largest neutrino detector currently in operation. It was constructed to explore a number of different topics including neutrino astronomy at the PeV-scale and particle physics at the GeV-scale. The detector consists of a cubic kilometer of ice outfitted with digital-optical modules (DOMs) composed of a 10" PMT encapsulated within a glass pressure sphere in the deep ice. These are used to detect the cherenkov radiation from particles travelling through the ice resulting from neutrino interactions. A sub-array that is more densely instrumented called DeepCore was used to measure atmospheric neutrinos and sets some of the best limits on the Δm^2 [48]. IceCube-DeepCore and SuperKamiokande [38] provide the current best statistics on atmospheric ν_μ flux, providing the primary contributions to the global fits on neutrino oscillation parameters.

1.4.3 Short Baseline Accelerator Experiments

Short baseline accelerator experiments consist of measurement of neutrinos from pion decays in flight, muon decay at rest, and beam dump experiments. In SBL accelerator experiments, neutrinos are measured via either the ν_μ channel from pion decay (eq 1.26) or muon decay (eq 1.27). Depending on the experimental setup, both appearance and disappearance experiments can be conducted using these beams. A table summarizing the various oscillation processes measured along with the experiments is found in table 1.2.

Pion decay in flight (DIF) experiments measure neutrinos from pion and kaon decay ($K \rightarrow \mu + \nu_\mu$), producing anti-neutrinos or neutrinos depending on the polarity of the magnetic focusing horn. Approximately 1% of the neutrinos produced are $\nu_e / \bar{\nu}_e$ and $\bar{\nu}_\mu / \nu_\mu$ from muons decaying after being produced from pion or kaon decay. The energy of the neutrinos produced is on the order of a GeV, but can be much higher depending on the proton beam energy. The source-detector distance is typically on the order of 1 km for these experiments. In order to produce $\nu_\tau / \bar{\nu}_\tau$ transitions from $\nu_\mu / \bar{\nu}_\mu$ the neutrino energy must at least 3.5 GeV.

Muon decay at rest (DAR) experiments utilize accelerators with lower energy proton beams than pion DIF experiments. The $\bar{\nu}_\mu$ energies are typically in the tens of MeV range. In these experiments the π^- are mostly absorbed by the nuclei of the target so the neutrinos produced come from π^+ decay 1.26. The source-detector distance for these experiments is on the order of tens of meters.

Beam dump experiments, also known as prompt neutrino experiments, utilize proton beams with energies in the 100s of GeV. A very thick target completely stops the proton beam, producing heavy hadrons which decay with roughly equal branching ratios into muons and electrons. ν_μ and ν_e are produced with energies on the order of 100 GeV and detectors are typically placed at a distance of 1 km.

Table 1.2: Short Baseline Accelerator experiments and the oscillation channel tested.

Experiment	Process	Type
LSND [49]	$\bar{\nu}_\mu \rightarrow \bar{\nu}_e$	Muon DAR
KARMEN [50]	$\bar{\nu}_\mu \rightarrow \bar{\nu}_e$	Muon DAR
LAMPF [51]	$\bar{\nu}_\mu \rightarrow \bar{\nu}_e$	Muon DAR
BNB-MiniBooNE [52, 53]	$\nu_\mu \rightarrow \nu_e$	Pion DIF
BNB-MiniBooNE [54, 55]	$\bar{\nu}_\mu \rightarrow \bar{\nu}_e$	Pion DIF
NumI-MB [56]	$\nu_\mu \rightarrow \nu_e$	Pion DIF
SciBooNE [57]	$\nu_\mu \rightarrow \nu_\mu$	Pion DIF
SciBooNE [58]	$\bar{\nu}_\mu \rightarrow \bar{\nu}_\mu$	Pion DIF
NOMAD [59]	$\nu_\mu \rightarrow \nu_e$	Pion DIF
CCFR [60]	$\nu_\mu \rightarrow \nu_\mu$	Pion DIF
CDHS [61]	$\nu_\mu \rightarrow \nu_\mu$	Pion DIF
FNAL-E531 [62]	$\nu_\mu \rightarrow \nu_\tau$	Pion DIF
BEBC [63]	$\nu_\mu \rightarrow \nu_e$	Beam Dump
CHARM [64]	$\nu_\mu \rightarrow \nu_\tau$	Pion DIF
CHARM [65]	$\nu_\mu \rightarrow \nu_\mu$	Beam Dump
CHORUS [66]	$\nu_\mu \rightarrow \nu_\tau$	Pion DIF
NOMAD [67]	$\nu_\mu \rightarrow \nu_\tau$	Pion DIF
CHORUS [66]	$\nu_e \rightarrow \nu_\tau$	Pion DIF
NOMAD [67]	$\nu_e \rightarrow \nu_\tau$	Pion DIF
CCFR [68]	$\bar{\nu}_\mu \rightarrow \bar{\nu}_\tau$	Pion DIF
CCFR [69]	$\bar{\nu}_e \rightarrow \bar{\nu}_\tau$	Pion DIF

1.4.4 Long Baseline Accelerator Experiments

Long baseline accelerator experiments are characterized by source detector distances greater than 100 km. The neutrinos are produced by pion and kaon decays in flight. Experiments in this category include K2K [70], MINOS [71], OPERA [72], T2K [73], and NO ν A [74] experiments.

Future planned experiments are the Hyper-K experiment [75] which will utilize a water Cherenkov type detector and DUNE [76] which will utilize a liquid argon time projection chamber.

1.4.5 Short Baseline Reactor Experiments

In general reactor neutrino experiments measure $\bar{\nu}_e$ in the few MeV range which come from beta decaying nuclei that result from the fission process. The detectors are designed to detect neutrino via the inverse-beta decay (IBD) process, see equation 1.2. The physics of reactor neutrino production is explained in detail in section 2.3. Short baseline reactor experiments consist of source-detector distances of meters. Because the distances are small and reactors are situated above ground, these experiments must deal with a significantly larger amount of backgrounds associated with cosmic radiation due to being at the surface with very little overburden compared to solar, atmospheric, and accelerator based experiments. They must also deal with the gamma and neutron backgrounds associated with reactor operations. These backgrounds are discussed extensively for the High Flux Isotope Reactor (HFIR) in chapter 3. Cosmic background radiation is discussed extensively in section 4.9 specifically for the PROSPECT experiment but the considerations are the same for any surface neutrino detector.

Short baseline experiments include Savannah River [77], BUGEY [78], Krasnoyarsk [79], ILL [80], Goesgen [81], ROVNO [82], PROSPECT [83], STEREO [84], SOLID [85], NEOS [86], and Neutrino-4 [87].

1.4.6 Long Baseline Reactor Experiments

Long baseline experiments for reactor neutrinos involve source-detector distances of 1km or greater. This allows for underground detectors which can provide a much larger overburden than the SBL reactor experiments. LBL experiments include Daya Bay [88], Double Chooz [89], Palo Verde [90], RENO [91], and JUNO [92]. KamLAND [93] is a reactor neutrino experiment which is situated at a flux-weighted average distance of 180 km from various Japanese nuclear reactors and could be considered in its own “very long” baseline class of reactor neutrino detection experiments.

1.5 Three Neutrino Oscillation Phenomenology

Solar experiments were the first to point to the existence of neutrino oscillations. The deficit first measured by Davis et al. [10] was later confirmed by several experiments listed in section 1.4.1. The hypothesis that vacuum oscillations into other active neutrino flavors is responsible for this deficit is disfavored due to a lack of observation of annual cyclical rate modulations due to the eccentricity of the Earth’s orbit. This led to other hypotheses for the measured discrepancy eventually leading to the realization that matter resonant enhanced transitions from electron neutrinos to other flavors as they pass through the sun due to interactions with the electrons in the sun provide a solution.

Matter effects on neutrino oscillations were first described in 1978 by Wolfenstein [94]. The correct sign of the matter potential effect was first discovered by Langacker et. al [95] in 1983. What is now dubbed the Mikheyev–Smirnov–Wolfenstein (MSW) effect [96], interactions between neutrinos and the medium through which it propagates is widely considered the correct solution to the solar neutrino problem [97]. This matter-enhanced oscillation was described as a potential solution to the solar neutrino problem in 1986 [98]. A number of possible parameterizations

were originally allowed by existing experiments, with what is known as the Large Mixing Angle (LMA) solution ultimately being confirmed by experiments such as KamLAND [99, 93] and SNO [97]. This solution provides a mixing angle such that $\tan^2 \theta \approx 0.4$ and a mass squared difference $\Delta m^2 \approx 7 \times 10^{-5} \text{eV}^2$.

Atmospheric neutrino experiments (see section 1.4.2 for a comprehensive list of such experiments) found deficits in the predicted muon neutrino flux relative to the electron neutrino flux which led to the hypothesis that oscillation could explain the discrepancies [100, 101, 102]. The best fit parameters within the two neutrino framework to explain the atmospheric data showed a maximal mixing where $\sin^2 2\theta = 1.0$ and $\Delta m^2 = 2.1 \times 10^{-3} \text{eV}^2$, taken from the SuperK experiment [38] which provided the most precise measurement of the atmospheric neutrino flux.

Given that solar and atmospheric experiments both found evidence of oscillation from ν_e and ν_μ respectively, in order to put these measurements in the correct context for a three neutrino oscillation paradigm one must examine the oscillation parameters relevant to both experiments to determine the overall best fit parameters. We denote the mass squared difference found by the solar experiments Δm_{SOL}^2 and the mass squared difference found by the atmospheric experiments Δm_{ATM}^2 , noting that $\Delta m_{\text{ATM}}^2 \gg \Delta m_{\text{SOL}}^2$ and that Δm_{SOL}^2 has been verified by the reactor $\bar{\nu}_e$ measurement by KamLAND [103] and that Δm_{ATM}^2 has been verified by the accelerator ν_μ measurement by K2K [70].

Since the two mass squared differences measured by solar and atmospheric experiments are independent, we can assign Δm_{SOL}^2 to Δm_{21}^2 and Δm_{ATM}^2 to $|\Delta m_{31}^2|$ which gives rise to two possible mass hierarchies as depicted in figure 1.2. The normal-ordering (NO) hierarchy is the one in which the mass of ν_3 is larger than ν_2 and ν_1 , whereas the inverted-ordering (IO) hierarchy is the one in which the mass of ν_3 is smaller than ν_2 and ν_1 .

Within the three generation paradigm, the full parameterization of the mixing matrix which is known in the literature as the Pontecorvo–Maki–Nakagawa–Sakata (PMNS) matrix [104], can be written using three squared-mass differences, three

mixing angles, and three CP-violating phases (two of which are Majorana phases which do not contribute to the oscillation phenomenon and are therefor omitted). The matrix is

$$U_{PMNS} = \begin{pmatrix} c_{12}c_{13} & s_{12}c_{13} & s_{13}e^{-i\delta_{CP}} \\ -s_{12}c_{23} - c_{12}s_{23}s_{13}e^{i\delta_{CP}} & c_{12}c_{23} - s_{12}s_{23}s_{13}e^{i\delta_{CP}} & s_{23}c_{13} \\ s_{12}s_{23} - c_{12}c_{23}s_{13}e^{i\delta_{CP}} & -c_{12}s_{23} - s_{12}c_{23}s_{13}e^{i\delta_{CP}} & c_{23}c_{13}, \end{pmatrix} \quad (1.28)$$

where $c_{ab} \equiv \cos \theta_{ab}$ and $s_{ab} \equiv \sin \theta_{ab}$. Here δ_{CP} is the CP violating phase and must be constrained to $\delta_{CP} \in [0, 2\pi]$. Given the oscillation probability in equation 1.12 and the 3 neutrino mixing matrix in equation 1.28, we can see that a global fit to the neutrino data would involve the parameters Δm_{21}^2 , Δm_{31}^2 or Δm_{32}^2 , θ_{12} , θ_{13} , θ_{23} , and δ_{CP} . Note that for the NO hypothesis, Δm_{31}^2 is positive and for the IO, Δm_{31}^2 is negative. Following the convention of the latest 2021 NuFit [105] result for the global parameter fit to the 3 neutrino model, Δm_{3l}^2 is reported corresponding to the larger of the two squared-mass difference depending on the assumed mass hierarchy ($l = 1$ for NO and $l = 2$ for IO).

Table 1.3 details the different experiment types and the three neutrino model oscillation parameters that they constrain. Table 1.4 lists the best fit parameters from the global fit and their margins of error. Note that the SBL reactor experiments are not listed because they are designed to probe the possible existence of sterile neutrinos, see section 2.2 for the motivation behind these experiments.

While the three neutrino model has been successful in explaining the solar and atmospheric anomalies as well as observed oscillation in long baseline reactor and beam experiments, there are still a number of experimental results from short baseline terrestrial experiments that point to this model not being the whole picture. These include the reactor antineutrino anomaly (RAA) showing deficits in $\bar{\nu}_e$ from short baseline reactor experiments [106, 107, 108], the Gallium anomaly showing deficits

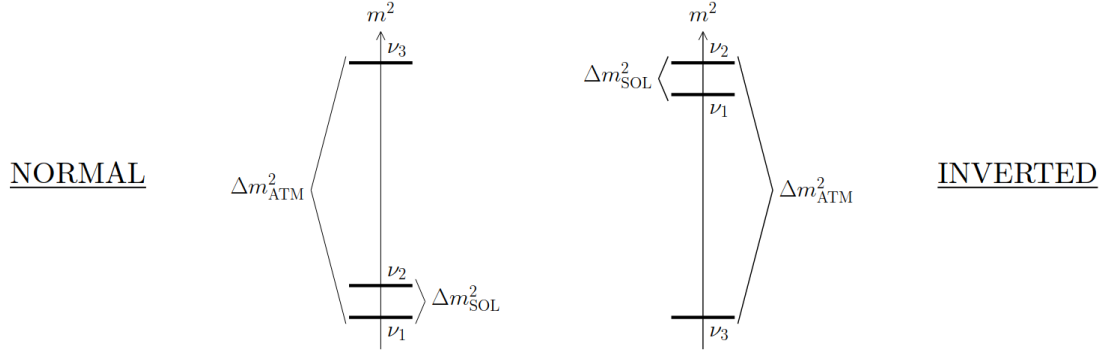


Figure 1.2: Visual depiction of the two possible mass hierarchies based on current atmospheric and solar measurements in which $\Delta m^2_{\text{SOL}} \ll \Delta m^2_{\text{ATM}}$. In the normal hierarchy. Figure taken from [23].

Table 1.3: Summary of experiment types and relevant oscillation parameters to which they contribute. (A. = accelerator, SK = SuperKamiokande, IC-DC = IceCube DeepCore) Source: [105]

Experiment	Dominant	Important
Solar Experiments	θ_{12}	$\Delta m^2_{21}, \theta_{13}$
Reactor vLBL (KamLAND)	Δm^2_{21}	θ_{12}, θ_{13}
Reac. LBL (Daya Bay, RENO, D. Chooz)	$\theta_{13}, \Delta m^2_{3l} $	-
Atmospheric Experiments (SK, IC-DC)	-	$\theta_{23}, \Delta m^2_{3l} , \theta_{13}, \delta_{CP}$
A. $(\nu_\mu, \bar{\nu}_\mu)$ dis. (K2K, MINOS, T2K, NOvA)	$ \Delta m^2_{3l} , \theta_{23}$	-
A. $(\nu_e, \bar{\nu}_e)$ app. (MINOS, T2K, NOvA)	δ_{CP}	θ_{13}, θ_{23}

in expected ν_e flux in Gallium based radiochemical experiments GALLEX [26, 109] and SAGE [110, 111] and recently confirmed by the BEST experiment [112], and the LSND anomaly [49] in which short baseline $\bar{\nu}_\mu \rightarrow \bar{\nu}_e$ oscillations were observed. Although analysis of the LSND and Gallium anomalies is beyond the scope of this dissertation, the RAA will be discussed in detail within section 2.2 as it provides one of the primary motivations behind the PROSPECT experiment [113].

The next section will detail the theory behind the *sterile* neutrino hypothesis which has been invoked to explain these anomalies.

1.6 Sterile Neutrino Hypothesis

One or more sterile neutrinos is motivated by the RAA (see section 2.2 for more details) and the Gallium anomaly. The data points to a potential mass splitting at the eV scale which is significantly larger than the mass splittings from the three neutrino model (see table 1.4 for current global fits). This would imply at least one additional neutrino exists that is sterile, meaning that it does not interact via any of the SM forces, and only interacts with other matter via gravity. We know this additional neutrino must be sterile because measurements of the Z boson resonance confirm that there exist three neutrino flavors that interact via the weak force [114]. Because it only interacts gravitationally, it is a candidate for dark matter and thus has some additional motivation to search for beyond the aforementioned anomalies.

In the following the relevant equations governing the oscillation into sterile neutrinos for short baseline experiments is shown. Note that these are the standard two-neutrino model results which is a good approximation for short distance oscillation effects.

1.6.1 Sterile Neutrino Impacts on Short Baseline Experiments

In a $3 + n$ framework where n is the number of sterile neutrinos, the matrix U from equation 1.11 will be a $(3 + n) \times (3 + n)$ matrix. For short baselines where oscillations in the 3 neutrino paradigm are not observed, we can approximate ν_e appearance from ν_μ with the relation [115]

$$P_{\mu e}^{\text{ssl}} \approx 4|U_{e4}|^2|U_{\mu4}|^2 \sin^2 \frac{\Delta m_{41}^2 L}{4E}. \quad (1.29)$$

Thus the effective mixing angle at short baselines will be $\sin^2 \theta_{\mu e} = 4|U_{e4}|^2|U_{\mu4}|^2$.

Similarly, for $\bar{\nu}_e$ disappearance we have the relation

$$P_{ee}^{\text{ssl}} \approx 1 - 4|U_{e4}|^2(1 - |U_{e4}|^2) \sin^2 \frac{\Delta m_{41}^2 L}{4E}. \quad (1.30)$$

This leads to an effective mixing angle at short baselines of $\sin^2 \theta_{ee} = 4|U_{e4}|^2(1 - |U_{e4}|^2)$.

1.7 Oscillation Parameter Statistical Analysis

In order to describe the statistical power of an oscillation experiment, one must understand how the measured statistics of propagation length and energy relate to the goodness of fit for different possible theoretical oscillation parameters. In general an experiment can measure a distribution of some observable x which is then used to infer the likelihood of some theoretical parameter μ . Following the convention of Feldman and Cousins [116], a variable with subscript t represents the true value of the parameter and 0 represents some experimental measurement of the parameter. The goal is to generate confidence intervals for a set of theoretical parameters μ_t given the measured x_0 distribution. In the following, the approach of classical statistics for discrete distributions as developed by Neyman [117] is utilized with the addition

of an ordering assumption based on likelihood ratios of the observed parameters introduced by Feldman and Cousins [116]. This allows for the ability to automatically change when a confidence interval changes from an upper limit to a two-sided interval, eliminating a statistical problem known as *undercoverage*.

Neyman’s confidence interval is a relationship such that

$$P(\mu \in [\mu_1, \mu_2]) = \alpha \quad (1.31)$$

where the observable x is some function of μ and μ is a set of theoretical parameters. This is in contrast to the Bayesian view which would attempt to describe the probability that μ_t is some value given the measurement x_0 :

$$P(\mu_t|x_0) = \mathcal{L}(x_0|\mu_t)P(\mu_t)/P(x_0) \quad (1.32)$$

where $\mathcal{L}$ is the likelihood function and P is the probability density function of the measured variables. Here the problem lies in the estimation of what is known as the *prior* in Bayesian statistics, $P(\mu_t)$, which in neutrino oscillation physics are the PDFs of the squared-mass differences. Typically when one does not have information about the parameter, a “uniform” prior is used, but this is not useful in the case of neutrino oscillations when the squared-mass difference parameter is unbounded. Thus, it makes more sense to use classical confidence intervals for oscillation experiments.

In Neyman’s construction, α represents the fraction of experiments with a fixed unknown μ_t which would yield a measured μ_0 in the range $[\mu_1, \mu_2]$. If the relation in equation 1.31 is satisfied, then the value μ is said to be *covered* at the stated confidence interval. If on the other hand there are any values of μ such that $P(\mu \in [\mu_1, \mu_2]) < \alpha$, then μ is undercovered and if there are any values of μ such that $P(\mu \in [\mu_1, \mu_2]) > \alpha$, then μ is overcovered.

A set of intervals is considered *conservative* if overcoverage exists for the given intervals. This is an issue because it limits the ability to reject false hypotheses for

a given experiment. A more problematic issue is undercoverage, in which limits are proposed which contain values that do not meet the statistical certainty claimed.

When one has a measured quantity and an unknown parameter, one can utilize the method of *confidence belts* as described in [118]. This is done by selecting an interval of measured values $[x_1, x_2]$ for a given value of μ which satisfies the relation

$$P(x \in [x_1, x_2] | \mu) = \alpha. \quad (1.33)$$

One can uniquely describe the acceptance region by choosing limits on x . In order to create an upper confidence limit, one can use

$$P(x < x_1 | \mu) = 1 - \alpha. \quad (1.34)$$

Alternatively, a central confidence interval can be described using the relation

$$P(x < x_1 | \mu) = P(x > x_2 | \mu) = (1 - \alpha)/2. \quad (1.35)$$

The procedure is complete once acceptance intervals on x are found for each possible value of μ . This is typically displayed as a contour on a 2-D plot of x versus μ . A problem arises where one will undercover the region specified if one attempts to use the statistics measured to determine whether or not to use a confidence interval or show an upper limit. This is resolved by the ordering principle outlined by Feldman and Cousins [116].

In order to construct the confidence interval over x for a given μ , one must find the value of μ which we will denote μ_{best} for each x . μ_{best} is the value of μ which maximizes $P(x | \mu)$. Once μ_{best} is determined, the ratio between the probability given the μ being considered and μ_{best} is calculated:

$$R = \frac{P(x | \mu)}{P(x | \mu_{\text{best}})}. \quad (1.36)$$

Once R is calculated for every x for a given μ , the probabilities $P(x|\mu)$ are added in order of descending R and the limit is found once the desired coverage is obtained. This procedure is repeated for each μ in the calculation. We will call this the Feldman-Cousins method, or FC for short.

1.7.1 Applying the Feldman-Cousins Method to Neutrino Oscillation Experiments

Recall in the simple case of two neutrino mixing the probability for a flavor transition from one flavor to the other is equation 1.16. The experiment will consist of a set of measurements $N \equiv \{n_i\}$ for each L/E bin i with a corresponding set of mean expected backgrounds $B \equiv \{b_i\}$. The goal then is to construct confidence regions in the $\sin^2 \theta - \Delta m^2$ plane. Denoting the set of expected contributions to the signal as $T \equiv \{\mu_i | \sin^2 \theta, \Delta m^2\}$, where μ_i is the oscillation contribution for measurement i , given the values $\sin^2 \theta, \Delta m^2$. The ordering principle for the FC method is then just based on the physically allowed $\sin^2 \theta, \Delta m^2$ pair that maximizes probability for the set of measurements N denoted $T_{\text{best}}(\sin^2 \theta_{\text{best}}, \Delta m_{\text{best}}^2)$:

$$R = \frac{P(N|T)}{P(N|T_{\text{best}})}. \quad (1.37)$$

When a sufficient number of measurements are used generating a Gaussian distribution, $\chi^2 = -2 \ln P$, which means that the ratio calculated is equivalent to the difference in χ^2 values between T and T_{best} . For the aforementioned Poisson process, this is equivalent to

$$\Delta\chi^2 = \sum_i \left[\frac{(n_i - b_i - \mu_i)^2}{\sigma_i^2} - \frac{(n_i - b_i - \mu_{\text{best}})^2}{\sigma_i^2} \right]. \quad (1.38)$$

In order to determine the $(\sin^2 \theta, \Delta m^2)$ pairs which satisfy the stated confidence value, one must simulate a large number of toy experiments with those oscillation parameters. The critical $\Delta\chi^2$ denoted $\Delta\chi_c^2$ is the difference such that α of the toy

simulated experiments have a $\Delta\chi^2 < \Delta\chi_c^2$. Once $\Delta\chi_c^2$ is determined for each $(\sin^2\theta, \Delta m^2)$ pair, the allowed region are the points where the $\Delta\chi^2$ of the data is smaller than $\Delta\chi_c^2$.

1.7.2 Different Statistical Approaches for Confidence Intervals in Neutrino Oscillation Experiments

In addition to the FC approach previously described, there are two other ways in which confidence regions in the Δm^2 - $\sin^2\theta$ space are constructed by modern oscillation experiments. The first is the *raster scan* (RS) method [116]. This is done by running through each value of Δm^2 and making a best fit to the value of $\sin^2\theta$ for the experiment. The interval is then constructed in $\sin^2\theta$ as being the points that contain a χ^2 less than 2.71 different from the minimum value (for a 90% CL). As Feldman and Cousins have shown, this approach leads to overcoverage within the region.

The second is known as the Gaussian CL_S method [119]. This method is employed when the FC approach is too computationally intensive due to the requirement of constructing a large number of toy MC experiments. For this method, three quantities must be calculated for each Δm^2 - $\sin^2\theta$ pair:

$$\Delta T = \Delta\chi_{min}^2(x)_1 - \Delta\chi_{min}^2(x)_0 \quad (1.39)$$

$$\overline{\Delta T}_0 = \Delta\chi_{min}^2(x_0^{Asimov})_1 \quad (1.40)$$

$$\overline{\Delta T}_1 = -\Delta\chi_{min}^2(x_1^{Asimov})_0 \quad (1.41)$$

In these equations the subscript 0 indicates that the χ^2 is calculated using predictions based on the null hypothesis (no oscillations) and 1 indicates calculation under the assumption of the chosen Δm^2 - $\sin^2\theta$ pair. x^{Asimov} is the Asimov dataset [120] either unoscillated or oscillated (subscript 0 or 1). $\Delta\chi_{min}^2$ is the difference in χ^2 between the chosen Δm^2 - $\sin^2\theta$ pair and the pair which yields the lowest χ^2 .

Once these quantities are known, one can construct confidence regions using the approximation to the p value:

$$\text{CL}_s = \frac{1 - p_1}{1 - p_0} \approx \frac{1 + \text{Erf}\left(\frac{\overline{\Delta T_1} - \Delta T(x)}{\sqrt{8|\Delta T_1|}}\right)}{1 + \text{Erf}\left(\frac{\overline{\Delta T_0} - \Delta T(x)}{\sqrt{8|\Delta T_0|}}\right)}. \quad (1.42)$$

When CL_s is less than $1 - \alpha$ where α is the stated confidence level, that point can said to approximately be excluded at that confidence level. For a 90% confidence interval, the points with $\text{CL}_s < 0.1$ would be excluded.

It should be noted that the usage of the Gaussian CL_s method is only valid when three conditions are satisfied. The first is that the nuisance parameter space is continuous under null and alternative hypotheses. The second is that the dataset is large so that the Gaussian approximation of the ΔT test is valid. The third is that the difference between the predictions of both hypotheses is small, which is typically the case for modifications to the standard model. If any of these conditions are not satisfied, one should use the FC method to calculate the exclusion region.

1.8 Conclusion

This chapter went into the background of neutrino oscillation physics which provides the motivation for the reactor measurements that will be discussed in upcoming chapters. Additionally, the sterile neutrino hypothesis was outlined which is one of the major hypotheses posited to explain various anomalies in reactor and beam measurements. The statistical framework used to analyze and generate exclusion contours in the space of oscillation parameters measured was described in order to give context for the results for the PROSPECT experiment that will be presented in [chapter 5](#).

Table 1.4: Best fit three neutrino oscillation parameters from 2021 NuFit analysis [105]. For normal ordering (NO), $l = 1$, for inverted ordering (IO), $l = 2$.

parameter	NO best fit $\pm 1\sigma$	IO best fit $\pm 1\sigma$
$\sin^2 \theta_{12}$	$0.304^{+0.012}_{-0.012}$	$0.304^{+0.013}_{-0.012}$
$\sin^2 \theta_{23}$	$0.405^{+0.019}_{-0.016}$	$0.570^{+0.016}_{-0.022}$
$\sin^2 \theta_{13}$	$0.02246^{+0.00062}_{-0.00062}$	$0.02241^{+0.00074}_{-0.00062}$
$\delta_{CP}/^\circ$	230^{+36}_{-25}	278^{+22}_{-30}
$\frac{\Delta m_{21}^2}{10^{-5} \text{eV}^2}$	$7.42^{+0.21}_{-0.20}$	$7.42^{+0.21}_{-0.20}$
$\frac{\Delta m_{3l}^2}{10^{-3} \text{eV}^2}$	$+2.510^{+0.027}_{-0.027}$	$-2.490^{+0.026}_{-0.028}$

Chapter 2

Reactor Neutrino Physics

This chapter gives an overview the field of reactor neutrino physics. In the first section the detection techniques utilized for reactor $\bar{\nu}_e$ energy spectrum measurements are detailed. Next, a section discussing two anomalies that have been measured in the data, namely a $\approx 6\%$ deficit in the measured $\bar{\nu}_e$ flux (called the *Reactor Antineutrino Anomaly* or RAA) along with a shape distortion in the 5 - 7 MeV range compared to predictions. The current state of these anomalies based on the most recent experiments will be described.

Subsequently the physics behind neutrinos at reactors will be detailed along with the major methods for calculating the expected flux. The issues calculating the flux will be mentioned and efforts to improve these calculations using total absorption spectroscopy (TAS) measurements will be detailed, along with a detailed description of the Modular Total Absorption Spectrometer (MTAS) experiment.

Finally, a description of the detection of coherent elastic neutrino-nucleus scattering along with the possibility of detecting this process at nuclear reactors is given.

2.1 Reactor Neutrino Detection

Reactor neutrinos are usually detected via the inverse beta-decay (IBD) reaction (see equation 1.2). There are also detectors that have utilized the CC interaction on deuteron, $\bar{\nu}_e + d \rightarrow n + n + e^+$ [121] and the NC interaction on deuteron, $\bar{\nu}_e + d \rightarrow n + p + \bar{\nu}_e$ [122]. These have been used to compare the CC and NC cross sections. However, for measuring the energy spectrum of the reactor $\bar{\nu}_e$, the IBD is the typical detection mode.

Currently research is underway to be able to detect reactor $\bar{\nu}_e$ utilizing coherent elastic neutrino-nucleus scattering (CE ν NS), but this will not be the focus of this section. See section 2.6 for more details on CE ν NS detection techniques and the feasibility of detection at reactors.

The cross section for the IBD process can be expressed to zeroth order in $1/M$ in terms of the weak axial-vector and vector coupling constants g_A and g_V in addition to the Cabibbo angle V_{ud} with the relation [123]

$$\sigma_0(E_{\bar{\nu}}) = \frac{1}{\pi}(G_F V_{ud})^2(g_V^2 + 3g_A^2)pE, \quad (2.1)$$

where p and E are the positron momentum and energy, and G_F is the Fermi constant. The positron energy is related to the neutrino energy via the formula $E_{\bar{\nu}} = E + 1.3$ MeV which comes from the mass difference between the neutron + positron and the proton, which neglects the small amount of kinetic energy carried by the outgoing neutron.

Corrections come in the form of outer and inner radiative corrections δ_{rad} and Δ_{rad} [124], nuclear recoil and weak magnetism corrections δ_{rec+WM} [125, 126], and threshold corrections δ_{thr} [124] which leads to a cross section of the form

$$\sigma = \sigma_0(1 + \delta_{rad})(1 + \Delta_{rad})(1 + \delta_{rec+WM})(1 + \delta_{thr}). \quad (2.2)$$

The form factor $(G_F V_{ud})^2(g_V^2 + 3g_A^2)$ can be expressed in terms of the neutron lifetime τ_N . The neutron lifetime contributes the largest uncertainty to the IBD cross section because the two methods of measuring the lifetime are in disagreement. It is measured via *bottle* and *beam* techniques, and these measurements currently yield the a value of $877.75 \pm 0.28_{stat} + 0.22 / - 0.16_{syst}$ s [127] and 888.0 ± 2.1 s [128] respectively. These two values yield form factors that are different by 1% which is the dominant uncertainty in the IBD cross section.

Different approaches have been made for measuring the IBD process. A commonality between the experiments is the requirement of a *prompt* signal representing the energy deposition of the positron and its annihilation gammas and the *delayed* signal representing the neutron capture on materials within the detector. The prompt and delayed signals must be seen in order within a specific time window set based on the mean capture time of the outgoing neutron. The capture time depends on the detector medium and the dopants used for the capture process. In the Savannah River experiment, Cadmium was added in the form of Cadmium Chloride to the liquid scintillator (LS) which formed the detector medium. [4] The detection of the gamma rays that result from neutron capture on Cadmium was used for the delay signal, significantly decreasing backgrounds from reactor gammas and neutrons.

Liquid scintillator is an organic liquid that fluoresces when charged particles pass through and ionize the medium. By coupling PMTs to the tank containing the LS, light from the charged particles is collected and measured to determine the energy deposited. By calibrating the detector response to the scintillation light with known radioactive source energies, one can obtain a precise determination of the energy of the positron in the IBD reaction.

A number of reactor experiments used Gadolinium doped LS. Gadolinium was chosen because the various isotopes of Gadolinium have large thermal neutron capture cross sections. Additionally, the high energy cascade of gamma-rays (totaling about 8 MeV) provide an easily distinguishable signal from typical reactor and cosmic

backgrounds. Palo Verde [90], Double CHOOZ [89], Daya Bay [88] and RENO [91] all used Gadolinium doped LS.

2.2 Reactor Antineutrino Measurement Anomalies

2.2.1 Reactor Antineutrino Anomaly

In 1981 a measurement of the electron spectrum from the high flux ILL reactor in Grenoble, France was performed by Schreckenbach et al. in order to provide a reference for experimental measurements of the reactor antineutrino spectrum [129]. This measurement provides the basis for the antineutrino spectra calculated by the so-called conversion method, in which the antineutrino spectra is calculated from the electron spectra [108], which takes into account coulombic repulsion of the outgoing electron not experienced by the antineutrino. The Huber-Mueller model is the combination of the conversion method and an *ab-initio* approach which is a summation of the beta spectrum for each beta decay transition coming from the fission products for a given actinide, relying on nuclear databases for fission branching ratios and transition strengths and energies of the decay [108, 107]. The details of conversion and ab-initio methods are given in section 2.3.

In 2011, a reevaluation of the reactor spectra with the Huber-Mueller model found that reactor experiments on average measure the antineutrino flux to be $94.4 \pm 2.3\%$ of the intensity predicted by the Huber-Mueller model, a discrepancy known as the reactor anti-neutrino anomaly [106] (RAA). These measurements include those taken at ILL-Grenoble [80], Gosgen [81], Rovno [82], Krasnoyarsk [79], Savannah River [77], and Bugey [78].

The deficit of reactor anti-neutrinos being detected cannot be explained by the current values of the oscillation parameters measured for θ_{13} and θ_{12} . While there are a number of systematic effects that could cause such a discrepancy, ranging from

errors in the ILL measurement to lack of accuracy in nuclear databases, there are also theoretical explanations for the deficit. The most popular explanation is one or more sterile neutrino flavors [130] which could provide oscillation at small distances (meter to kilometer scale). Oscillations at this length scale would be detectable by anti-neutrino measurements near reactors.

2.2.2 Shape Anomaly

In addition to a discrepancy detected in the overall rate of neutrinos coming from reactors, the θ_{13} measurements by Daya Bay [88], Reno [91], and Double Chooz [89] provide anti-neutrino spectra with shapes inconsistent with the Huber-Mueller model, specifically finding the flux in the 5-7 MeV region is higher than expected [131]. See figure 2.1 for the spectrum measurements relative to prediction. Note that Bugey3 does not exhibit this same spectral shape distortion that is consistent among the other reactor experiments [132].

2.2.3 Sterile Neutrino Search Status

A number of short baseline experiments were conducted at research reactors in order to resolve these anomalies. These include SoLiD [85], STEREO [133], PROSPECT [83], DANSS [134], Neutrino-4 [87], and NEOS [135]. Additionally, Double Chooz, RENO, and Daya Bay have some sensitivity to sterile neutrinos at smaller mass splittings than the short baseline reactor experiments. A table summarizing the different experiments and their relevant parameters and the statistical techniques used is shown in 2.1.

The experiments utilize two major techniques for measuring the sterile neutrino parameters. The first is the *rate* technique in which the total IBD rate is compared to the predicted detected rate based on a model of the reactor $\bar{\nu}_e$ flux and the setup detection efficiencies. The second is the *shape* technique which checks the energy and position of each detected event and checks different values of the sterile parameters

to find which ones best fit the data. The shape technique has the advantage that systematics due to the uncertainties in the flux prediction and detector efficiencies are cancelled. It is enabled by the segmentation of the detectors at short baselines. The relative counts in L/E bins allows for a direct test of the sterile neutrino oscillation hypothesis with less dependence on the model of the neutrino source.

Several different statistical techniques have been used by the different experiments in order to generate exclusion contours for allowed parameter spaces of the squared-mass difference and mixing angle of a sterile neutrino [136]. These are explained in sections 1.7.1 and 1.7.2. It is important to note these distinctions given in the last column of table 2.1 because their exclusion contours, and in the case of Neutrino-4 their discovery claim, must be recognized in the context of these methods used.

With regard to the rate anomaly, PROSPECT, STEREO, NEOS did not find evidence for a 3+1 sterile neutrino oscillation within the Kopp best fit space. The exception is Neutrino-4, which did claim a discovery at 3σ of a sterile neutrino [87], although its results are in contention [84]. The contention is due to the fact that the full FC approach was not used, and the χ^2 analysis done overestimates the statistical significance of the oscillation signal due to Wilk’s theorem not being satisfied. A joint analysis between PROSPECT, STEREO was recently completed, showing both good agreement between experiments and confirming the RAA and shape anomaly [138].

More recent calculations of the reactor flux show that the reactor anomaly nearly disappears when using a new normalization of the ^{235}U to ^{239}Pu β spectrum ratio calculated by the Kurchatov Institute [139] and reevaluating the conversion method. Additionally, using the most up to date summation method [140], the RAA also mostly disappears, with statistical significance of the deficit between 1 and 1.5σ [141].

In light of this reanalysis of the overall rate deficit, a recent analysis of the sterile neutrino hypothesis using all of the reactor data plus the Gallium experiments and utilizing the full FC approach with MC simulations disfavor the hypothesis [142].

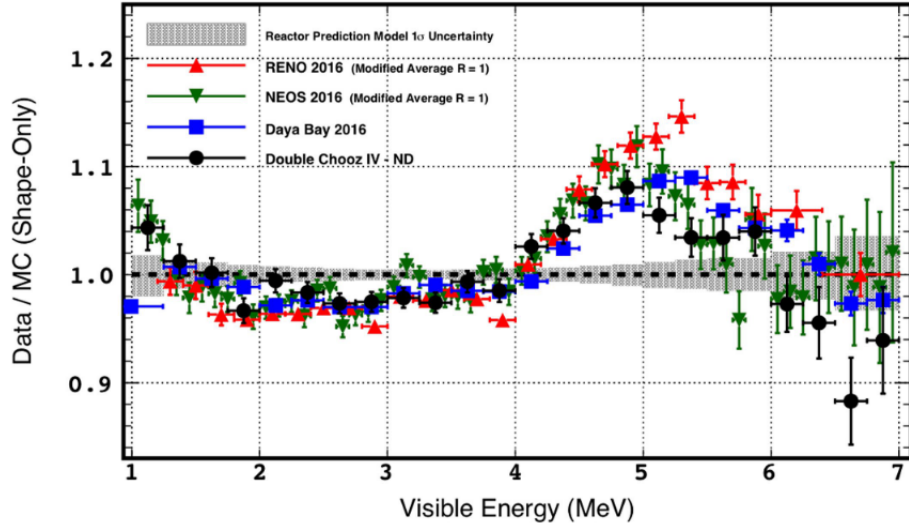


Figure 2.1: Ratio of measured reactor $\bar{\nu}_e$ spectra to Huber-Mueller prediction for medium baseline reactor experiments. The "bump" is evident as an excess at 5 MeV. Source: [132]

Table 2.1: Summary of experiments searching for sterile neutrino oscillations at reactors. Reactor power, detector overburden, reactor-detector distance, detector mass, detector type, and statistical method for oscillation analysis displayed. Source: [137]

Experiment	P_{th}	D/m.w.e.	L/m	m/t	Detection	Method
SoLid	80	10	6-9	1.6	^6Li -PS	n.a
NEOS	2800	20	24	1.0	Gd-LS	RS
DANSS	3100	50	11-13	0.9	Gd-LS	CL_S
STEREO	58	15	9-11	1.7	Gd-LS	RS,FC, CL_S
PROSPECT	85	1	7-9	4.0	^6Li -LS	FC, CL_S
Neutrino-4	100	5-10	6-12	1.5	Gd-LS	CL_S
Daya Bay	17,400	250, 860	550, 1650	80, 80	Gd-LS	FC, CL_S
D-Chooz	8500	120, 300	400, 1050	8, 8	Gd-LS	RS
RENO	16,800	120, 450	294, 1383	16, 16	Gd-LS	FC, CL_S

2.2.4 Shape Anomaly Status

In order to better understand the reactor spectrum shape anomaly, improvements to the beta decay spectrum of the largest contributors to the anti-neutrino spectrum have been conducted by the Modular Total Absorption Spectrometer (MTAS) [143] (see section 2.5.1 for details on this experiment) and Total Absorption Gamma-ray Spectroscopy (TAGS) [144] experiments. These measurements were needed in order to correct older measurements of the beta decay spectra and level schemes that were taken with high resolution Ge detectors done in the 80s, of which ENDF and ENSDF decay libraries were relying on extensively. Ge detectors do not have the efficiency to resolve the large number of transitions for beta decaying isotopes with large Q values (several MeV), which results in an apparently smaller number of larger energy transition than exists in reality (known as the "pandemonium effect" [145]). This has the effect of artificially increasing the predicted antineutrino energy from these isotopes [146]. A full analysis of the effect of these newly measured transitions on the anti-neutrino spectrum prediction is currently underway, but initial results point to the discrepancies increasing due to lower overall anti-neutrino energies predicted by MTAS and TAGS. See section figure 2.3 for the impact of the MTAS measurements on the $\bar{\nu}_e$ energy spectrum.

Sonzogni, et al. show that the anomaly is not consistent with a distortion in the calculated ^{238}U spectrum and show that shape corrections to the underlying $\bar{\nu}_e$ spectra for both individual FPs in the summation calculation and experimental shape factors used in the conversion method cannot be ruled out as the source of the anomaly [147].

Additionally, theoretical calculations combining experimental knowledge of spin-parity assignments for odd-odd nuclei using a framework developed by Nakata et al. [148] was utilized to refine the summation model and results show greater consistency with experimental measurements [149], pointing to a combination of both Pu isotopes and ^{235}U being the cause of the shape anomaly.

While these recent improvements to the reactor flux predictions tend to reduce the size of the rate anomaly, reactor $\bar{\nu}_e$ measurements with greater statistics will be needed to definitively address this. Discovery claims of a sterile neutrino by Neutrino-4 will also be addressed by further experiments. This will be accomplished by the planned PROSPECT-II experiment, which is looking to get several more years of data taking at HFIR beginning in 2024. Additionally, the shape anomaly will require more TAS style measurements of fission products in order to definitively address. As predictions of the spectrum improve, greater resolution from higher statistics measurements will be crucial in understanding the source of the shape discrepancies.

2.3 Reactors as a Neutrino Source

Power from fission reactors comes from the fission of the actinides U and Pu plus the radioactive decay of the fission products. The $\bar{\nu}_e$ comes from beta decay of the fission products. The energy spectrum of $\bar{\nu}_e$ can be expressed as [150]

$$S(E_{\bar{\nu}}) = \sum_i f_i \left(\frac{dN_i}{dE_{\bar{\nu}}} \right), \quad (2.3)$$

where $E_{\bar{\nu}}$ is the antineutrino energy, f_i is the number of fissions from actinide i and $dN_i/dE_{\bar{\nu}}$ is the cumulative neutrino spectrum normalized per fission of each actinide i .

In order to determine f_i , the reactor thermal power must be known along with the contributions of each actinide isotope that power. The number of fissions can then be determined with the effective thermal energy per fission denoted e_i from each actinide i . Values of e_i are listed for each of the major fissioning isotopes which contribute 99.99% of the thermal power at reactors in table 2.2. Using these values along with the thermal power W_{th} we can calculate the neutrino spectrum with the equation

$$S(E_{\bar{\nu}}) = \frac{W_{th}}{\sum_i (f_i/F) e_i} \sum_i \frac{f_i}{F} \left(\frac{dN_i}{dE_{\bar{\nu}}} \right), \quad (2.4)$$

where the number of fissions for each actinide is expressed as a fraction of the total number of fissions F .

This calculation is complicated by the fact that not all beta decaying isotopes are in secular equilibrium and there are also low energy neutrinos coming from spent fuel which is typically stored near the reactor core. The details of the spent fuel must be obtained from the reactor operators.

The reactor power W_{th} is measured using temperature measurements of the cooling system along with coolant flow rate calculations. This typically results in errors on the order of 2% of the total power [150]. The fuel composition for a reactor will typically vary throughout the power cycle and will depend largely on the reactor design. Many of the reactor neutrino experiments operate at pressurized water reactors, so it is useful to discuss the fuel evolution for such a setup. The reactor cycle typically lasts about a year, beginning with fuel rods consisting of around 3% enriched ^{235}U , with the remainder being ^{238}U . Despite the high composition of ^{238}U , the percentage of fissions from ^{238}U is typically around 10% which is due to the energy threshold of fission for this isotope requiring neutrons in the fast energy range (few MeV). Throughout the cycle, ^{239}Pu is bred in due to neutron capture on ^{238}U and eventually becomes the dominant fissioning nuclei. Any experiment will have to take into account the time variation of the fuel composition contributing to the fissions when calculating the expected $\bar{\nu}_e$ spectrum. Figure 2.2 shows an example of such a calculation for two different initial ^{235}U enrichments at the start of the pressurized water reactor cycle. [152].

The fission process will produce two nuclei of unequal masses, and the products will undergo decays until they reach a stable isotope. On average about 6 neutrons are converted to protons per fission, meaning that there will be $\approx 6\bar{\nu}_e$ emitted per fission due to beta decay of the nuclei undergoing transformations to stability. This is due to the fact that larger mass elements have a higher fraction of neutrons relative to protons for a stable nucleus. The subsequent beta decays result in $\approx 6 \times 10^{20} \bar{\nu}_e$ per GW of thermal power. It is important to note that while many of the beta decaying

Table 2.2: Energy per fission for the primary fissioning actinides. Energies are expressed in units of MeV/fission. Values taken from [151].

Nucleus	Energy from mass excess	Without ν	E_{tot} including n-captures
^{235}U	202.7 ± 0.1	192.9 ± 0.5	201.7 ± 0.6
^{238}U	205.9 ± 0.3	193.9 ± 0.8	205.0 ± 0.9
^{239}Pu	207.2 ± 0.3	198.5 ± 0.8	210.0 ± 0.9
^{241}Pu	210.6 ± 0.3	200.3 ± 0.8	212.4 ± 1.0

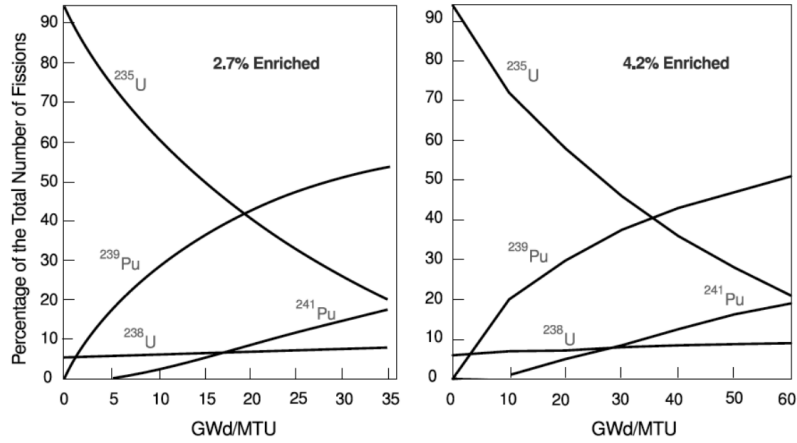


Figure 2.2: Percentage of fissions coming from the four major isotopes in a typical pressurized water reactor. The x-axis shows the energy output in Gigawatt-days per metric ton of Uranium (MTU) supplied as fuel. This is proportional to the operating lifecycle. Note that the time evolution of the different fission contributions is similar between the two cases while the power output is increased for the higher ^{235}U enrichment.

isotopes reach equilibrium within a few hours of the reactor turning on, some isotopes that contribute to the detectable energy spectrum (> 1.8 MeV for detectors utilizing the IBD mechanism) take several days to reach equilibrium, and this must be taken into account for an accurate prediction of the $\bar{\nu}_e$ flux [153].

There are two methods of calculating the $\bar{\nu}_e$ spectrum for the fission products. These are the *summation* and *conversion* methods. The *summation* method involves utilizing fission yields for measured for each isotope that can result from the fission process for each fissioning isotope and summing their respective measured $\bar{\nu}_e$ spectra. The *conversion* method relies on a measured electron spectrum for each fissioning actinide and converting this to the $\bar{\nu}_e$ spectra. These two methods are described in detail below.

2.3.1 Summation Method

The summation method (also referred to in the literature as the ab-initio approach), first described in the early 1980s [154, 155, 156], involves summing each of the contributions from each beta decay branch for each isotope multiplied by the number decaying at a given time for that isotope and the branching ratios. The contribution from a beta decay branch i is given as

$$\frac{dN_i}{dE_{\bar{\nu}}} = \sum_n Y_n(Z, A, t) \sum_{n,i} b_{n,i}(E_0^i) P_{\bar{\nu}}(E_{\bar{\nu}}, E_0^i, Z) \quad (2.5)$$

where Y is the number of beta decays for the isotope with atomic number Z and mass number A at time t , n denotes whether the isotope is in its ground or isomeric state, $b_{i,n}$ is the branching fraction for the beta decay branch i, n which has a unique endpoint energy E_0^i which determines the $\bar{\nu}_e$ spectrum $P_{\bar{\nu}}(E_{\bar{\nu}}, E_0^i, Z)$ which is normalized to unity. The branching fractions b are normalized to 1 so that $\sum_i b_{i,n}(E_0^i) = 1$.

Note that Y will converge to the cumulative fission yield for the isotope Z, A after sufficient burn time has gone by. Any of these fission products can be produced

directly from the fissioning actinide which contributes to its *independent* yield or from a more neutron rich nuclei directly produced which subsequently decays into the isotope via a series of beta decays. Thus the cumulative yield is the sum of the independent yield for that isotope plus the yield from the different pathways to it through beta decay of more neutron rich nuclei.

There are a few different sources of nuclear data one could utilize to perform this calculation. Cumulative fission yields for most of the relevant isotopes along with the electron spectra for beta decay of isotopes have been measured experimentally. Cumulative fission yields are provided by the European based Joint Evaluated Fusion and Fission (JEFF) [157] nuclear data library, the Japanese Evaluated Nuclear Data Library (JENDL) [158], and the U.S. Evaluated Nuclear Data File (ENDF) [159] libraries. Beta decay branching fractions, endpoint energies, level schemes, and spin / parity assignments are also obtained via databases from these sources. The different databases use different studies to base their numbers on which means that the calculated neutrino spectra for a given actinide will differ depending on the choice of database used. This contributes a source of uncertainty to the expected neutrino flux in any given reactor neutrino experiment.

Additional sources of uncertainty arise due to the fact that not all beta spectra have been measured for the different isotopes, spin and parity aren't known for all of the different levels that have been measured, and corrections to the spectra needed for Gamow-Teller and especially those of the first-forbidden type require accurate knowledge of the spin and parity. Also older measurements of the beta spectra using high resolution low efficiency Germanium detectors suffer from a bias known as the *pandemonium effect* [145] which tends to miss lower energy beta decays to higher energy states of the daughter nucleus. Decay schemes generated using relatively low efficiency detectors overestimates the beta population of low energy levels and underestimates or misses feeding at high excitation energies. Currently efforts to correct these effects by utilizing total absorption spectrometers consisting of arrays of highly efficient NaI detectors are underway by the Modular Total Absorption

Spectrum (MTAS) [160] and the Total Absorption Gamma Spectrum (TAGS) [144] experiments which will be covered in greater detail in section 2.5. Theoretical corrections to the forbidden transitions will be detailed in section 2.4.

2.3.2 Conversion Method

The conversion method relies on measurements of the electron spectra for ^{239}Pu , ^{241}Pu and ^{235}U taken at the ILL reactor in Grenoble, France in the 1980s [161, 162, 163] and the ^{238}U spectrum measured at the FRMII neutron source in Garching, Germany [164]. These spectra must then be converted to $\bar{\nu}_e$ spectra and corrected for the fact that the electron spectra were measured before equilibrium was reached. In order to perform the conversion, 30 virtual decay branches were used [165, 166, 167]. The procedure involved dividing the measured ILL electron spectrum into 30 bins. First the highest energy bin is used for finding the branching ratio of the first virtual branch. The contribution of this first, highest energy virtual branch is subtracted from the experimental spectrum. This process of fitting the virtual branch with the endpoint at the next lowest energy bin after the previous subtraction is performed is repeated for each branch down to the lowest energy bin. The antineutrino spectrum is then the sum of all virtual branches. The conversion to the $\bar{\nu}_e$ spectra is performed by calculating the antineutrino energy $E_{\bar{\nu}}$ from the electron energy E_e with the formula $E_{\bar{\nu}} = E_0 - E_e$ with the branch's endpoint energy E_0 . Then the spectrum is corrected for radiative corrections which result from the coulomb forces between the electric field of the isotope undergoing the decay and the emitted electron which the neutron antineutrino does not experience.

The main limitation with the conversion method was shown by Vogel [168] to be the fact that an artifact of the method appears around each virtual endpoint energy in the form of a shape oscillation relative to the true spectrum. In order to correct for these oscillations, the measured electron spectrum must utilize finer energy bins which must be then rebinned to the desired antineutrino energy bins, and the size

of these finer bins is smaller than the resolution provided by the ILL measurements. Additionally, accurate reproduction of the antineutrino spectrum at high energies requires a more accurate knowledge of the effective average Z for the virtual branch than is known. Huber and Mueller provide an improvement of the conversion method by utilizing a hybrid approach between the conversion and summation methods where they utilize the summation method for all of the measured fission products and use a conversion procedure to estimate the contributions from the remainder of the fission products taken as the remainder of measured ILL spectrum and the summation spectrum [108], henceforth referred to as the Huber-Mueller model.

2.4 Calculating Beta Decay Antineutrino Spectra

The currently used theory of beta decay was first described by Fermi in 1934 [2]. In order to calculate $P_{\bar{\nu}}$ from equation 2.5, the spectrum shape can be calculated by utilizing the Fermi function F and applying shape corrections based on the spin and parity of the parent and daughter states. This is expressed in the equation

$$P_{\bar{\nu}}(E_{\bar{\nu}}, E_0^i, Z) = K p_E E_e (E_0 - E_e)^2 F(Z, E_e) C(Z, E_e) (1 + \delta(Z, A, E_e)), \quad (2.6)$$

where K is a normalization factor, $p_E E_e (E_0 - E_e)^2$ is the phase-space factor, E_0 is the endpoint energy of the transition, E_e is the electron energy, $F(Z, E_e)$ is the Fermi function which contains the effect of the coulomb field of the daughter nucleus on the electron, $C(Z, E_e)$ is a shape factor which accounts for the momentum dependence of the nuclear matrix elements and δ is the corrections to the spectrum shape based on weak magnetism, finite size, and radiative corrections described below.

The Fermi function calculated assuming a point nuclear function is

$$F_0(Z, E_e) = 4(2p_e R)^{-2(1-\gamma)} \left[\frac{\Gamma(\gamma + iy)}{\Gamma(2\gamma + 1)} \right]^2 e^{\pi y}, \quad (2.7)$$

where p_e is the electron momentum, R is the radius of the nucleus in units of the electron Compton wavelength, Γ is the gamma function, $\gamma = \sqrt{1 - (\alpha Z)^2}$, $y = \alpha Z E_e / p_e$, and α is the fine structure constant.

In order to correct the Fermi function for the finite size of the nucleus, Behrens et al. [169] calculated a numerical solution to the Dirac equation for the resulting electron in the Coulomb potential of the daughter nucleus. This was evaluated at $r = 0$ in order to calculate the function $L_0(Z, E_e)$ which allows for the more accurate Fermi function $F(Z, E_e) = F_0(Z, E_e) \times L_0(Z, E_e)$.

2.4.1 Finite Size Correction

In addition to taking account the finite size of the nucleus in the Fermi function, one must also consider the weak interaction effects of the finite size on the outgoing electron first derived by Holstein et al. [170]. The correction is expressed in terms of the weak force density and the charge density ρ_W and ρ_{CH} [171]:

$$\delta_{FS} = -\frac{3}{2} \frac{Z\alpha}{\hbar c} \langle r \rangle_{(2)} \left(E_e - \frac{E_{\bar{\nu}}}{27} + \frac{m_e^2 c^4}{3E_e} \right). \quad (2.8)$$

Here $\langle r \rangle_{(2)}$ is the Zemach moment which is the first moment of the nuclear weak isovector transition density convolved with the electromagnetic ground state charge density. This is expressed as

$$\langle r \rangle_{(2)} = \int d^3r \rho_W(r) \int d^3s \rho_{CH}(s) |\vec{r} - \vec{s}|. \quad (2.9)$$

Assumptions about these densities can then be made to calculate δ_{FS} using perturbative expansions in αZ , see references [172, 171, 170, 124] for details.

2.4.2 Radiative Correction

Quantum electrodynamics corrections to the $\bar{\nu}_e$ spectra were performed by Sirlin [173]. For the shape of the spectrum only the energy dependent corrections matter; this correction takes the form

$$\delta_{QED} = \frac{\alpha}{2\pi} h(E_e, E_0), \quad (2.10)$$

where $h(E_e, E_0)$ is defined as

$$\begin{aligned} h(E_e, E_0) = & 3 \ln \left(\frac{m_p}{m_e} \right) + \frac{23}{4} - \frac{8}{\hat{\beta}} \text{Li}_2 \left(\frac{2\hat{\beta}}{1+\hat{\beta}} \right) \\ & + 8 \left(\frac{\tanh^{-1} \hat{\beta}}{\hat{\beta}} - 1 \right) \ln \left(\frac{2\hat{E}\hat{\beta}}{m_e} \right) \\ & + 4 \frac{\tanh^{-1} \hat{\beta}}{\hat{\beta}} \left[\frac{7+3\hat{\beta}^2}{8} - 2 \tanh^{-1} \hat{\beta} \right], \end{aligned} \quad (2.11)$$

where m_p is the proton mass, $\hat{E} \equiv E_0 - E_{\bar{\nu}}$, $\hat{p} \equiv (\hat{E}^2 - m_e^2)^{1/2}$, $\hat{\beta} \equiv \hat{p}/\hat{E}$, and $\text{Li}_2(z) = -\int_0^z (dt/t) \ln(1-t)$.

2.4.3 Weak Magnetism Correction

The daughter nucleus has a magnetic moment which will interact with the outgoing electron. This interaction is relevant for Gamow-Teller transitions where the change in total spin is 1 and has the form [170]

$$\delta_{WM} = \frac{4E_e}{3g_A M} \left(1 - \frac{m_e^2 c^4}{2E_e^2} \right) \left[\frac{\langle \vec{l} \rangle}{\langle \vec{\sigma} \rangle} + (\mu_p - \mu_n) \right], \quad (2.12)$$

where $\mu_p - \mu_n = 4.7$ is the nucleon isovector magnetic moment, $M = \frac{1}{2}(M_1 + M_2)$ is the average mass of the parent (M_1) and daughter (M_2) nuclei, g_A is the axial-vector coupling constant, and $\frac{\langle \vec{l} \rangle}{\langle \vec{\sigma} \rangle}$ is the ratio of the matrix elements of the spin and angular momentum operators which must be calculated for each transition.

Hayes shows that this can be approximated using a truncated orbital correction which yields a correction of the form [174]

$$\delta_{WM} \approx \frac{4}{3} \frac{\mu_p - \mu_n - 1/2}{g_A M} E_e \left(1 - \frac{m_e^2 c^4}{2E_e^2} \right). \quad (2.13)$$

The impact of the finite size and weak magnetism corrections on the electron and antineutrino spectra is displayed as a function of energy using the summation method for a typical reactor composition in figure 2.3. It is apparent that these corrections are important in that they tend to shift the prediction for the antineutrino up as energies increase above 2 MeV up to the 2% level.

2.5 Total Absorption Spectroscopy for Beta Decay Measurements

Historically beta decay schemes were measured using gamma ray spectroscopic techniques which was useful for measuring energy levels of different excited daughter states for simple decay schemes and the lower excitation levels for more complex ones [175]. However, when the decay has a large Q value, the intensity feedings derived from such techniques are prone to systematic errors due to the failure of observing the numerous low energy gamma rays which is described by Hardy et al. as the *Pandemonium effect* [145]. The Total Absorption Spectroscopy (TAS) approach instead attempts to measure the distribution of various beta decay feedings via a near 100% efficient gamma ray detector with a nearly 4π coverage. This allows one to measure each of the gammas in any cascade from an excited state at energy level E so that the sum of all detected gammas equates to that energy. This provides an unambiguous signature for a feeding to the excited state at energy E [175].

The first TAS style measurement was performed by Duke et al. [176] to study various electron capture reactions. The measurement was performed using two small NaI(Tl) crystals, each 15 cm diameter x 10 cm length, placed face-to-face with a small

gap between for the source such that the detection efficiency was less than 90% of 4π .

Improvements to the design were used to study spallation produced beta decaying isotopes by Bykov et al. [177] at the isotope separation on-line (ISOL) source. The spectrometer utilized one cylindrical NaI(Tl) crystal 20 cm diameter x 20 cm long with the radioactive source placed in a 4 cm diameter x 10 cm long axial well. The detector included auxiliary NaI(Tl) detectors at the end of the well in order to provide $\approx 99\%$ of 4π coverage. Inside the well was situated a Si charged particle detector to discriminate between beta and electron-capture decays.

More recent TAS measurements were performed in the 90s by Greenwood et al. [178] in order to measure beta-decay intensity distributions for fission product radionuclides. This design was the basis for modern measurements by MTAS [143] and TAGS [144] experiments. The design was an improvement on previous designs in that the NaI(Tl) crystal utilized was larger and surrounded by an array of 7 7.6 cm diameter PMTs [175]. The measurement was done at the Idaho National Engineering Laboratory (INEL) ISOL facility. After mass separation at the ISOL, the selected fission isotope was collected on a tape which was moved via microprocessor control to a position in front of the Si detector inside the well of the NaI(Tl) crystal.

Modern measurements have scaled up the designs of the previous TAS systems in order to provide detailed and accurate beta decay feedings for isotopes that have been identified to be important in the determination of the reactor $\bar{\nu}_e$ spectra.

2.5.1 Modular Total Absorption Spectrometer

The Modular Total Absorption Spectrometer (MTAS) [143, 179] was constructed at ORNL and a first commissioning run was performed in 2012 at the Holifield Radioactive Ion Beam Facility [180] (HRIBF). The detector consists of 18 NaI(Tl) hexagonal crystals produced by Saint-Gobain Crystals based in Hiram, OH. Each crystal is 21 inch long x 6.93 inch wide. Additionally, a central module with the same

dimensions contains a 2.5 inch diameter hole which is used to place the radioactive source. The active mass is roughly one ton which makes it very efficient to gamma radiation.

Each hexagonal detector module is arranged in a hexagonal lattice (see figure 2.4) and the modules are referred to as the Central (C) detector, the Inner ring (I) detectors, the Middle ring (M) detectors and the Outer ring (O) detectors. Each of these assignments are based on the distance of each module to the central axis of the detector.

The detector utilizes 48 PMTs. The Central detector is connected to 6 1.5 inch diameter PMTs on each end. The remaining 18 detectors have a 5 inch diameter ETI9390 PMT attached on each end. In order to reduce background count rates two layers of 1/4 inch thick lead blankets are attached to the support frame of the detector. 2 inch thick lead bricks are placed underneath the detector and the front and back sides of the detector are also covered with additional lead blankets amounting to an inch thickness. Rubber sheets for absorbing neutrons consisting of 9% borated polyurethane covers the sides and top of the detector as space permits. With the shielding in place background count rates at HRIBF were reduced from 15,000 hz to 2,400 hz between 100 keV and 10 MeV.

In addition to the NaI(Tl) crystals, the setup contains two I-1000 1 mm thick 7-strip silicon detectors for beta measurements. The silicon detectors have an active area of 60 x 40 mm² and are placed perpendicular to the detector center. They surround the radioactive source which is transported to the detector via a tape collection device. This gives a 80% of 4π solid angle coverage. Online isotope separation using the HRIBF magnetic spectrometers allows experiment operators to implant the isotope of interest and subsequently move to position within the detector within 500-780 ms.

The energy resolution of each crystal is $> 6\%$ at 1.33 MeV and 7 - 8% at 0.66 MeV. The efficiencies for MTAS in running conditions is displayed in figure 2.5. The detector response is modelled using a detailed Geant4 [181] simulation. Simulated efficiencies are displayed with a solid line and measured efficiencies with sources of

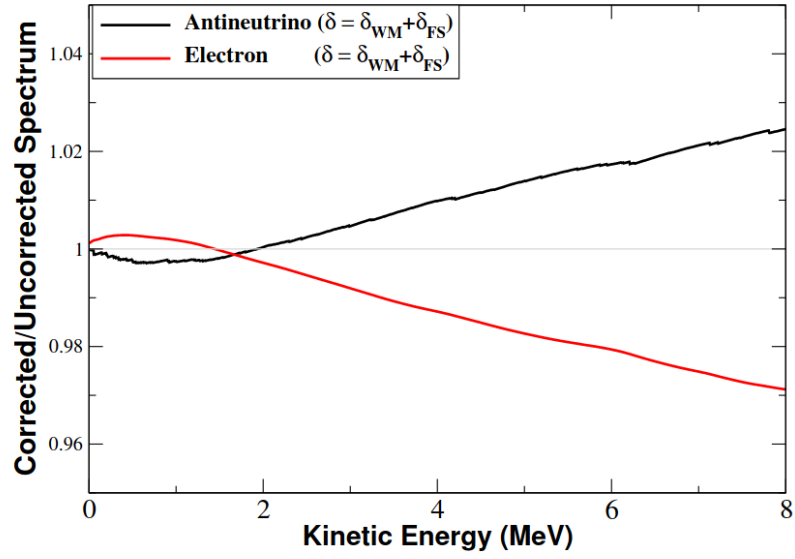


Figure 2.3: Magnitude of the impacts of the finite size and weak magnetism corrections applied to a typical reactor spectrum using the summation method. Source: [150]

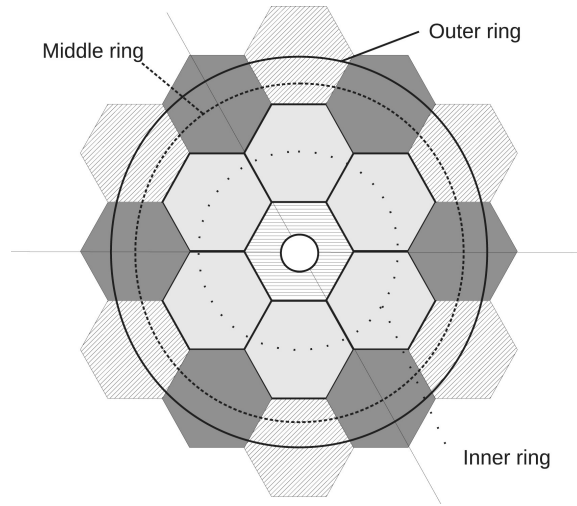


Figure 2.4: Honeycomb arrangement of NaI(Tl) crystals utilized in the MTAS spectrometer. The Inner-ring modules are light grey, Middle-ring modules dark grey; the Outer-ring modules are hatched at 45°, and the Central detector is hatched horizontally. Source: [179]

known intensities are shown with data points. The efficiency for full-energy (partial energy) deposition of a single gamma-ray is about 78% (98%) at 300 keV and 71% (96%) for a 4-MeV single gamma-ray transition.

Between 2011 and 2016 the beta decay spectrum of ^{86}Br , ^{89}Kr , ^{89}Rb , $^{90\text{gs}}\text{Rb}$, $^{90\text{m}}\text{Rb}$, ^{90}Kr , ^{92}Rb , ^{139}Xe , and ^{142}Cs were measured by MTAS at HRIBF [182]. The beta intensities and ground state feedings were calculated using the maximum entropy method described by Tain and Ott [183]. These nuclei were identified as having high importance for decay heat calculations relevant for nuclear safety and efficiency applications. Because they contribute substantially to the heat released in the fission process, they are also important in the summation method of calculating the $\bar{\nu}_e$ spectrum. The MTAS measurements revised the existing level scheme and ground state feeding significantly for ^{89}Kr , ^{90}Kr , ^{139}Xe and ^{142}Cs . The feeding to the ground state reduced from 23(4)% to 11(1)% for ^{89}Kr , from 29(4)% to 7(1)% for ^{90}Kr , and from 56(5)% to 43(3)% for ^{142}Cs .

By recalculating the $\bar{\nu}_e$ spectra for the different fissioning actinides with the updated MTAS measurements and comparing to the same calculation using the ENDF B-VII [184] library, the trend of decreasing the ground state feedings tends to decrease the overall electron energies and hence the $\bar{\nu}_e$ energies, shifting more of the spectrum below the 1.8 MeV detection threshold. This results in an overall lower number of detectable neutrinos predicted, tending to decrease the anomaly. For the isotopes measured, the impact is 0.976, 0.986, 0.983, and 0.984 for ^{235}U , ^{238}U , ^{239}Pu and ^{241}Pu respectively. Figure 2.6 shows the change in $\bar{\nu}_e$ spectra for the different actinides.

2.6 Coherent Elastic Neutrino-Nucleus Scattering

Coherent Elastic Neutrino-Nucleus Scattering (CE ν NS) is a weak neutral-current interaction between neutrinos and nuclei first proposed in 1974 by Freedman [185]. The CE ν NS process was first detected by the COHERENT collaboration at the Spallation Neutron Source (SNS) using CsI [186]. Their measurement of the

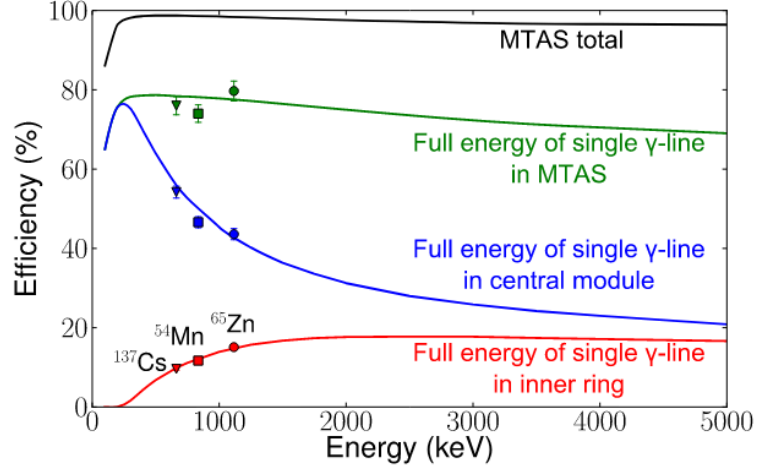


Figure 2.5: MTAS efficiency for different detector layers, data points from sources with known activity and lines are from Geant4 simulation. Source: [143]

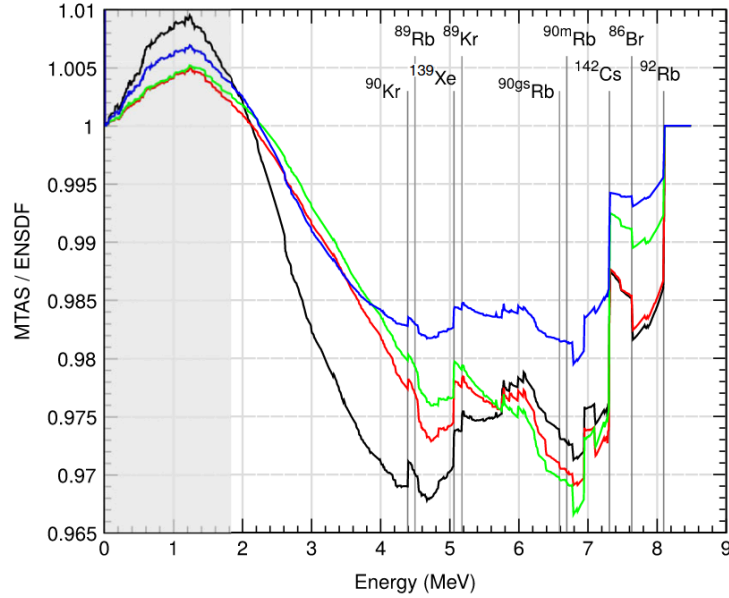


Figure 2.6: Ratio of calculated $\bar{\nu}_e$ spectrum from MTAS measurement and data from ENDF database. Spectra from the different actinides are shown, ^{235}U in black, ^{238}U in blue, ^{239}Pu in red, and ^{241}Pu in green. The shaded region shows the energy region inaccessible to detection via IBD. Vertical lines denote beta endpoint energies for the measured isotopes. Source: [182]

CsI cross section for $\text{CE}\nu\text{NS}$ agreed with the Standard Model within 1σ [187]. Future high precision measurements of the $\text{CE}\nu\text{NS}$ process will serve as additional tests of the SM, including a measurement of the Weinberg angle [188]. Other applications include measurements of the neutron nuclear form factor [189], nuclear reactor monitoring [190], and understanding backgrounds for direct Dark Matter detection [191].

Detection of $\text{CE}\nu\text{NS}$ requires the measurement of low energy nuclear recoils. This is because the momentum transfer between the neutrino and the nucleus is small, leading to recoil energies of 10s of keV for neutrinos with energies in the 10s of MeV range. The differential cross section with recoil energy T for a spin-0 nucleus of mass M at rest with Z protons and N neutrons is [192, 188]

$$\frac{d\sigma_0}{dT} = \frac{G_F^2 [N - (1 - 4s_W^2)Z]^2 F^2(q^2) M^2}{4\pi M} \left(1 - \frac{T}{T_{\max}}\right). \quad (2.14)$$

G_F is the Fermi constant, $s_W \equiv \sin \theta_W$ is the Weinberg angle and $F(q^2)$ is the form factor of the nucleus which tends to unity in the coherent limit (as $q^2 \rightarrow 1$). $T_{\max}$ is the maximum recoil energy determined by the neutrino energy E_ν :

$$T_{\max}(E_\nu) = \frac{2E_\nu^2}{M + 2E_\nu}. \quad (2.15)$$

At MeV scale neutrino energies, the weak mixing angle is small [193]; $s_W \approx 0.238$, implying $N - (1 - 4s_W^2)Z \approx N - 0.045Z$ which indicates the cross section has a strong dependence on N^2 . Note that for spin-1/2 fermions (e.g. odd $A = N + Z$ nuclei), the term in parentheses turns into $(1 - \frac{T}{T_{\max}} + \frac{T^2}{2E_\nu^2})$, with the term T^2/E_ν^2 being negligibly small for the coherent scattering process. The $\text{CE}\nu\text{NS}$ cross section is quite large compared to other neutrino interaction cross sections. A plot displaying the $\text{CE}\nu\text{NS}$ cross section for various nuclei in addition to IBD, neutrino induced neutron, and other interactions is shown in figure 2.7.

A detector will have some low energy threshold T_{th} . Thus, the reduced cross section for detectable nuclear recoils is

$$\bar{\sigma}(T_{\text{th}}, E_\nu) = \int_{T_{\text{th}}}^{T_{\text{max}}} \frac{d\sigma}{dT} dT = G_F^2 [N - (1 - 4s_W^2)Z]^2 F^2(q^2) M^2 \frac{(T_{\text{max}} - T_{\text{th}})^2}{8\pi M T_{\text{max}}}. \quad (2.16)$$

Converting the detectable lower energy limit of the recoil energy, we can get the lower limit of the detectable neutrino energy

$$E_{\nu,\text{th}} = \frac{1}{2} \left(\sqrt{2MT_{\text{th}} + T_{\text{th}}^2} + T_{\text{th}} \right) \approx \sqrt{\frac{M}{2}} T_{\text{th}} A. \quad (2.17)$$

2.6.1 Detection

In order to detect the $\text{CE}\nu\text{NS}$ process, one must be able to measure low energy recoiling nuclei above backgrounds that typically dominate the detected energy for this process. So far this has only been done by the COHERENT collaboration using CsI[Na] [187] and liquid Argon [195] wherein a 6.7σ and 3σ preference for $\text{CE}\nu\text{NS}$ is found above the no signal hypothesis for CsI and Ar measurements respectively.

In both of these detectors the ionization caused by the recoiling nucleus is detected via scintillation light. The percentage of the deposited recoil energy T that is deposited in the form of ionization energy I is called the quenching factor, $Q = I/T$. The quenching factor is dependent on the detection medium and process. As an example for the case of CsI, the COHERENT collaboration measured the CsI[Na] detector scintillation response to 3-60 keV energy nuclear recoils was measured in a neutron elastic scattering experiment [196]. The results of the scintillation response is displayed in figure 2.8. The quenching factor ranges from 5 to 10% for nuclear recoils with energies < 60 keV.

The successful detection of $\text{CE}\nu\text{NS}$ by the COHERENT experiment relied on the pulsed beam nature of the SNS source. The SNS is a π^+ decay at rest (DAR) facility located at ORNL. The advantage of this source over other manmade neutrino sources such as a reactor is that the beam timing is well known, and therefor events will only

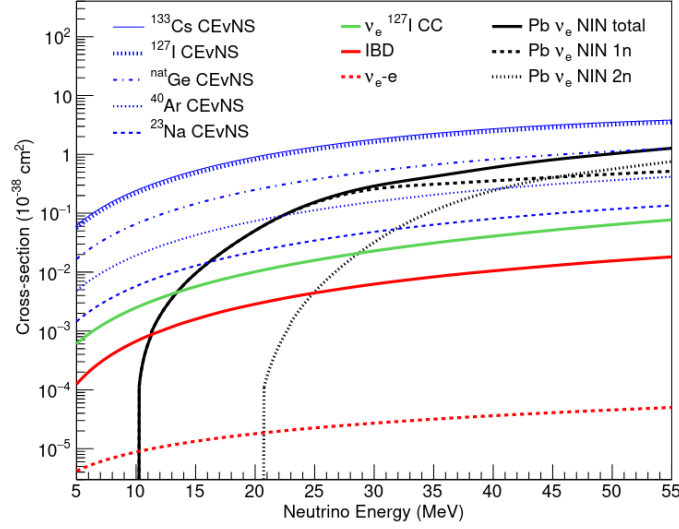


Figure 2.7: CE ν NS cross section as a function of neutrino energy for a variety of interactions and different nuclei. Also shown are neutrino induced neutron (NIN) cross sections on lead, inverse beta decay of $\bar{\nu}_e$ on free protons (IBD), and elastic scattering of ν_e on electrons. Source: [194]

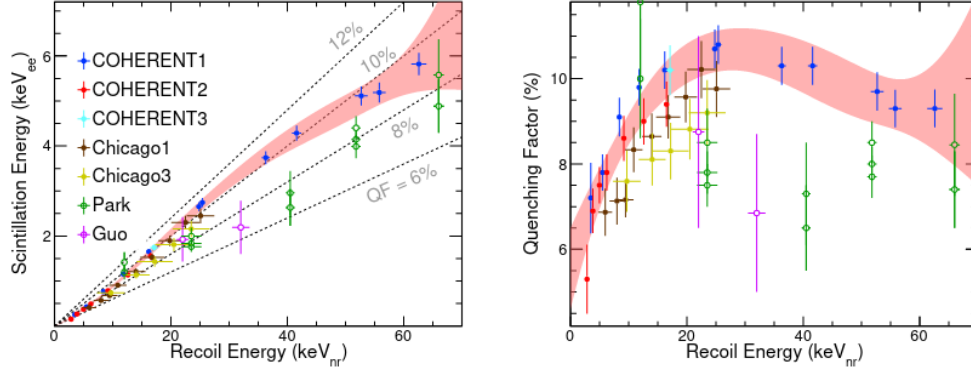


Figure 2.8: Scintillation light response neutron recoils measured in electron-equivalent energy for CsI[Na]. Data points are from a variety of measurements including 3 measurements performed by the COHERENT collaboration [196] and measurements made by Collar et al in Chicago [197]. Highlighted region shows best fit with 1σ error. Right is the corresponding data in the form of a quenching factor. source: [196].

occur within the pulse duration of the beam allowing for background subtraction when the beam is off. A 14.6 kg CsI[Na] detector was placed in a basement hallway within the SNS located 19.3 m from the source and collected data for 13.99 GWhr of integrated beam power. The crystal was attached to a PMT and the signal was digitized with a 500 MHz digitizer. The detector was shielded with lead and low-Z materials to shield from gamma and neutron backgrounds associated with the source [198]. Muon veto panels are deployed above the setup to reject cosmogenic-related backgrounds.

Beam-correlated backgrounds modelled were beam-related neutron (BRN) and neutrino-induced neutron (NIN) backgrounds. The normalization for these backgrounds was determined by a measurement where the outer water shielding of the setup was drained and the neutron background was characterized with simulations. An MCNPX-PoliMi [199] simulation was used to estimate the incident neutron flux due to the beam. The MARLEY [200] simulation package was modified for ^{208}Pb to estimate the NIN flux. With the neutron fluxes determined via simulation and validated with measurement, the fluxes were propagated through the full shielding in a simulation in order to determine the background component due to these beam related sources. These were estimated to make up 7% of the excess signal events detected. Uncorrelated steady state backgrounds comprised 98% of the backgrounds, indicating a 1/3.5 signal to background ratio. The reported $\text{CE}\nu\text{NS}$ event count was 306 ± 20 , consistent with the SM prediction of 341 ± 11 (theory) ± 42 (experiment). The results showing the detected $\text{CE}\nu\text{NS}$ spectrum from the different sources (ν_μ , ν_e , and $\bar{\nu}_e$) along with beam-correlated backgrounds are displayed in figure 2.9. The results from the Argon experiment validate the N^2 dependence of the $\text{CE}\nu\text{NS}$ cross section [195].

2.6.2 Future Experiments Planned by the COHERENT Collaboration

Several experiments are planned by the COHERENT collaboration [201] at the SNS. A heavy water detector designed to measure the neutrino flux of the SNS beam will utilize the deuteron beta decay reaction (equation 1.23) to do so and operate on similar principles as the SNO detector. This will constrain the largest systematic for the current measurements which is a 10% uncertainty in the neutrino flux.

A Germanium array will be deployed in 2022 to measure $\text{CE}\nu\text{NS}$. The crystals are p-type point-contact high-purity Ge detectors designed for a low energy threshold and low intrinsic background. The energy resolution will be much greater than the existing CsI and Ar measurements albeit with a lower timing resolution. The timing resolution is still enough to leverage the pulsed beam and the time separation between neutrino flavors from the muon decay process. Several dewars will be deployed with a number of 2 kg detectors, each containing layers of copper, polyethylene and lead shielding. Muon veto panels similar to the CsI measurement will be used to reject cosmic backgrounds. Ultimately 50 kg of detector mass is planned for deployment.

A multi-tonne array of repurposed NaI(Tl) detectors is being deployed currently. Each detector consists of a 7.7 kg NaI crystal with thallium doping. This would represent the lowest N value measured for the $\text{CE}\nu\text{NS}$ process thus far.

Finally, upgrades to the CsI and Argon experiments are planned with significantly larger detector masses.

2.6.3 Detection of $\text{CE}\nu\text{NS}$ at a Reactor

Currently a number of efforts have been made to detector the $\text{CE}\nu\text{NS}$ process at a reactor. This is challenging because of the high neutron and gamma backgrounds associated with reactor operations (see chapter 3 for a detailed assessment of reactor backgrounds at a research reactor). Unlike the IBD process which is the standard for detecting neutrinos at a reactor, the $\text{CE}\nu\text{NS}$ process does not have a time correlated

signal that it can utilize to reject ambient backgrounds. Thus, one must rely on reducing the backgrounds in the region of interest (ROI) to acceptable levels such that the signal can be viewed as a residual above the reactor-off signal.

Using the example of a Ge detector with a recoil energy detection threshold of 0.1 keV, we can see the relation between the reduced detection cross section of equation 2.16 and a typical reactor flux in figure 2.10. Using the relation in equation 2.17, a 0.1 keV threshold corresponds roughly to a 2 MeV neutrino energy detection threshold. Because the large portion of the reactor $\bar{\nu}_e$ spectrum resides below 2 MeV, it is apparent that lowering the detection threshold of a reactor-based CE ν NS detector is paramount.

The CONUS experiment was performed in 2018-19 [202]. It set an upper limit on the detection rate of CE ν NS at a reactor. This experiment was performed using a cryo-cooled 1.9 kg Ge detector inside an onion-like layer of shielding consisting of lead, borated polyethylene, polyethylene, plastic muon veto panels, and steel. The experiment reported an upper limit of 85 counts in the region of interest below 1 keV electron-equivalent (keV_{ee}) and above $0.3 keV_{ee}$ across the exposure time of 248.7 kg d. The detection was based on the ionization of the medium by the recoiling Ge particles.

Next generation efforts involve the use of cryogenic bolometers which detect thermal vibrations within the detector. The advantage of such a system is very low thresholds and a much more linear energy response compared to the ionization style approach. MINER [203] is a proposed experiment at the Nuclear Science Center at Texas A&M University which will operate within 2 meters of the TRIGA reactor core. The experiment will use cryogenic Si and Ge detectors with a target fiducial mass of 10 kg and a low energy threshold of 200 eV.

The NuCLEUS experiment [204, 205] is proposed to operate at the CHOOZ reactor using cryogenic CaWO₄. Its advantages lie in a low detector threshold of 10 eV which is achieved with low mass (gram scale) detectors and the high CE ν NS cross

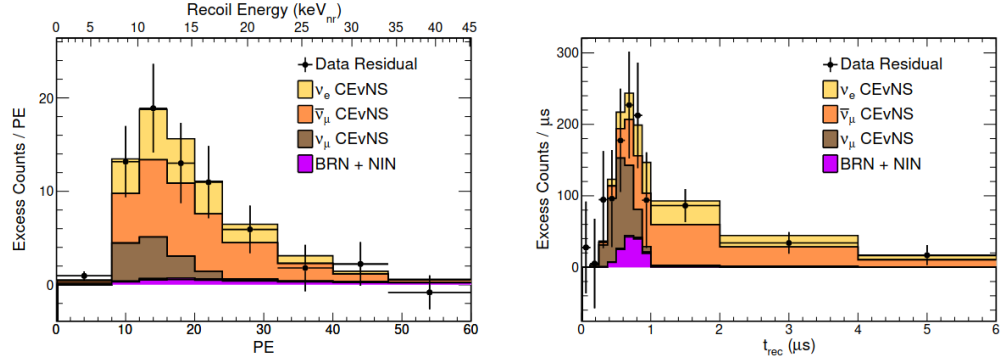


Figure 2.9: Left is the CEνNS event rate for the different neutrino sources and the estimated beam-correlated backgrounds. Right is the same data displaying the timing distribution from the start of the beam pulse. Source: [187].

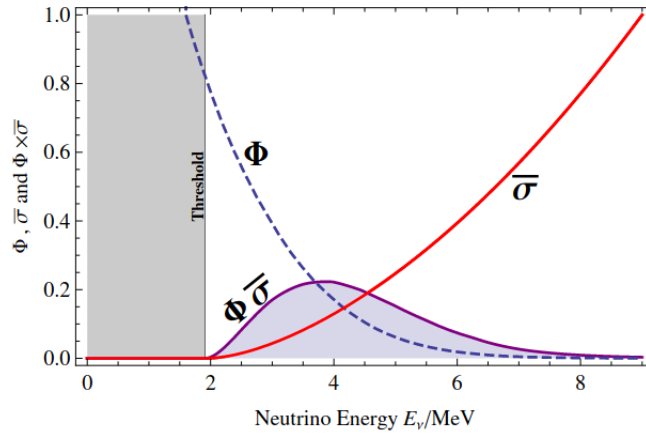


Figure 2.10: Demonstration of a typical reactor flux Φ and reduced detection cross section $\bar{\sigma}$ and their product for a Ge detector with a 0.1 keV recoil energy detection threshold. Shaded region represents undetectable region due to the low energy detection threshold. Source: [188].

section from the use of Tungsten. They will also utilize veto detectors for active background suppression in addition to passive shielding.

The Ricochet experiment [206, 207] will utilize an array of 27 Ge detectors cooled to 10 mK using an ultra low noise cryostat. Their mass will be about 38 g each, leading to roughly 1 kg of active material. The detectors will utilize germanium neutron transmutation doped sensors in order to reach thresholds as low as 50 eV. The detectors will be equipped with both heat and ionization readout in order to determine particle identification.

2.7 Conclusion

This chapter discussed various aspects of antineutrino detection at a reactor. The primary mechanics of detection via inverse-beta decay were outlined, with a focus on detection via liquid scintillator detectors. Next, the primary anomalies associated with $\bar{\nu}_e$ detection at a reactor were outlined along with their current status. The details of calculating a $\bar{\nu}_e$ flux from the reactor fuel composition were then given in order to provide background for how the predictions are generated. Issues with the calculation are discussed along with current generation of measurements using TAS detectors for correcting older measurements of beta decay spectra. Details were provided for the MTAS experiment which the author of this thesis was involved. Finally, CE ν NS style measurements at a reactor were described to provide context for the next chapter which will go into detail about the reactor backgrounds at HFIR.

Chapter 3

Reactor backgrounds at HFIR for neutrino experiments

This chapter describes the deployment of a Germanium detector at Oak Ridge National Lab’s High Flux Isotope Reactor (HFIR) for the purpose of understanding the energy and spatial distribution of the gamma field in the experiment hall where PROSPECT took data and future neutrino experiments will be located. The sources from both the reactor and the beamlines are described in detail, along with their temporal variations due to reactor power and their spatial variations due to the geometry of the beamlines and building materials in the vicinity. Additionally, a shielding study was performed to assess the amount that backgrounds in tens of keV range can be mitigated.

This work helps inform backgrounds for future experiments at reactors such as IBD-based neutrino measurements, CEvNS measurements, and fission fragment gamma spectroscopy like those done at ILL [208] and those that were proposed at MAFF [209].

3.1 Introduction

The High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory in Oak Ridge, TN USA is an 85 mega-watt highly enriched Uranium (HEU) reactor utilized by a number of research groups for its neutron source. Recently it was shown that reactor antineutrino measurements differ from expectation in both the overall rate and the shape of the energy spectrum. This has prompted a number of experiments deployed to measure reactor antineutrino spectra around the world, including a measurement done at HFIR by the PROSPECT collaboration in 2018 [83]. A major challenge when operating an antineutrino detector at a reactor are the backgrounds associated with reactor operation primarily coming from neutrons that diffuse through the building into the area of the experiment. Thermalized neutrons can capture on the building materials and experiment shielding materials generating gamma radiation which can provide backgrounds to neutrino detection if not properly shielded. In this work we describe a deployment of a Germanium detector with a 1kg active volume at the experiment hall within HFIR in order to provide a detailed characterization of the spatial and temporal variation of the gamma radiation within. The detector was deployed in two modes, one utilizing a mobile lead collimator shield, and another utilizing a series of cylindrical layers of polyethylene and lead shielding. The reactor gamma background is characterized and implications for future neutrino experiments are discussed.

3.1.1 HFIR Building and Reactor Description

The experiment hall of the reactor is located one floor above and approximately 6 meters south of the reactor core. The pressurized reactor vessel is immersed in a pool of water which is surrounded by concrete. The top of the reactor vessel guide them to experiments. There are 4 beamlines, two of which are below the experiment hall - HB3 and HB4. These beamlines provide pathways for thermal neutrons to diffuse into the materials in the floor below the experiment hall. The experiment hall

contains a lead shield wall that is a 0.1 m thick and surrounded by steel supports. The wall was constructed before the start of the PROSPECT experiment to mitigate the largest source of backgrounds in the experiment hall which are gammas coming from the reactor pool wall. The central portion of the wall is 3.0 m wide and 2.1 m tall. It is completed by two shorter flanking portions on either end containing 0.05 m thick lead. Refer to figure 3.1 for a diagram displaying the core and beamlines relative the features in the experiment hall.

3.2 Materials and Methods

Two configurations were used during deployment. The first is a lead collimator attached to a movable cart. The collimator is able to rotate up to 180 degrees. This allows us to aim the detector in any direction. This setup was used to scan throughout the room and point to various sources of background. A catalogue of these measurements is reported in section 3.4.

The second configuration is a "Russian doll" style arrangement of concentric cylindrical shielding surrounding the Ge detector. The shielding layers were chosen to mitigate thermal neutron and gamma backgrounds.

3.2.1 Germanium Detector Specifications

The detector is an OrtecTM GEM P-type coaxial High Purity Germanium detector. The crystal has a 62 mm diameter by 69.7 mm length and a hole with an 8.5 mm diameter by 56.1 mm depth. The quoted dead layer thickness is 0.7 mm for the lithiated outer dead layer and a 0.3 um borated inner dead layer. The active volume calculated from the quoted dimensions is 1.02 ± 0.01 kg.

An aluminum case surrounds the detector and a copper cold finger is thermally coupled to the bottom of the crystal. The detector is cooled via an OrtecTM ICS mechanical cryo-cooler.

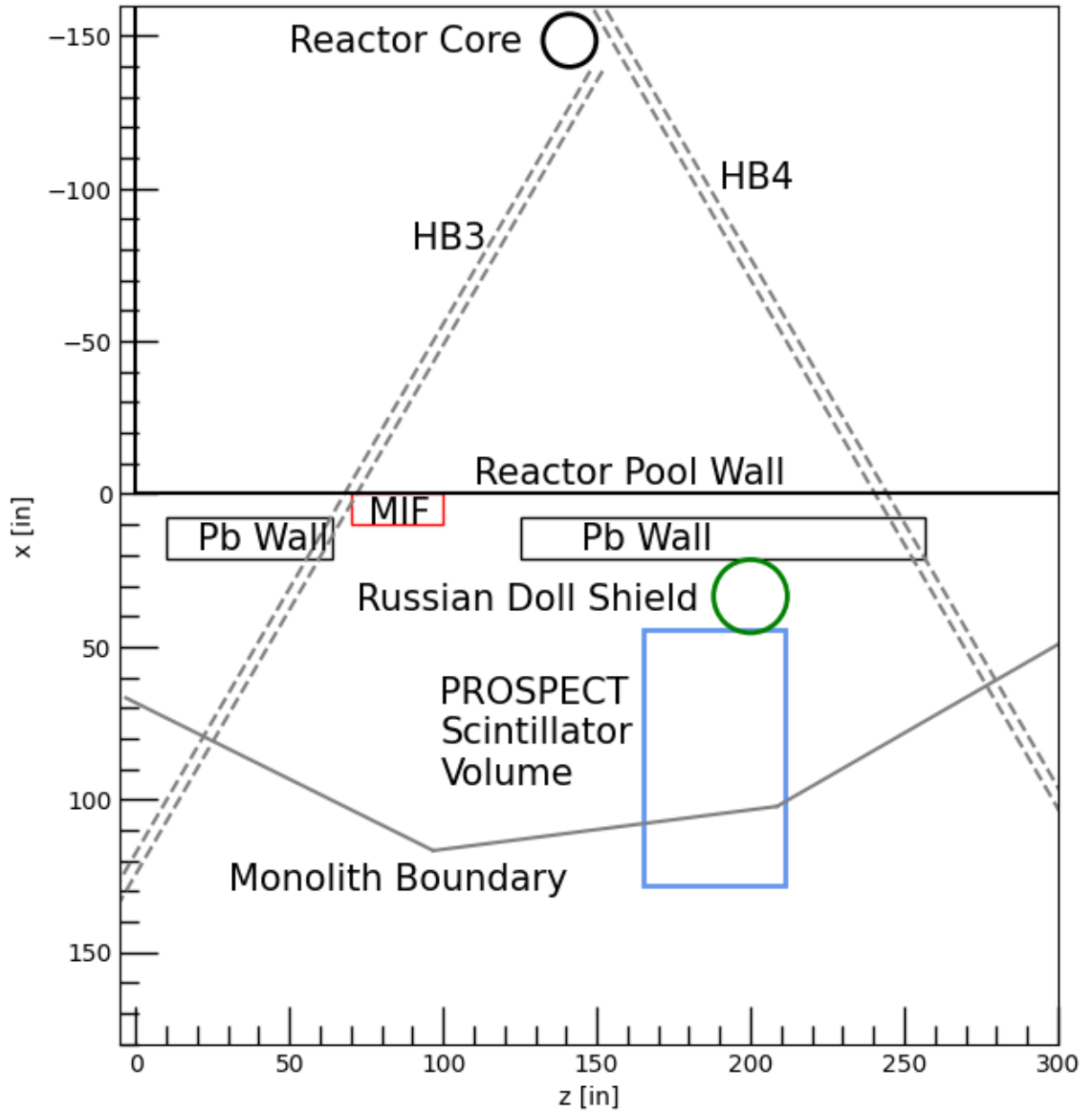


Figure 3.1: Top down diagram of the core and beamlines HB3 and HB4 relative to the experiment hall. The placement of the Russian Doll shield (refer to section 3.5 for more details) is located at the green circle at the lowest point of background radiation in front of the lead shield wall. The inner scintillator volume of where PROSPECT took data is displayed in blue. The concrete monolith is displayed in grey. The location of the Materials Irradiation Facility (MIF) valve box is denoted in red. Note that the center of the core and the beamlines are 4 meters below the floor of the experiment hall.

3.2.2 Data Acquisition and Metadata Database

Signals are processed with a Canberra™ Lynx digital signal analyzer and analyzed using the Genie-2000 Spectroscopy Software from Canberra™.

Spectra are written out to files for each run taken. A coordinate system was created to locate the cart's position and orientation. The room coordinate system used was x being the distance from the reactor wall, z being the distance from the western edge of the reactor wall, and y being the height above the floor.

In order to record the location and angle of the cart, the x,z coordinates of the front right and front left corners of the cart were recorded for every measurement. Additionally, the angle of the collimator was recorded with a magnetic protractor which was attached to the lead shield (see figure 3.3). An angle of 0 indicates the detector is pointing straight down.

A sqlite database was constructed to organize the detector coordinates, data acquisition settings, detector bias, shielding, and calibrations used for each file. Data files were logically organized into runs which denote several sequential measurements taken with the same detector settings. The database schema is depicted in figure 3.2. Python functions were developed to retrieve spectra based on metadata such as position, acquisition time, gain settings, shield type, and acquisition length.

3.2.3 Movable Shield Cart

The shield cart used is the ISOXSHLD produced by Mirion Technologies. It is movable with 4 iron caster wheels and utilizes a wheel lock rotational mechanism for rotating the shield and detector system. The lead collimator is cylindrical with a 111 mm outer radius, a 57 mm inner radius, and a 180 mm length. The lead end cap of length 43.5 mm contains a 30 degree opening cone at its center with an initial opening radius of 18 mm. Figure 3.3 shows an isometric drawing of the shield cart with the detector placed in the horizontal position and a picture of the cart deployed at the reactor.

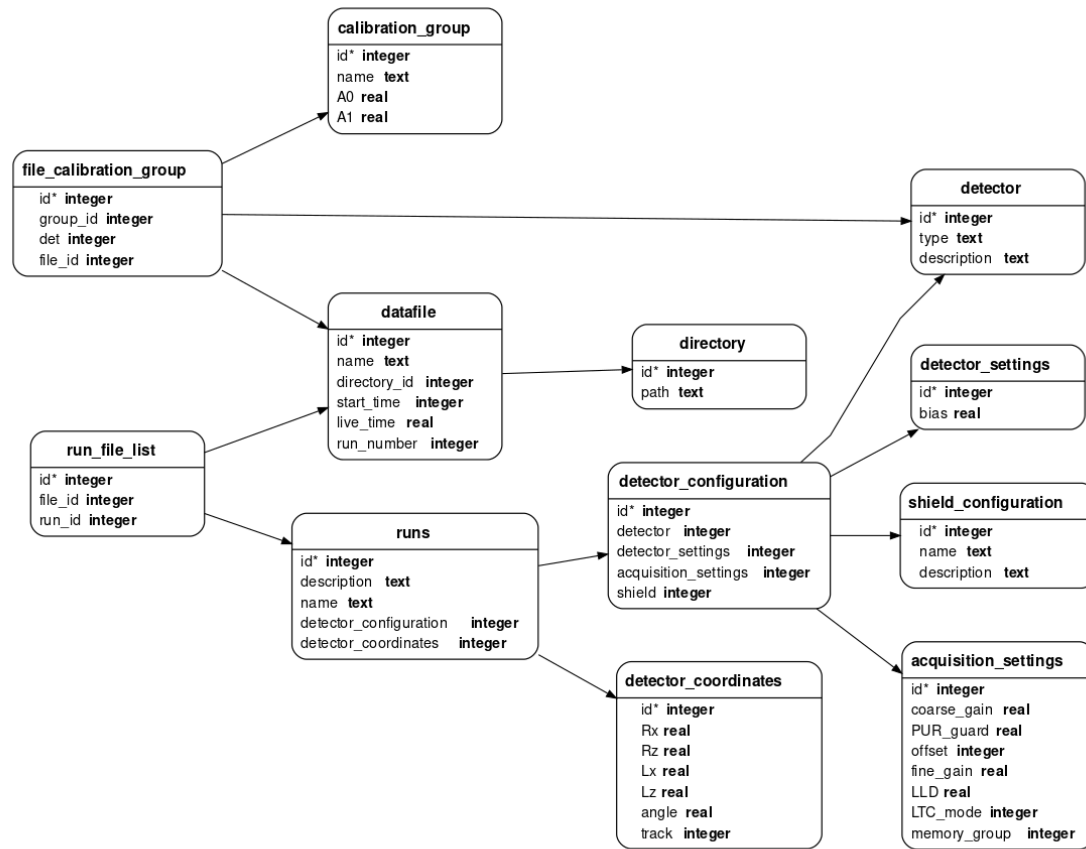


Figure 3.2: Database schema used for the experiment. Lines denote foreign key relationships.

3.2.4 Russian Doll Shielding

The Russian doll shield was constructed by AMETEK-AMT; it consists of a series of concentric cylindrical shields. From outer to inner there is a half inch thick steel casing, 3.5" of lead, .02" tin, 1/16" copper, 2 7/8" borated polyethylene and 0.9" lithiated polyethylene at the innermost layer. A cutout of the layers along with the detector placed within are depicted in the picture in figure 3.4. The inner lithiated polyethylene layer was chosen in order to absorb neutrons via the ${}^6\text{Li}(n, \alpha){}^3\text{H}$ reaction which does not produce gammas reaching the Ge detector.

The shielding sits atop a steel stand 32 inches off the ground. The stand has a 24" x 24" base with 2" thick rectangular columns on each corner. We also added a layer of water bricks around the shield apparatus, pictured in figure 3.5. Each water brick contains 3.5 gallons of water has dimensions 9" x 18" x 6". We took measurements both with and without water bricks to see the impact on backgrounds. More details of the Russian doll measurements are found in section 3.5.

3.3 Experiment Hall Gamma Characterization

In order to measure the gamma radiation coming from the reactor, the detector cart was placed next to the lead shield wall with the collimator facing the direction of the core. The cart and detector angles were adjusted until the orientation with the maximum integral count rate was found. The detector was left in this position for 20 hours while the reactor was at 100% operating power in order to get a high statistics measurement of the gamma energy spectrum. This measurement was repeated when the reactor was turned off. Figure 3.6 shows the measured spectra in this location.

Visible spectral lines are identified and pictured in appendix A. Gamma lines above 5000 keV are due to neutron capture on isotopes present in structural steel throughout the building such as iron, nickel, and chromium. Also visible at this

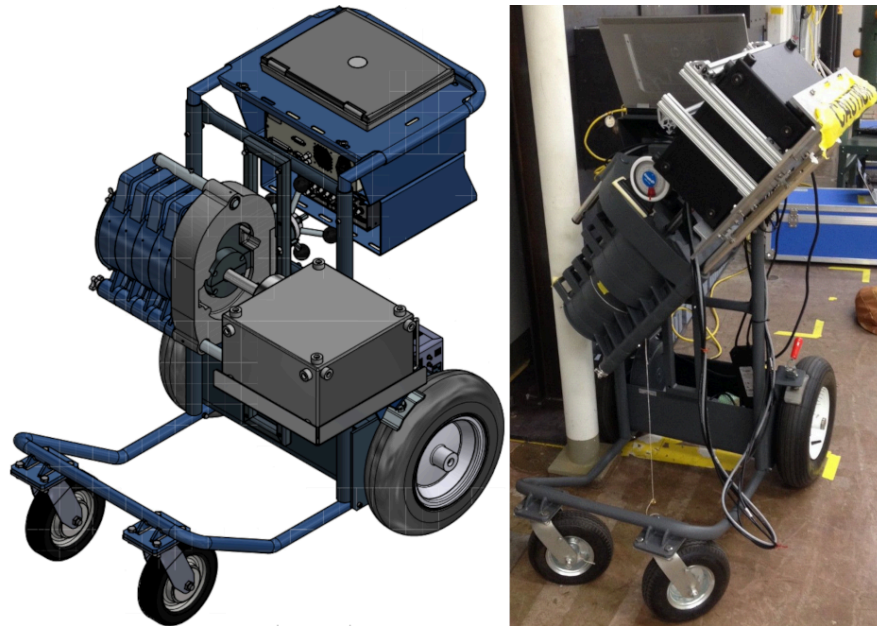


Figure 3.3: Left: isometric view of shield cart, right: picture of shield cart in position east of the lead shield wall pointing towards the reactor core.

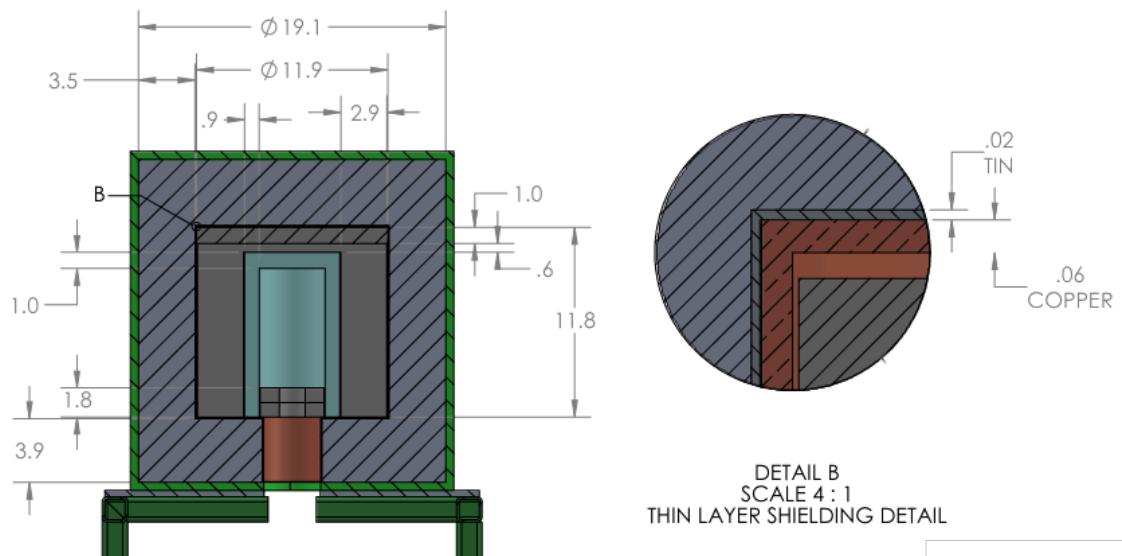


Figure 3.4: Cutout drawing of Russian doll shielding. From outer to inner shielding layers are steel (green), lead (light grey), tin (see detail B), copper (see detail B), borated polyethylene (dark grey) and lithiated polyethylene (teal). Measurements in inches.



Figure 3.5: Russian doll shielding water bricks. Background shows the lead shield wall.

location are neutron capture lines from aluminum which forms the reactor vessel, and beryllium from the neutron reflector surrounding the core.

At the 1-2 MeV range there are gammas from beta decaying radioactive isotopes such as ^{60}Co , ^{152}Eu , ^{154}Eu , ^{41}Ar and ^{40}K . The Europium is present in the reactor pool due to the control plates composed of Eu_2O_3 . Cobalt is present from residual contamination from past experiments at the Materials Irradiation Facility (MIF) which has a valve box attached to the wall just above where the detector was placed. Each of these sources which are related to residual activity of radioactive isotopes from reactor activities are also present when the reactor is off. ^{41}Ar circulates through the building while the reactor is operational due to neutron capture on ^{40}Ar present in the air around the pool. See table [A.1](#) for a list of all gamma lines and their sources.

3.3.1 Beamline 4 Gamma Characterization

Beamline HB4 runs East of the PROSPECT location at a 30 degree angle counter clockwise from south through the floor below. As can be seen in the position scan in figure [3.10](#), there is a region of larger gamma rates roughly 100 inches East of the southern edge of the PROSPECT detector. The center of this “hot spot” corresponds to a protective steel block surrounding the beamline at the cold source of beamline 4. The large amounts of steel provides material that absorbs neutrons that are scattered by the cold source and subsequently generate neutron capture gammas. This is important for consideration of future experiments in the PROSPECT location because this source of radiation is the dominant source due to the attenuation of the primary component coming from the reactor pool by the lead shield wall. This is the source of radiation that caused larger amounts of gamma backgrounds in the bottom two layers of segments on the south side of the PROSPECT detector. This required treating two additional segments as fiducial segments because the HB4 gammas caused too many accidental backgrounds to be able to effectively detect antineutrino events. For a future experiment such as PROSPECT-II [\[210\]](#), mitigating HB4 gammas from the

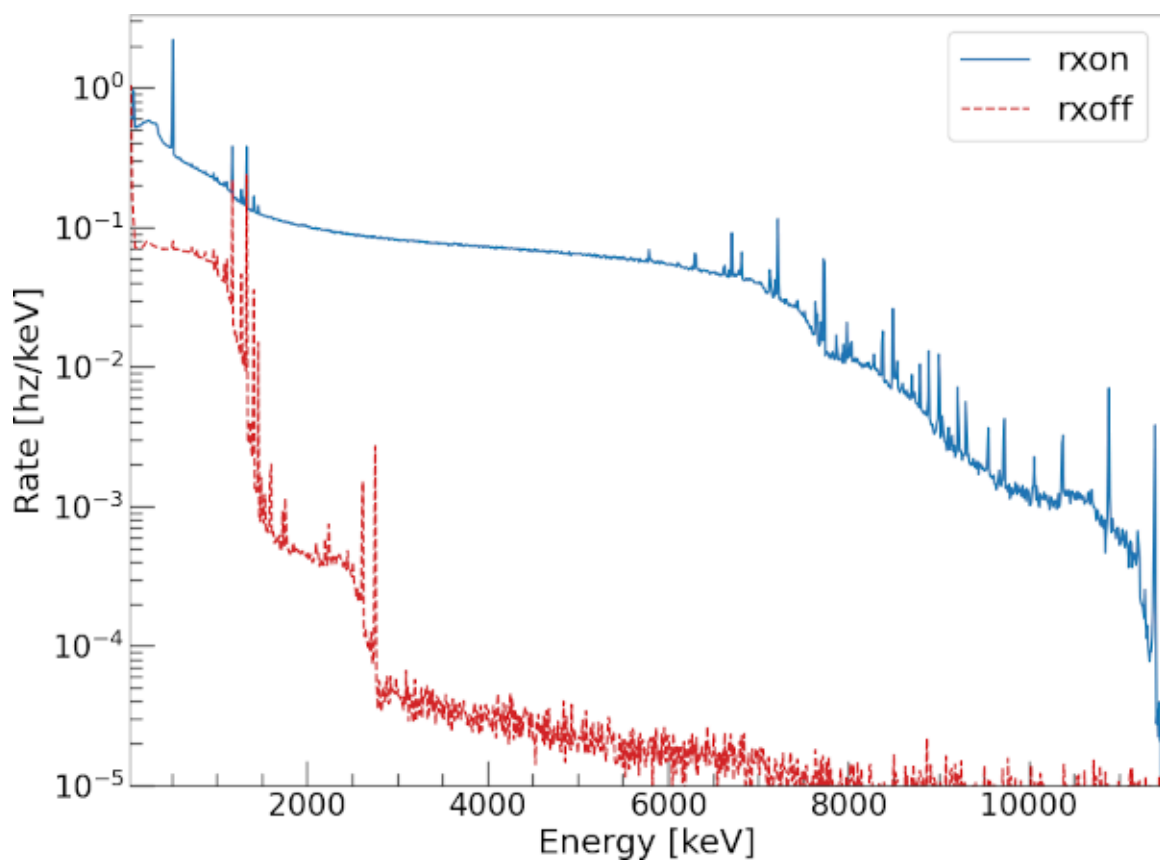


Figure 3.6: Measured energy spectrum with collimator facing the reactor positioned west of the lead shield wall, just under the MIF box (see figure 3.1). Reactor on in blue, off in red. High energy lines are from neutron capture on building and reactor materials.

source would reduce the accidentals in this region of the detector allowing for a larger active region.

An overnight run was made with the detector placed at the center of the hot spot with the detector pointed down in order to obtain a high statistics energy spectrum. This spectrum can be found in figure 3.7 along with the spectra taken facing the reactor both through and around the lead shield wall for comparison. The major difference between the HB4 radiation and the reactor gammas are the lack of reactor specific sources such as neutron capture on Beryllium, Aluminum, and ^{59}Ni and the presence of neutron capture on ^{48}Ti . The presence of Titanium suggest a different steel composition in the beamlines compared to the structural steel surrounding the reactor. The HB4 location has a larger flux of gammas coming from capture on iron.

Due to the radiation from HB4 primarily coming from neutrons scattered at the shutter, the ideal method for shielding would be to place neutron and gamma absorbing materials in the alcove above the beamline on the floor below. This would allow for absorption of the neutron before they can reach the floor while also attenuating gammas from the neutron interactions in the shielding layers. By placing the materials in the floor below, no additional shielding needs to be placed in the experiment hall which has floor loading limits and space requirements for walkways. [113].

3.3.2 Gamma Rates Correlated with Reactor Power

The measured rate of gamma rays in the experiment hall have a strong correlation to the reactor power. In general the rates in the experiment hall will correlate most strongly with reactor power, beamline activities in the floor below, and the amount of time the reactor has been on during the current cycle. In general rates will increase throughout the duration of the cycle as see in figure 3.9.

In order to illustrate the correlation with reactor power, the detector was placed in the MIF position facing the reactor as was used for the spectrum in figure 3.6. During

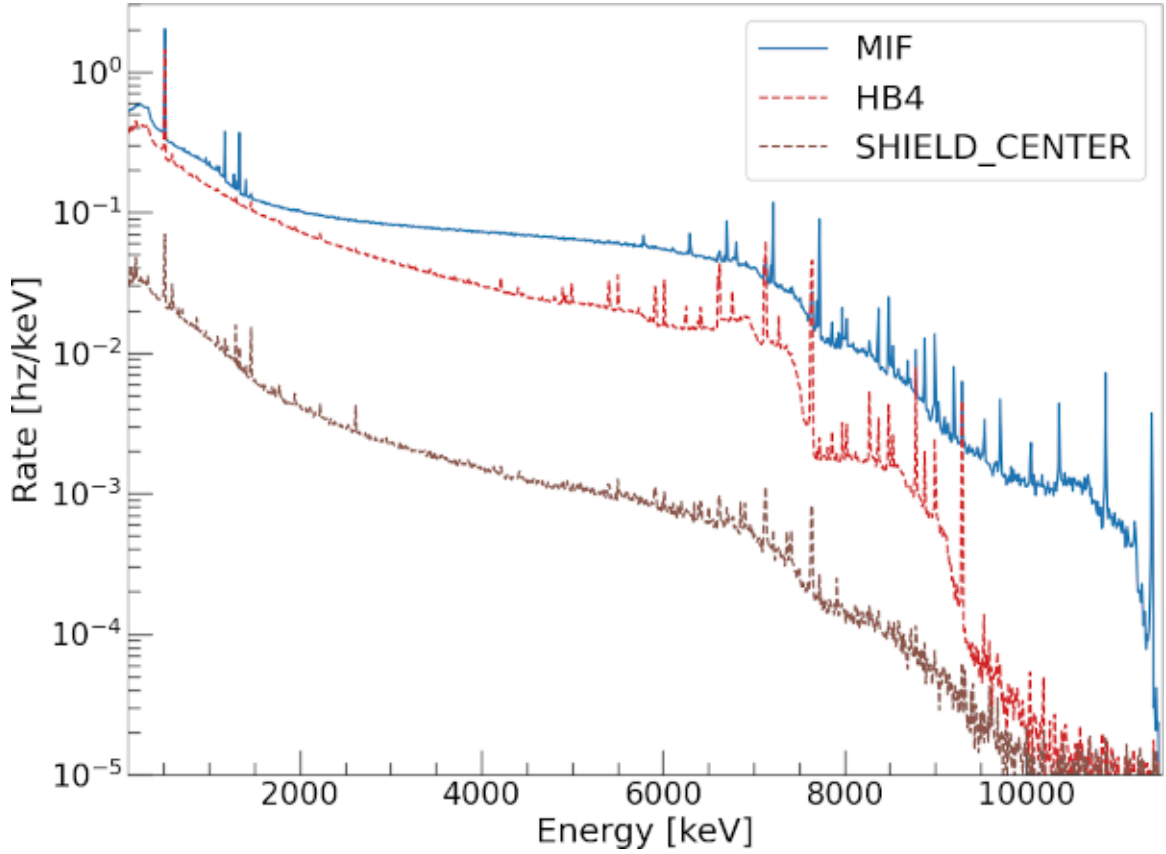


Figure 3.7: Comparison of reactor on spectra taken at three different locations. Blue is taken under the MIF box with collimator pointing at the reactor (no lead shield wall attenuating this location), red is taken over the HB4 hot spot, and brown is at the lowest background location situated close to the center of the lead shield wall. Gamma lines such as neutron capture on beryllium and ^{59}Ni are only coming from near the reactor core whereas gammas from neutron capture on ^{49}Ti are only present in the HB4 beamline area due to structural materials unique to that region of the building. Brown line relative to blue demonstrates the effectiveness of the lead shield wall.

the startup procedure, the operators will announce over a loud speaker the beginning of the ramp up to a target power level. Once the announcement is heard, we start a new run with the detector to get a spectrum for each ramp up period. This was done during the ramp up for cycle 491 on April 13, 2021. A reactor off spectrum taken with 5 days of data before the startup procedure commenced was used to subtract from the measured spectra. Rates for the subtracted spectra were then calculated by summing 23 500 keV increments from 100 keV to 11,600 keV. Each of these rates were then divided by a reactor off subtracted spectrum sampled for 1 hour after the reactor reached 100% power. The results are plotted in figure 3.8. Because we don't have access to granular power data within each of these sampled periods, we cannot provide a correlation coefficient with the reactor power, but one can qualitatively see from this plot that the various portions of the gamma energy spectrum do correlate well with the power. Note that during this ramp up, a pause was taken at 10% power while the reactor operators performed various safety diagnostics. The measured data here is consistent with this power level with most energy ranges showing about 10% of the rates of the 100% spectrum.

3.3.3 Gamma Rates Time Series

During the 2 day lead up to Cycle 491 and the first 2 days of the cycle, the detector was placed in the MIF position facing the reactor. Before this particular cycle some reactor tests were performed the day before the startup. This involved bringing the reactor up and down between 0 and 10% power which is illustrated in the rates observed in figure 3.9.

One can see that on 21-04-13 between 05:00 and 10:00 the rates spiked at certain times. This is due to instrumentation in the floor below from beamline 3 changing settings causing larger amounts of neutrons to scatter up into the experiment hall. A neutron diffractometer [211] and spectrometer [212] are instruments capable of these

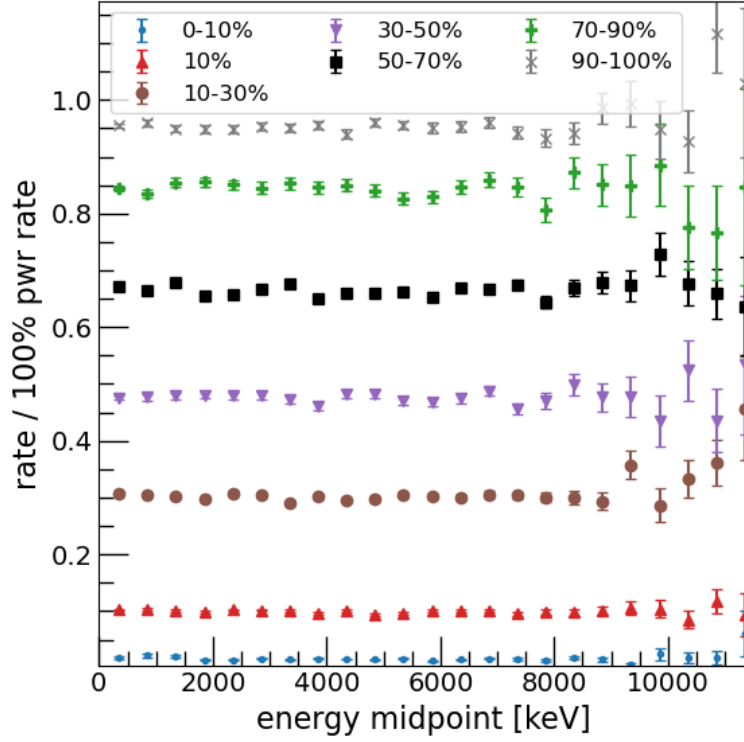


Figure 3.8: Ratios of rates in 500 keV increments to the spectrum at 100% power for various periods during the ramp up for cycle 491. Note that only power ranges are known based on the operator announcing the beginning of a ramp up to a set power level with the exception of the 10% power level which the reactor was kept at for the duration of the 10% sample.

changes in neutron flux observable in the experiment hall. The 30% variation seen in this plot is typical of such variations seen during a reactor cycle.

3.4 Spatial Survey

One goal of the measurement campaign was to characterize the spatial variation of the gamma field in order to better understand the sources of radiation. There are two primary regions of larger gamma fluxes due to the features of the building such as the shape of the concrete monolith, the location of the beamlines and associated beam shutters, and the volume of the reactor pool. A thorough scan was done with the detector cart in the downward facing position. The cart was placed at various locations along experiment floor, covering the area where PROSPECT was located along with the surrounding vicinity. Runs were done in a low gain mode that allowed for an energy range of up to 11.4 MeV which covers the largest energy gamma of 11386.5 keV from the neutron capture reaction $^{59}\text{Ni}(n, \gamma)^{60}\text{Ni}$. Approximately 100 positions were scanned with 4 minutes of live time. A contour plot showing total rates for energies from 30 keV to 11400 keV is shown in figure 3.10. The highest rates are found west of the lead shield wall where radiation from the reactor is able to shine through. The lead shield wall does a good job of mitigating backgrounds in the region of PROSPECT. A hot spot is visible east of the PROSPECT location which is due to large amounts of steel near the cold source within the HB4 beamline on the floor below. This hotspot is the dominant source of gamma backgrounds for the PROSPECT experiment.

Another scan was done along the east face of the PROSPECT inner volume with the detector pointed east towards the HB4 hotspot. This was done in order to quantitatively determine the contribution of the hotspot towards the gamma rates in the PROSPECT detector by simulating the measured gamma spectrum. The rates from the scan are depicted in figure 3.11. Simulation of the gamma backgrounds in the PROSPECT detector are detailed in section 3.7.

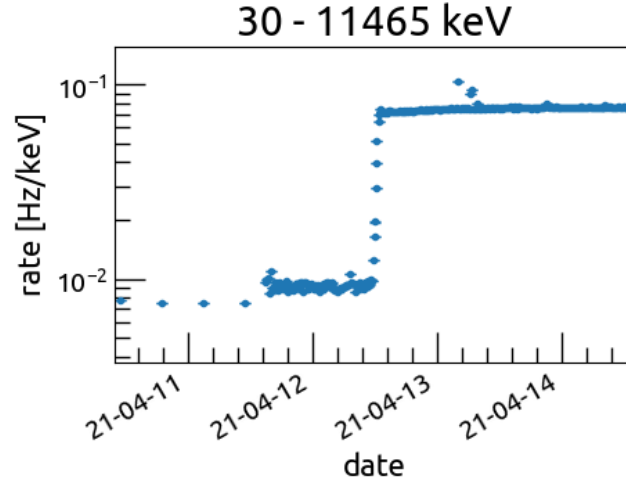


Figure 3.9: Rates between 30 keV and 11465 keV over time in the collimated Ge detector while in the MIF position facing the reactor. First couple of days is during reactor off. Oscillations before ramp up are due to tests performed by reactor technicians. Reactor ramp up was measured as detailed in section 3.3.2. After at full power a slow ramp up in rates is observed throughout the remainder of the cycle, as is typical of gamma backgrounds seen in the experiment hall during a cycle. Spikes in rate correspond to changes in neutron diffractometer [211] and spectrometer [212] instrument settings downstream of beamline 3 in experiments on the floor below.

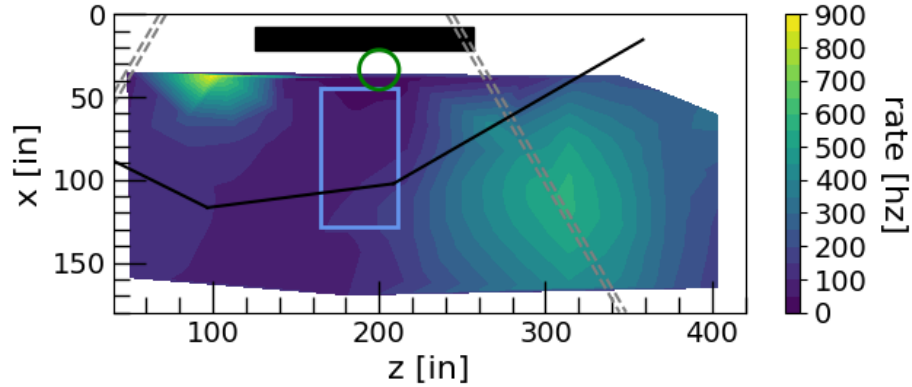


Figure 3.10: Rates between 50 keV and 11400 keV measured with the Ge detector inside the lead collimator facing down towards the floor. Blue box indicates the region of the PROSPECT active scintillator volume, the green circle represents the location of the Russian doll shield, the grey dashed lines represent the path of beamline 4 through the floor below, and the black rectangle represents the lead shield wall. The black line denotes the boundary of the concrete monolith positioned below the floor. The $y = 0$ position is the reactor wall, coordinates are in inches.

3.4.1 Track Scan Measurements

In order to precisely position the shield cart in a repeatable manner, the shield cart was placed on a track with wheel mounted sleds (figure 3.12). The track was placed parallel to the shield wall, with one end terminating at the Eastern edge of where the PROSPECT liquid scintillator volume was located and the other end terminating 30 inches West of the lead shield wall termination point. Measurements were taken for about 5 minutes in 10 positions along the length of the track. Each of these positions was repeated with the detector collimator pointing at 5 different angles between 48 and 58.5 degrees. The idea was to see if we could "locate" the profile of the reactor using the detected gamma rate. This did not work as can be seen in figure 3.13; the rates looking through the shield wall were too attenuated to see granular enough differences to distinguish the reactor direction. Significantly higher statistics runs would be needed to distinguish fine scale features in the radiation field.

3.5 Russian Doll Measurements

After taking various measurements with the movable collimator configuration, the Germanium detector was placed in the Russian doll shielding in July, 2021 where it took data until February, 2022 during which 4 reactor on/off cycles took place. Two gain configurations were used during the runs, one the same gain which was used to measure up to 11.5 MeV as shown with the collimator scans. The other gain was a high gain mode used to examine the energy space below 90 keV. This was done in order to examine the backgrounds at low energy for the purpose of understanding backgrounds at energies relevant for CE ν NS detection. At one point during the run a layer of lead .025 m thick was placed below the shield. This was accomplished with a 3x4 arrangement of .025 x .1 x .2 m bricks. 6 water bricks were also added to mitigate thermal neutrons at this time. After a set of measurements were made in this configuration with both gain settings, a third configuration where a wall of

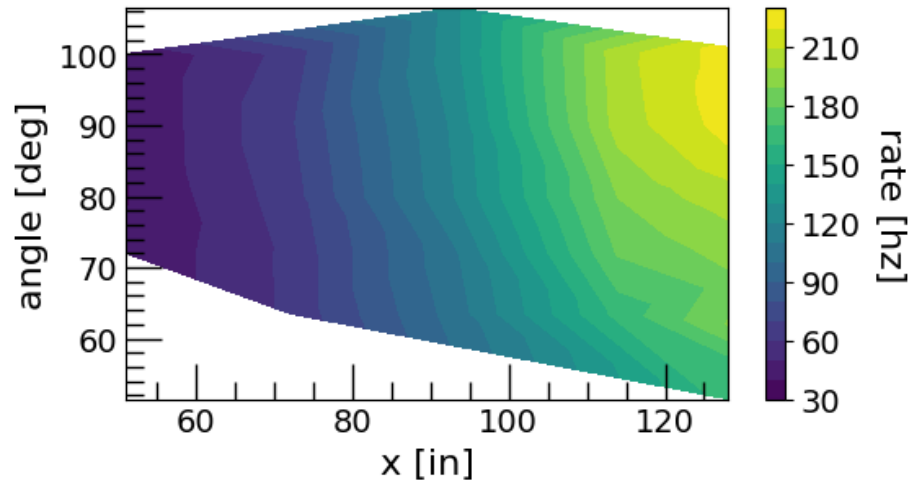


Figure 3.11: Measured gamma rates between 50 and 11400 keV. Scan is along the east face of the PROSPECT detector active volume. Low x values correspond to the north side of the detector. High rates correspond to the detector being pointed at the HB4 hot spot.

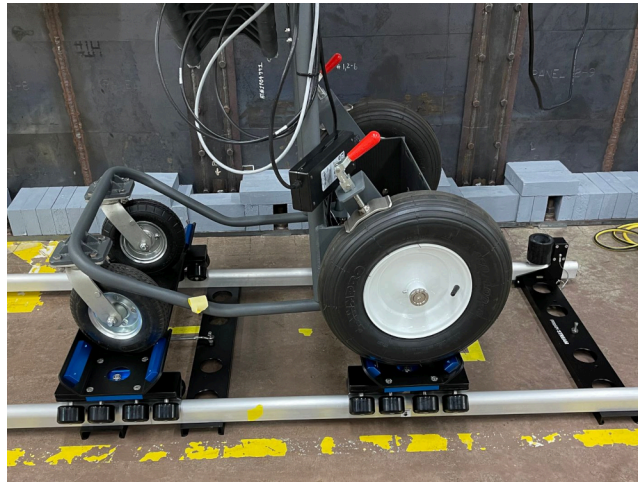


Figure 3.12: Picture showing the shield cart placed on the sliding track. The track was positioned parallel to the shield wall 20 inches away from it. The positions measured ranged from the east side of the PROSPECT active volume to 30 inches past the west edge of the lead shield wall.

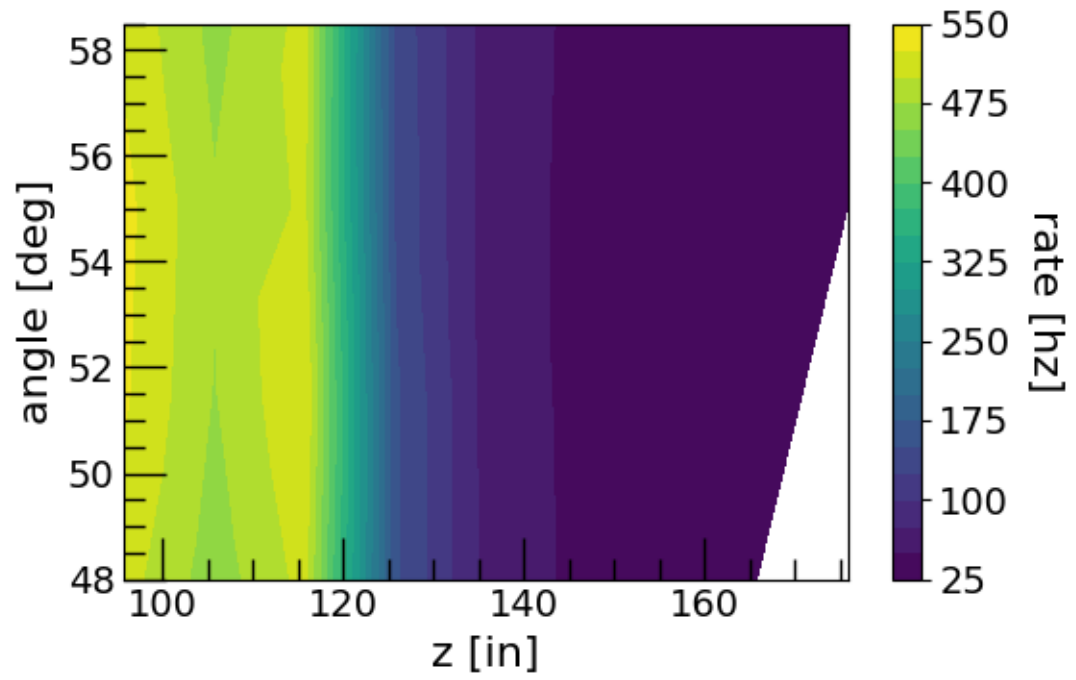


Figure 3.13: Gamma rates between 50 and 11400 keV as seen from the Ge detector cart placed on track sleds at different positions along the length of the track. Abrupt increase in rates are due to the detector moving past the lead shield wall. Reactor is at $z = 141.5$ in.

water bricks was constructed around the shield, as pictured in figure 3.5. This wall comprised of 54 water bricks in 7 layers.

After taking data with the wall for a reactor on and off period, the stand upon which the detector sat was modified to allow fitting water bricks on the detector stand and a final set of measurements was performed with this arrangement where water was more tightly packed to the bottom of the shield. These water bricks were taken from the 7th layer of the surrounding wall. Finally, the 7th layer was replaced by an additional 8 water bricks brought in.

A detailed characterization of the gamma sources found within the RD shield is found in section 3.5.1. The impact of the different shielding configurations on the gamma rates is detailed in section 3.5.2.

3.5.1 Primary Gamma Sources within the Russian Doll

Due to the large amount of lead in the RD shield, most of the gamma sources present in the experiment hall are attenuated to levels where no peaks are visible in the spectrum. Additionally, the borated and lithiated polyethylene shielding attenuate the thermal neutrons from the reactor before they can capture on the germanium. What remains are gammas from neutrons capturing on the shielding materials, natural radioactivity in the shielding materials, the radon decay chain from radon in the air, and gammas scattering off the shield into the detector.

The main lines visible are listed in table 3.1. ^{113}Cd is very prevalent in the spectrum. This was a surprise since there was no Cadmium listed in the shielding materials as per AMETEK specifications. However, tin has a very similar atomic mass (118.7 AU) as cadmium (112.4 AU), so some trace amounts will be present in tin alloys. Some tin alloys are made with cadmium. A simulation was performed in order to estimate the percentage of cadmium atoms in the tin mixture. To do this an isotropic thermal neutron flux was simulated in Geant4. The number percentage of cadmium was then varied so that the ratio of the area of the neutron capture peak

on ^{207}Pb (7368 keV) to the area from the primary ^{113}Cd line (558 keV) matched the data. A Maxwell-Boltzmann energy distribution was used for the neutrons with a temperature of 0.025 eV (290 K). From this simulation we estimate $\approx 15\%$ of the atoms in the tin mixture was natural cadmium, indicating about 2% is ^{113}Cd . This number should only be taken as a rough order of magnitude estimate because the neutron simulation would need more extensive validation in order to verify this, and the ^{207}Pb peak has low statistics. Additionally, we are making assumptions about the neutron distribution that likely are not accurate.

The feature that is yet to be identified is the collection of peaks between 472 and 484 keV. A three peak fit to this region results in peaks at 437, 480, and 484 keV with relative amplitudes of .83, 1.0, and 0.58 respectively. As can be seen in figure 3.14, the feature can also be seen when the reactor is off, albeit with lower intensity and a slightly different shape.

3.5.2 Shield Configuration Comparison

Shielding from thermal neutrons is important to mitigate secondary gammas from capture on shielding materials. Water is an economical means of such shielding, with a low average mass per nucleon it is a great absorber of neutrons. Measurements were taken with four configurations of shielding. The first is just the layered shielding as described in section 3.5. We then added 6 water bricks below the shielding apparatus and 7 layers of water bricks around the shield for a total of 60.5 bricks (some half bricks of dimension 9 x 9 x 6 inch were used) and took data for a reactor cycle in this configuration. This configuration had some empty space below the RD shield which could be filled with more water bricks. We wanted to test if placing water from the top layer of the water brick wall down below the shield to fill in this space would help further decrease rates. So the third configuration is with the top layer removed and placed underneath in a tighter packed arrangement underneath the shield. For the

Table 3.1: Gamma peaks visible within the Russian doll while reactor is on. "n,g" denotes neutron capture on the listed isotope, "b-" denotes radioactive beta decay of the isotope. The radioactive decays are also visible during reactor off.

energy [keV]	ID	yield [%]
7916.3	^{63}Cu n,g	100
7367.9	^{207}Pb n,g	100
5824.6	^{113}Cd n,g	3.96
5433.1	^{113}Cd n,g	1.55
2767.5	^{113}Cd n,g	1.5
2660.1	^{113}Cd n,g	3.7
2614.533	^{208}Tl b-	100
2550.1	^{113}Cd n,g	2.05
2455.8	^{113}Cd n,g	0.511
2398.6	^{113}Cd n,g	1.03
2223	^1H	100
2204.2	^{214}Bi b-	5.08
1764.5	^{214}Bi b-	15.4
1660.368	^{113}Cd n,g	3.75
1489.56	^{113}Cd n,g	3.19
1399.6	^{113}Cd n, g	4.67
1377.7	^{214}Bi b-	4
1364.3	^{113}Cd n,g	6.23
1293.6	^{41}Ar b-	99.1
1281	^{214}Bi b-	1.43
1238.1	^{214}Bi b-	5.8
1209.7	^{113}Cd n,g	5.57
1120.3	^{214}Bi b-	15.1
805.9	^{113}Cd n,g	6.8
768.4	^{214}Bi b-	4.9
725	^{113}Cd n,g	5.99
707.4	^{113}Cd n,g	1.55
651.3	^{113}Cd n,g	18.9
609.3	^{214}Bi b-	46.1
558.5	^{113}Cd n,g	100
351.9	^{214}Pb b-	37.6
295.2	^{214}Pb b-	19.3
242	^{214}Pb b-	7.43
238.6	^{212}Pb b-	43.3

final arrangement we brought in 8 more water bricks and restored the 7th layer of bricks to the surrounding wall to get the configuration pictured in figure 3.5.

A plot comparing the spectrum at low energies (30 - 60 keV) in a high gain acquisition mode is shown in figure 3.15. From this plot we can see that the 7th layer of water bricks is very important for mitigating gamma rates. This is due to the fact that the Ge crystal within the shield is situated between 40 and 43 inches off the ground, so the 7th water brick shields gammas and neutrons coming in nearly parallel to the crystal. Ideally a hermetic enclosure would be used to further mitigate backgrounds. The rates for the different shield configurations are displayed in table 3.2. Note that runs were not taken in low gain mode (11.4 MeV range) for all of the shielding configurations, but rates are displayed for those ranges for the data available.

3.6 Detector Response Model

In order to estimate the incident gamma flux from the measured spectrum, a detector response model was created using the simulation package Geant4[181]. Detector geometry along with the lead collimator and Russian doll shielding were constructed virtually. Gammas are simulated using the package's standard electromagnetic physics model. Locations and energies are recorded for all energy depositions within the Germanium crystal. A spherical charge distribution model is used to approximate the charge collection physics of the detector. A sphere with a volume proportional to the energy deposited is assumed to contain a uniform distribution of charge; charge within the overlaps of this sphere with the dead layer of the detector is then discarded. The dead layer thicknesses at the top, bottom, and sides of the detector are varied based on a fit to efficiency measurements. See section 3.6.1 for more details. Total energy from each energy deposition after dead layer corrections are summed. The detected energy is approximated by sampling a Gaussian with a width proportional to $A + B * E$. E is the energy of the peak centroid; A and B are coefficients fit

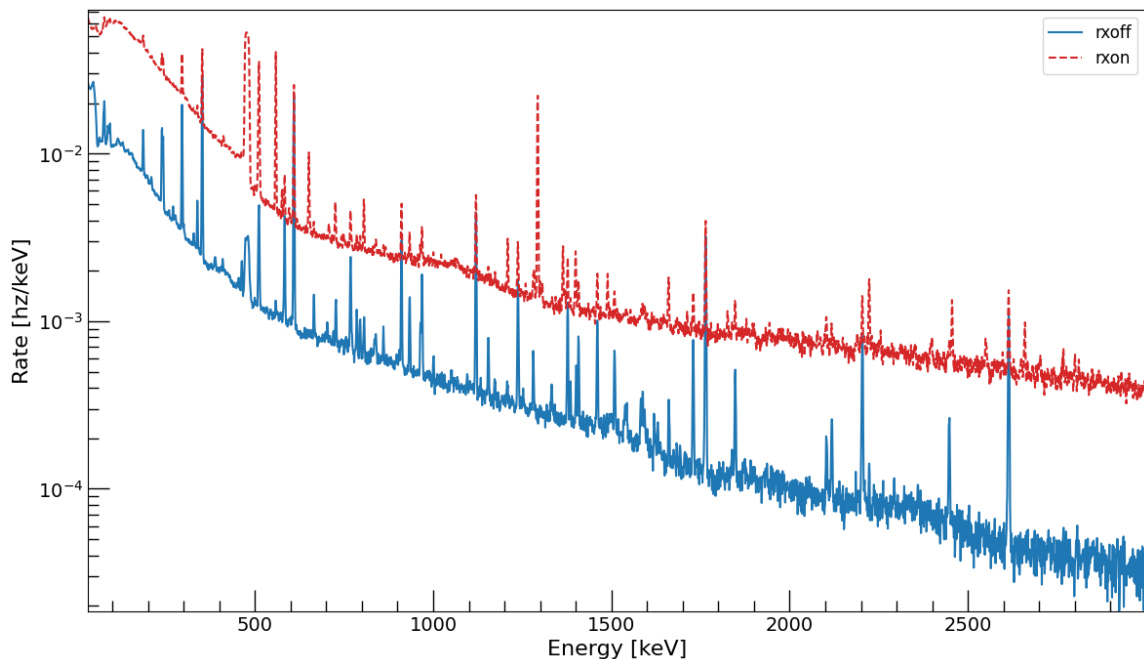


Figure 3.14: Energy spectrum with Russian doll shielding, red reactor on blue reactor off. Reactor on features are due to neutron captures on shielding materials, especially ^{113}Cd .

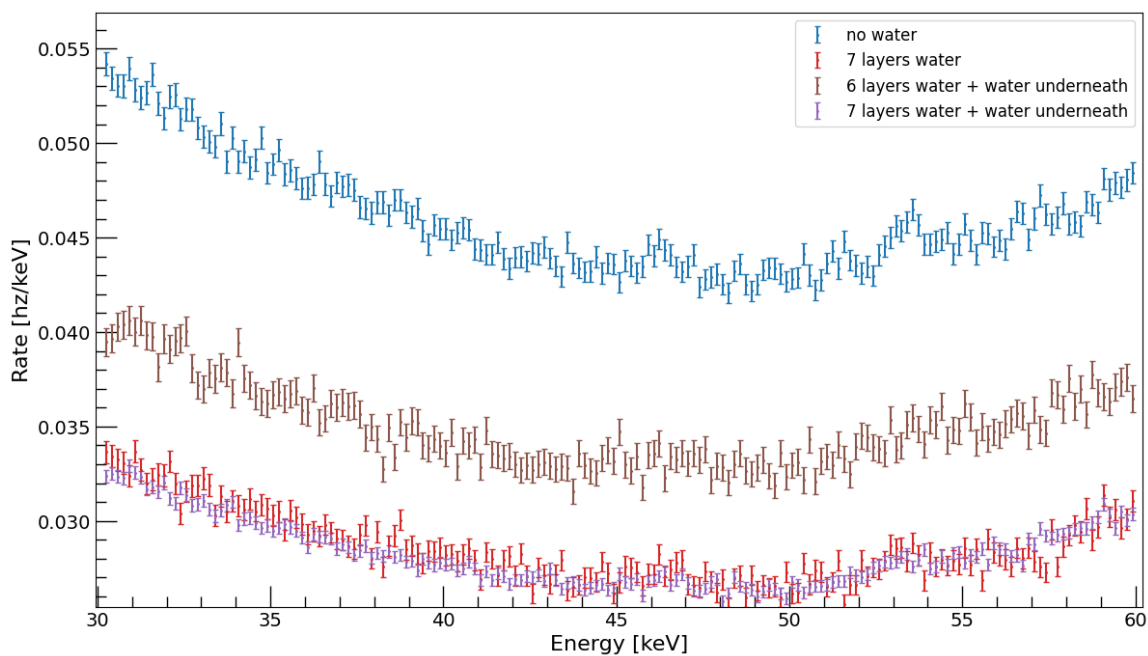


Figure 3.15: Energy spectra taken in the Russian doll shield in high gain mode. Comparison shown is between different shield configurations described in section 3.5.2. Error bars are from counting statistics.

to measured spectral line widths. More details on determining the energy resolution across the full energy range are found in section 3.6.2.

The simulated energy spectrum is calculated for energies in 1 keV increments from 30 to 11500 keV. This is accomplished by sending particles originating outside of the detector into the active volume at a specified energy. The simulated spectra at energy bin i , $\mathbf{S}_i$, are then used to reconstruct an observed spectra $\mathbf{O}$ by solving the linear equation

$$\mathbf{O} = \sum_i w_i \mathbf{S}_i, \quad (3.1)$$

where w_i is the multiplicative weight for the i th energy bin. The Richardson-Lucy [213] [214] algorithm was used to solve the deconvolution. A 1 hz/mm² isotropic flux is used in the simulation so that the deconvolved spectrum will consist of the sum of the weights for each energy bin multiplied by this flux.

3.6.1 Efficiency Measurements Validation

A series of efficiency measurements were performed using the bare Ge detector. A radioactive source was placed at three different distances from the top face of the detector along the cylindrical axis of symmetry. Photopeak efficiency was measured for 13 different energies by using the sources as summarized in table 3.3. The setup was simulated in Geant and the dead layers and charge radius parameter as described in section 3.6 were varied to best match the efficiency data. The optimal values found were a top dead layer thickness of 1.3 mm, an inner dead layer thickness of 3.6 mm, a side dead layer thickness of 0.65 mm, a bottom dead layer thickness of 3.5 mm, a charge radius parameter of 0.22 mm/MeV^{1/3}.

A lack of efficiency data at high energy means we have to rely on the accuracy of the Geant simulation for reconstructing the gamma flux. An experiment to determine the efficiency at higher energies is difficult due to the issue of finding a source in the 7+ MeV range with a well known activity. We can instead use the high energy photopeaks

from neutron capture sources in the reactor to measure the relative intensity of the full absorption peak and the first and second escape peaks to validate the simulation at high energies. This is shown in section 3.6.3.

3.6.2 Photopeak Resolution

Spectra taken when the detector is pointing towards the reactor at the MIF location is ideal for measuring the detector resolution at the full range of energies. The 11.4 MeV peak from ^{59}Ni provides a near background-free measure of the resolution at the upper end of the energy range. Additionally, the 7.7 MeV peak from ^{27}Al and the 7.65 MeV, 7.63 MeV pair from ^{56}Fe are well above background. This data is also useful for validating the simulation at high energy. The simulation should be able to accurately determine the relative intensities of the full absorption peak, the first escape peak, and the second escape peak for a given energy. This is shown in section 3.6.3.

Peaks are fit using a gaussian plus a skew gaussian plus a quadratic background. The functional form of the fit f is

$$f(E) = H(1 - R) \exp \left[-\frac{(E - c)^2}{2\sigma} \right] + HR \exp \left[\frac{E - c}{b} \right] \text{erfc} \left[\frac{E - c}{\sqrt{2}\sigma} + \frac{\sigma}{\sqrt{2}\beta} \right] + A + BE + CE^2 \quad (3.2)$$

where E is the energy, H is the height, R is the height of the skew gaussian relative to the height of the gaussian, c is the centroid, σ is the standard deviation, β is the skewness parameter, and erfc is the complementary error function. The skew Gaussian accounts for charge loss due to impurities in the crystal while the Gaussian accounts for variations in the amount of charge collected due to thermal fluctuations and electronic noise.

A linear function $A + B * E$ is used to fit the sigma widths of the peaks as a function of energy. The fit values are $A = 0.97$ eV, $B = 0.00018$ and the reduced chi square of the fit is 2.37 with 10 degrees of freedom. The fit is displayed in figure 3.16.

3.6.3 Simulation Validation at High Energy

Without known rates of high energy sources we cannot measure the detector efficiency at these energies, but we can measure the ratio of the full peak area to the first and second escape peaks. These ratios should be captured accurately by the simulation if the geometry is correct and the compton scattering, photoelectric effect, and pair production physics are accurately being reproduced. The area of peaks are measured by taking the background from the fit used in equation 3.2 and subtracting this from the histogram values 3.5σ to the left and the right of the peak centroid. Linear interpolation between samples is used to approximate partial bin area. The spectrum used for this study is the same reactor on spectrum as in figure 3.6. The results are shown in table 3.4.

In general, the ratios agree better when gammas are simulated coming from all directions rather than just coming through the collimator. The next section describes a study done to understand the effectiveness of the lead collimator, and shows that a much larger number of gammas will be detected coming through the lead rather than through the collimator opening due to the much larger available surface area for gammas to pass.

3.6.4 Collimator Effectiveness

In order to determine the effectiveness of the lead collimator at attenuating gammas, simulations were done using an isotropic flux of gammas at various energies. We compare the rates detected by the detector between two cases, one being the case of radiation coming through the collimator and the other being the case of radiation coming from any direction. The results are shown in figure 3.17 which plots the rates

Table 3.2: Rates measured within the RD shield for different configurations of surrounding water bricks. “layers” refers to the number of water bricks stacked to form the wall, “+” denotes 6 additional water bricks placed underneath the shield. 30 - 60 keV range is measured with a high gain mode, 50 - 11380 keV measured with the nominal low gain mode used for the position scan studies. Rates for both reactor on and off displayed.

shield	30 - 60 keV	30 - 60 keV	50 - 11380 keV	50 - 11380 keV
config	rates rxon [hz]	rates rxoff [hz]	rates rxon [hz]	rates rxon [hz]
no water	1.382 ± 0.001	0.2923 ± 0.0008	18.957 ± 0.009	3.725 ± 0.002
7 layers	0.859 ± 0.001	0.2791 ± 0.0003	11.770 ± 0.004	3.516 ± 0.002
6 layers+	1.052 ± 0.002	0.2785 ± 0.0004	—	—
7 layers+	0.850 ± 0.001	0.2814 ± 0.0006	—	—

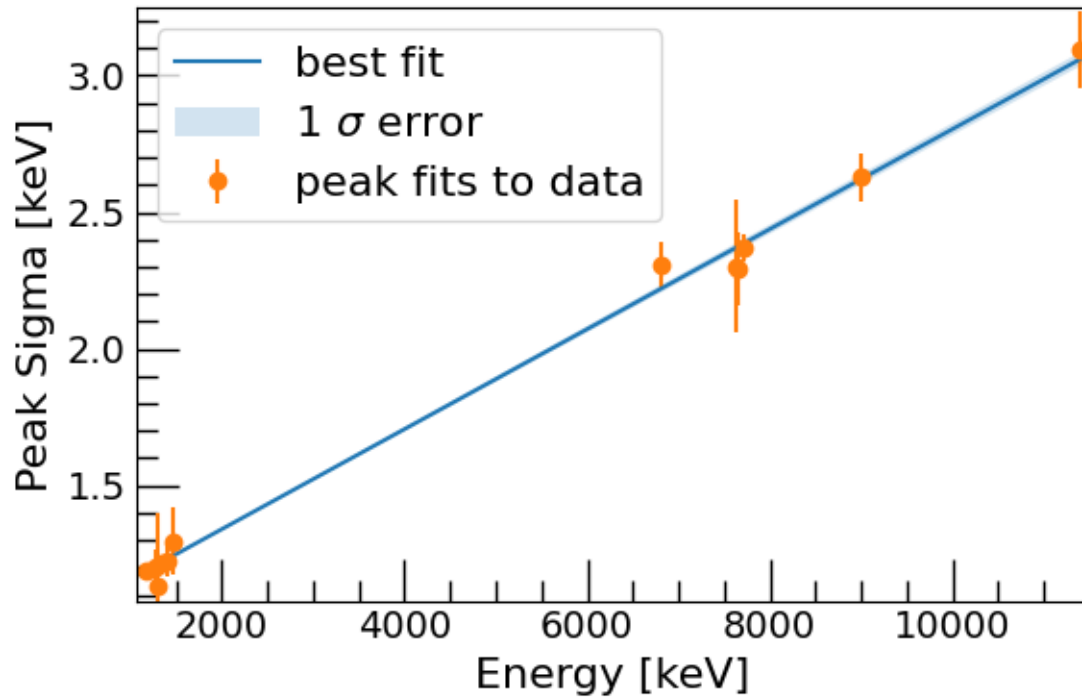


Figure 3.16: Linear fit to sigma widths as a function of energy. Fits were performed on the major gamma lines from ^{59}Ni , ^{58}Ni , ^{27}Al , ^{56}Fe , ^9Be , ^{41}Ar , ^{40}K , and ^{60}Co .

Table 3.3: Efficiency measurement results and simulated values. E = energy, D = distance, Eff = efficiency, meas = measurement, sim = simulation.

source	E [keV]	D [mm]	Eff (meas)	Eff (sim)	% diff	% meas err
²⁴¹ Am	59.5	103.7	0.00385	0.00392	1.85	5.01
²⁴¹ Am	59.5	203.7	0.00118	0.00119	1.32	5.03
²⁴¹ Am	59.5	403.7	0.000317	0.000323	1.90	5.01
¹⁰⁹ Cd	88	103.7	0.00832	0.00660	-20.68	4.26
¹⁰⁹ Cd	88	203.7	0.00249	0.00200	-19.70	4.24
¹⁰⁹ Cd	88	403.7	0.000693	0.000537	-22.55	4.29
⁵⁷ Co	122.1	103.7	0.00974	0.00947	-2.82	3.01
⁵⁷ Co	122.1	203.7	0.00292	0.00288	-1.51	3.02
⁵⁷ Co	122.1	403.7	0.000814	0.000793	-2.57	3.01
⁵⁷ Co	136.5	103.7	0.00979	0.00979	-0.08	3.47
⁵⁷ Co	136.5	203.7	0.00299	0.00300	0.42	3.51
⁵⁷ Co	136.5	403.7	0.000826	0.000836	1.21	3.48
¹³³ Ba	276	103.7	0.00724	0.00750	3.53	6.56
¹³³ Ba	276	203.7	0.0023	0.00239	3.79	6.59
¹³³ Ba	276	403.7	0.000655	0.000681	3.96	6.59
¹³³ Ba	302.9	103.7	0.00667	0.00658	-1.32	5.89
¹³³ Ba	302.9	203.7	0.00213	0.00212	-0.64	5.90
¹³³ Ba	302.9	403.7	0.000609	0.000603	-0.99	5.90
¹³³ Ba	356	103.7	0.00595	0.00616	3.47	5.83
¹³³ Ba	356	203.7	0.00191	0.00197	3.38	5.84
¹³³ Ba	356	403.7	0.000548	0.000565	3.08	5.84
¹³³ Ba	384	103.7	0.00563	0.00550	-2.35	5.51
¹³³ Ba	384	203.7	0.0018	0.00176	-2.38	5.52
¹³³ Ba	384	403.7	0.000519	0.000502	-3.34	5.52
¹³⁷ Cs	661.7	103.7	0.00368	0.00371	0.80	3.02
¹³⁷ Cs	661.7	203.7	0.0012	0.00120	0.39	3.03
¹³⁷ Cs	661.7	403.7	0.000349	0.000349	-0.12	3.04
⁵⁴ Mn	834.8	103.7	0.00311	0.00311	0.11	3.01
⁵⁴ Mn	834.8	203.7	0.00102	0.00102	-0.05	3.02
⁵⁴ Mn	834.8	403.7	0.000296	0.000296	-0.07	3.05
⁶⁰ Co	1173.24	103.7	0.00238	0.00241	1.05	3.01
⁶⁰ Co	1173.24	203.7	0.000798	0.000795	-0.35	3.03
⁶⁰ Co	1173.24	403.7	0.000233	0.000232	-0.28	3.07
²² Na	1275	103.7	0.00221	0.00227	2.69	3.01
²² Na	1275	203.7	0.000747	0.000753	0.78	3.02
²² Na	1275	403.7	0.000221	0.000220	-0.49	3.03
⁶⁰ Co	1332.5	103.7	0.00217	0.00219	0.72	3.01
⁶⁰ Co	1332.5	203.7	-	0.000727	-	-
⁶⁰ Co	1332.5	403.7	0.000215	0.000213	-0.71	3.06

Table 3.4: Peak ratios for selected neutron capture gammas taken at the MIF position facing the reactor. In general the ratios are better reproduced by the simulated gammas from all directions. E = energy, R = ratio, dR = ratio uncertainty.

E [keV]	type	R 0/1	dR 0/1	R 0/2	dR 0/2	R 1/2	dR 1/2
11386.50	data	0.58	0.07	1.28	0.50	2.19	0.90
11386.50	sim through	0.77	0.05	1.49	0.26	1.95	0.37
11386.50	sim all	0.59	0.04	1.08	0.19	1.84	0.34
9718.79	data	0.72	0.35	1.25	1.96	1.74	2.77
9718.79	sim through	0.86	0.05	1.68	0.22	1.95	0.28
9718.79	sim all	0.67	0.04	1.16	0.16	1.73	0.26
8998.63	data	0.67	0.28	1.36	1.41	2.04	2.20
8998.63	sim through	0.97	0.08	1.88	0.26	1.93	0.30
8998.63	sim all	0.75	0.05	1.24	0.14	1.65	0.22
7724.03	data	0.87	0.27	1.85	1.49	2.12	1.79
7724.03	sim through	1.11	0.07	2.09	0.21	1.88	0.23
7724.03	sim all	0.85	0.05	1.49	0.15	1.75	0.20
7693.40	data	0.99	2.40	1.52	7.28	1.55	7.98
7693.40	sim through	1.15	0.08	2.08	0.20	1.81	0.21
7693.40	sim all	0.86	0.06	1.45	0.14	1.68	0.19
7645.58	data	0.86	1.56	1.53	6.45	1.78	7.90
7645.58	sim through	1.16	0.09	2.17	0.24	1.88	0.25
7645.58	sim all	0.89	0.05	1.48	0.15	1.67	0.20
7631.18	data	0.90	1.44	1.83	7.09	2.04	8.30
7631.18	sim through	1.14	0.07	2.13	0.21	1.87	0.22
7631.18	sim all	0.87	0.05	1.49	0.16	1.70	0.21
6809.61	data	1.02	1.93	2.13	6.83	2.08	6.88
6809.61	sim through	1.34	0.09	2.42	0.20	1.81	0.19
6809.61	sim all	1.05	0.07	1.70	0.17	1.63	0.20

of the detected photopeak as a function of energy for both cases. By normalizing to the total surface area of the flux in both cases we can interpret the ratio of the two curves as the relative probability that a gamma will be detected passing through the collimator versus coming from a random direction. This shows maximal effectiveness of the collimator at low energies, with about an 80 times higher normalized rate at 50 keV, and a minimal effectiveness at 2000 keV with only a 12 times higher probability of gammas being detected through the opening. The collimator is relatively more effective at energies higher than 2000 keV because the gammas coming in from the side are less likely to be fully absorbed in the detector than coming in from the front due to the shorter path length through the crystal which outcompetes the larger probability of passing through the lead.

3.7 PROSPECT Gamma Background

Source calibrations with the PROSPECT detector rely on source feed-throughs which allow radioactive source capsules to be placed in between segments at any position along their length. This is described in more detail in the chapter describing the PROSPECT experiment, section 4.4. A planned upgrade to the PROSPECT experiment will not utilize these source feed-throughs, opting for a simplified enclosure for the liquid scintillator volume. This means that energy calibrations will have to be done with sources external to the detector.

In this section we explore if there are features in the gamma background at HFIR that can be used to aid the energy calibration of a future experiment.

3.7.1 Gamma Measurements at PROSPECT Boundary

Gamma measurements were made at the boundary of the PROSPECT inner scintillator volume as described in section 3.4. This section showed how the rates throughout the region of the PROSPECT detector varied, as seen in figures 3.10 and

3.11. A comparison of energy spectra taken with the collimated Ge detector at two locations along the PROSPECT boundary is displayed in figure 3.18. This shows that not only are the background rates changing as a function of position, but so is the relative energy spectrum. This is due to the varying sources of background within the vicinity.

From studying the spectra at the MIF location and the HB4 hotspot (see figure 3.7 for the gamma spectra), we see that gammas coming from HB4 do not have lines from neutron capture on Be, Cr, Cu, or ^{59}Ni . Conversely, no Ti lines are seen in the spectra coming from the reactor. Additionally, the Al and Fe lines which are dominant will be present in varied amounts depending on the location due to the varying amounts and compositions of structural material throughout the building.

For these reasons, the gammas present throughout the PROSPECT volume will vary in energy composition. This makes it challenging to precisely simulate the features of the PROSPECT gamma spectrum. However, as is clearly indicated in the high statistics spectrum taken at the MIF location, the $^{59}\text{Ni}(n,\gamma)^{60}\text{Ni}$ line at 11.39 MeV is the only gamma line clearly visible above 10.5 MeV. The fact that it does not have other reactor related gamma backgrounds at this energy and its high energy far above typical calibration sources (such as ^{60}Co at 1.33 MeV) makes it an ideal feature to use for an additional energy calibration point.

3.7.2 PROSPECT Gamma Simulation

In order to determine the viability of using the ^{59}Ni 11.39 MeV line for calibration, a simulation of the gamma spectrum as taken at the NW location pictured in figure 3.18 was created. This was done by inverting the spectrum using the detector response as detailed in section 3.6 and feeding this gamma flux spectrum into the PROSPECT simulation package which will be described in depth in section 5.3. The NW spectrum was chosen because it was taken close to the reactor and therefore contains some of the ^{59}Ni gammas. It is observed within the PROSPECT data that

a broad peak around 11.39 MeV is visible, but only in a few segments near the North face of the detector and close to floor (recall that the reactor is situated $\approx 5\text{m}$ below the experiment hall). Thus, the NW data is most representative of the gammas that will be seen in those segments.

The result of this simulation is shown in figure 3.19. Features visible in the data energy spectrum are the Compton edges at ≈ 7.8 MeV from neutron capture on Fe and Al, a broader Compton edge at ≈ 9 MeV from the higher energy Fe and Ni neutron captures, and the Gaussian feature at 11.4 MeV from neutron capture on ^{59}Ni . The simulation underestimates the width of this last feature. However, the location of this Gaussian peak should line up between simulation and data if the energy calibration is good. The next section shows the results of these fits.

3.7.3 Simulation Comparison

A Gaussian plus a linear polynomial is fit to both the data and simulation for segments 15, 16, and 30 for the energy range 10.0 to 12.0 MeV. These segments were chosen because they are the closest segments to the reactor that had working PMTs on both ends of the segments for the duration of the neutrino measurement campaign (see figure 5.8 for the numbering scheme of the PROSPECT segments, note that the reactor is down and to the left of this figure). It is found that segment 16 did not have a large enough bump at 11.4 MeV, indicating that this would not be a suitable segment to perform the energy calibration. However, both segments 15 and 30 spectra resulted in fits with centroids matching the simulated energy spectrum. The results of these fits along with the simulation fits are shown in table 3.5.

These fits were performed for three sets of data, one being a week of reactor on data, another 3 weeks of reactor on data, and a third being the same 3 weeks of reactor on data plus a background subtraction with 1 week of reactor off data. This was done in order to see if a week's worth of statistics was sufficient to fit the feature. The background subtraction was performed to check if cosmic backgrounds which

are appreciable at this energy range were large enough to interfere with the fit. As can be seen from the fit results, a week’s worth of data was indeed sufficient. The background subtraction did not appreciably change the fit centroid, indicating that cosmic backgrounds won’t be an issue if this feature were to be used for an energy calibration for a future measurement.

It should be noted that the fit centroids line up well indicating a good match between simulation and data energy scale normalization but the widths do not. This could indicate that the energy source is more downscattered than is being simulated or it could indicate an incorrect energy resolution used in simulation for energy smearing. A study was performed to determine if an incorrect energy resolution scaling could be responsible for the mismodelling at high energies. This is detailed in the next section.

3.7.4 Energy Resolution Study

The energy resolution of the simulated gammas is scaled by a fraction of its nominal value and a grid search is performed to determine the optimal scale factor that minimized the chisquare difference between simulation and data for the energy bins between 10.5 and 12.0 MeV. This is done for several segments in the corner of the PROSPECT detector closest to the reactor excluding the outer fiducial segments. The result of this optimization is shown in table 3.6. Plots of four of the selected segments after optimizing the energy resolution is shown in figure 3.20. After improvements to the energy resolution for this energy region, the simulation and data compare much more favorably with the best χ^2/ndf of 15/15 for segment 45 resulting in a p-value of .45 and the worst χ^2/ndf of 40/15 for segment 29 with a p-value of .0005. The remaining discrepancies are statistically significant for several segments indicating that the incorrectly modelled resolution is not the sole reason for the difference.

Table 3.5: Fit results using a Gaussian plus linear polynomial for the energy range between 10.0 and 12.0 MeV. Varying amounts of statistics were used to test the viability of using this feature for an energy scale calibration which would need to be done roughly every two weeks. Abbreviations used are seg = segment number, On = reactor on live time, off = reactor off live time, C = fit centroid value, dC = 1σ uncertainty in the fit centroid, σ = gaussian width, d σ = 1σ uncertainty in the gaussian width. The chi-square value of the fit is shown in the final column, the number of degrees of freedom is 195.

Seg	On [days]	Off [days]	C [MeV]	dC [MeV]	σ [MeV]	d σ [MeV]	χ^2
15	7.2	—	11.36	0.014	0.32	0.019	461
15	18.7	—	11.33	0.008	0.34	0.011	394
15	18.7	7.4	11.34	0.012	0.35	0.016	320
16	7.2	—	12.71	0.31	1.8	0.4	396
16	18.7	—	12.45	0.039	1.51	0.05	293
16	18.7	7.4	—	—	—	—	—
30	7.2	—	11.34	0.017	0.31	0.02	493
30	18.7	—	11.4	0.02	0.38	0.024	333
30	18.7	7.4	11.42	0.039	0.41	0.046	247
Sim	—	—	11.34	0.011	0.23	0.011	326

Table 3.6: χ^2 values quantifying the degree of compatibility between PROSPECT gamma simulation and reactor off subtracted data between 10.5 and 12.0 MeV for selected segments. χ^2_{smear} shows the comparison after unified resolution smearing of 325 PE/MeV for all segments, χ^2 shows the comparison using the measured resolution of each segment for the simulation smearing, and χ^2_{min} shows the minimized χ^2 value after optimizing the resolution scaling factor f_{res} . There are 15 degrees of freedom in this χ^2 comparison.

seg	χ^2_{smear}	χ^2	f_{res}	χ^2_{min}
15	117	166	0.328	20
16	96	138	0.232	19
17	53	87	0.248	17
18	64	118	0.336	22
29	89	112	0.2	40
30	192	238	0.264	31
31	58	85	0.36	13
43	38	44	0.256	20
45	46	118	0.208	15
46	106	121	0.24	19
57	44	43	0.2	19
58	41	58	0.208	22
59	69	86	0.232	25

3.7.5 Discussion

The simulation energy scale is calibrated with the procedure described in section 5.3.2 and the data energy scale is calibrated as described in section 5.2.5. Since the simulation is already well validated against the PROSPECT data including for the ^{12}B spectrum which goes up to 13 MeV, we can safely assume that a match between the simulated gamma feature and the data would indicate that this is a useful feature to use in the future for an energy scale calibration.

While the centroids of the Gaussian fits tend to match, the large difference in χ^2 between simulation and data needs to be understood before using this as a calibration feature. By varying the energy resolution we find much better agreement indicating that the simulated energy resolution does not scale properly out to large energies beyond 10 MeV. However, this is not the sole source of the discrepancy because the differences in most segments are still statistically significant with p-values < 0.05 . This indicates that both the energy resolution is not properly modelled and the input source term is not accurate. It is possible that the shielding of PROSPECT contains enough $^{10}\text{B}(n,\gamma)^{11}\text{B}$ to see the 7% yield 11.45 MeV gamma line. This would not be measured by the Ge detector since the PROSPECT shielding was no longer present in the room at the time of the Ge measurements. Additionally, the measured Ge spectrum has a very small number of counts in the 10+ MeV energy region. This makes the reconstruction in that region much more uncertain. This also limits our ability to model the energy region accurately in the PROSPECT detector.

3.8 Conclusion

This chapter provided a detailed characterization of the gamma radiation field in the experiment hall at HFIR. The sources of radiation were identified along with their major locations. The beamline 4 source was shown to be the largest component contributing to radiation at the location of the PROSPECT detector after the local

shield wall was placed which greatly mitigated gammas coming directly from the reactor.

Additionally, due to the usage of a high resolution Germanium detector, a source of energy at 11.4 MeV was identified as coming from the neutron capture on ^{59}Ni . This is a source that only is visible from the direction of the reactor. It was shown that this is an isolated gamma which could be useful for helping to constrain the energy scale at high energies for a future detector in the experiment hall. However, more work needs to be done to understand why simulation deviates from data in this energy region before using it in a future calibration.

Finally, an investigation into how low one can lower the backgrounds with the “Russian Doll” shielding setup showed that thermal neutrons become the primary source of background at low energies once gammas have been mitigated with enough lead. Low-Z material such as water is great for attenuating these neutrons. We also show that the thermal neutron flux can vary greatly depending on the activities of the neutron experiments on the floor below. A detailed characterization of the thermal neutron spectrum and its variations with the experimental activity would be required to be able to determine the feasibility of a future $\text{CE}\nu\text{NS}$ measurement at the experiment hall.

Next we will detail the PROSPECT experiment which took place in the experiment hall where the background measurements were performed.

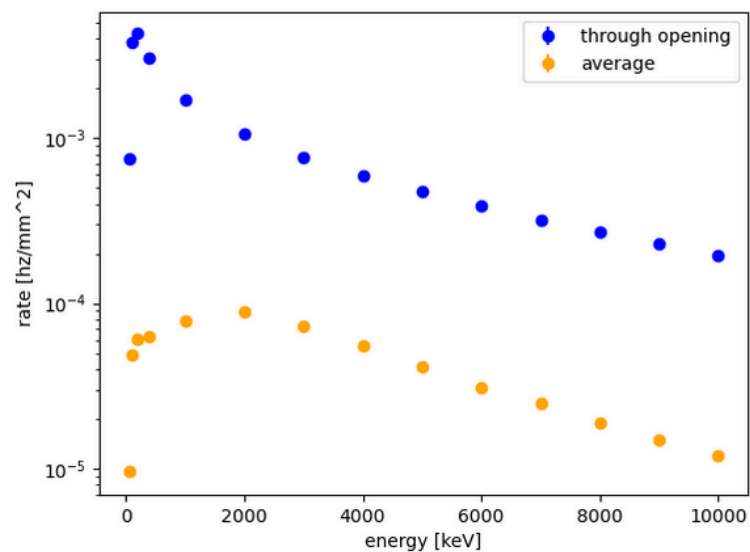


Figure 3.17: Detected rates from a simulated 1 hz/mm^2 gamma flux at different energies. The y axis is scaled by the surface area over which the radiation is coming through in order to show the relative probability of a gamma being detected going through the collimator vs not.

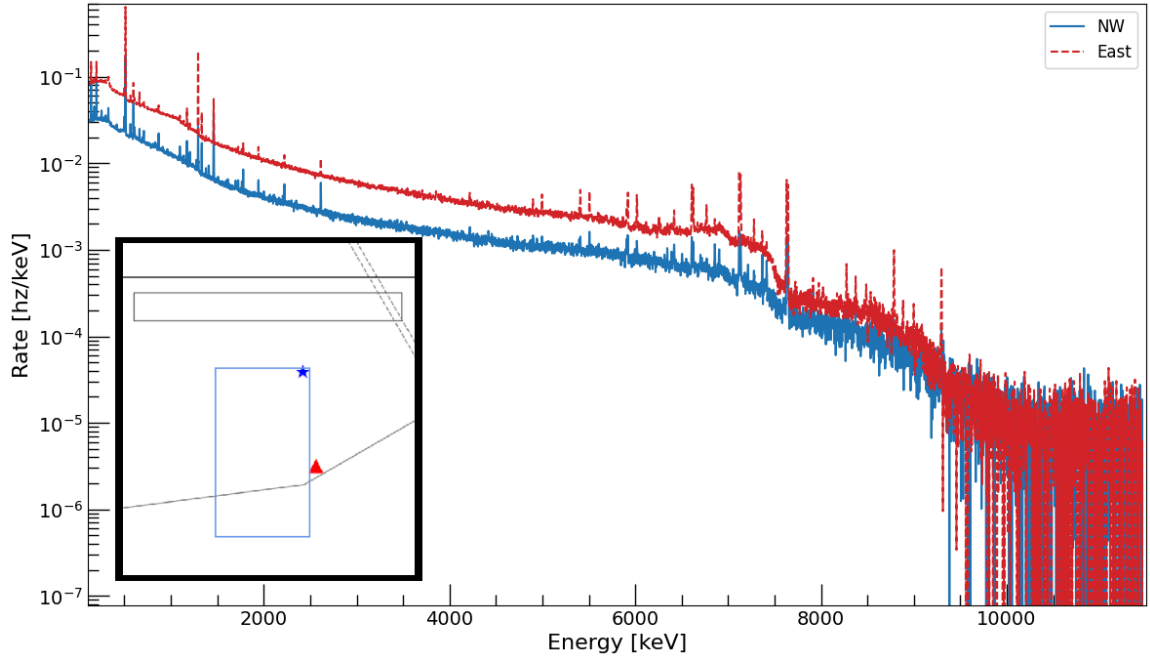


Figure 3.18: Comparison between overnight spectrum taken with the collimated Ge detector at two different locations along the boundary of the PROSPECT detector. Inset shows the location of each measurement with respect to the boundary (light blue), with the solid line above the points representing the reactor pool wall and the grey rectangle the lead shield wall. Dotted lines on upper right is beamline 3 and grey lines beneath the detector region is the monolith boundary. Red triangle indicates the location taken for the spectrum in red (East), blue star the location of the blue spectrum (NW).

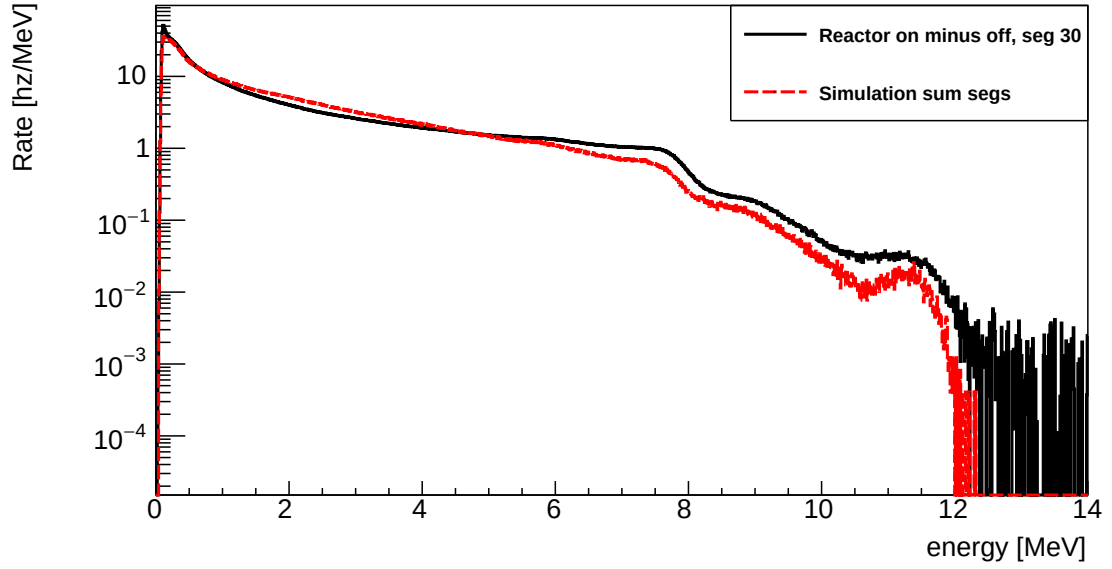


Figure 3.19: Data (black) vs simulation (red) for gamma backgrounds in the PROSPECT detector. The data is gamma energy spectrum in segment 30 from 3 weeks of reactor on data taken in September 2018 with a background subtraction performed using 1 week of reactor off data to remove cosmic backgrounds. Simulation uses spectra taken with the collimated Ge detector at the northwest boundary of the PROSPECT detector as input. Note the simulation uses the sum of all segments spectra in order to save computational time, this is not expected to appreciably change the feature at 11.39 MeV.

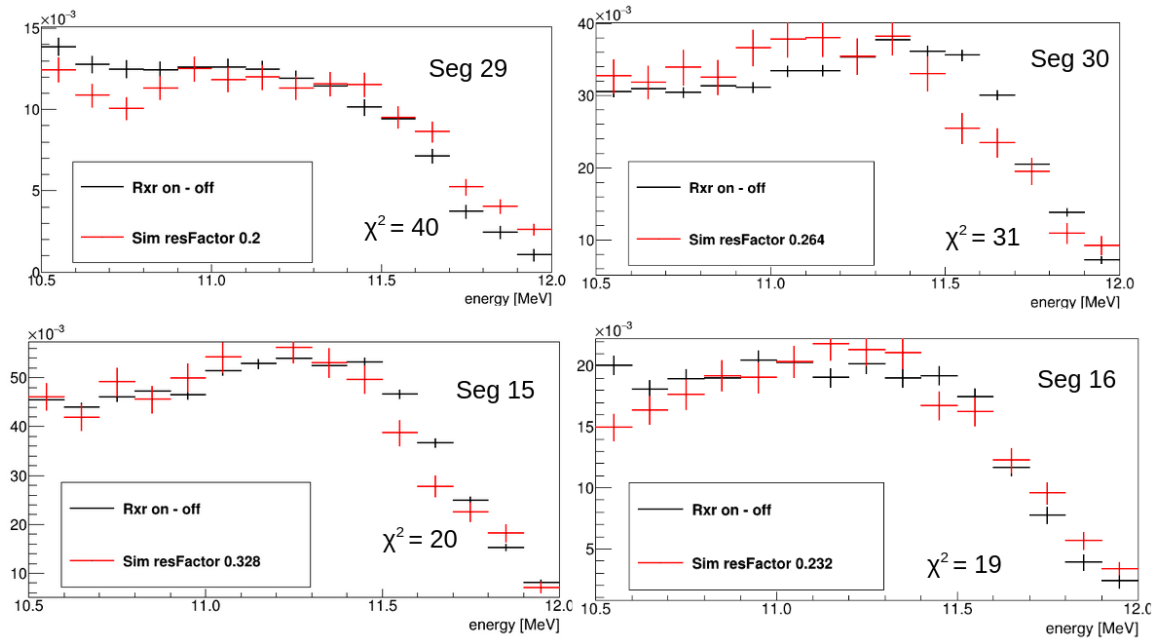


Figure 3.20: Comparison between simulation and data for 4 selected segments after optimizing simulated energy resolution. Resolution factors used for each simulated segment are labelled.

Chapter 4

The PROSPECT experiment

4.1 Introduction

The PROSPECT experiment was designed in order to measure the $\bar{\nu}_e$ flux from the High Flux Isotope Reactor (HFIR) at ORNL and to test for potential sterile neutrino oscillations. The experiment took data in 2018 across five reactor on cycles.

This chapter details the detector construction and its passive shielding. A description of the detection principles is given. Backgrounds due to cosmic ray interactions and accidental coincidences from reactor correlated gammas are described along with a background subtraction method.

4.2 Experiment Site

The PROSPECT collaboration originally considered three locations for its experiment [215]. These were the research reactors at the National Institute of Standards and Technology (NIST), Idaho National Laboratory (INL) and ORNL. HFIR at ORNL was ultimately chosen. With a typical operating power of 85 MW, the reactor is much lower power than commercial reactors. However, the ability to place an experiment close to the reactor (5-10 m) makes up for this in neutrino flux. The close

distance also allows to probe potential neutrino oscillations with lengths on the order of a few meters.

Although the reactor at INL has a larger power of 110 MW, the site resides farther above sea level which results in larger amount of cosmic background radiation. The reactor at NIST typically operates at 20 MW which means a lower neutrino flux would be available for measurement.

Other aspects of HFIR have already been described in the previous chapter and will not be covered here. The next section will detail the unique aspects of the HFIR reactor that need to be taken into account for modelling its neutrino spectrum.

4.2.1 Modelling HFIR Reactor Neutrinos

In section 2.3 we described how the beta decaying products that are not in secular equilibrium must be taken into account when modelling the $\bar{\nu}_e$ from the reactor. This is calculated for HFIR using their fuel composition of primarily ^{235}U based on the procedure in reference [108].

Additionally, $\bar{\nu}_e$ from neutron capture daughters that are being produced in large quantities close to the reactor must be taken into account. It was found that the aluminum in the aluminum-clad fuel will produce an appreciable number of antineutrinos due to the beta decay of ^{28}Al which is produced from the $^{27}\text{Al}(n,\gamma)^{28}\text{Al}$ reaction. ^{28}Al will beta decay with a half life of 2.25 minutes. The beryllium reflector of the core will capture neutrons and produce ^6He from $^9\text{Be}(n,\alpha)^6\text{He}$. ^6He beta decays with a half life of 807ms. Using a model of the core the $\bar{\nu}_e$ contribution can be calculated for these isotopes, and is displayed in figure 4.1 along with the non-equilibrium corrections. The $\bar{\nu}_e$ from these three sources account for less than 1% of the antineutrinos from the reactor.

4.3 Detector Design

The detector consists of 14 (wide) x 11 (tall) optically separated segments of ^6Li doped liquid scintillator. Each segment contains a lithiated liquid scintillator (LiLS) volume with dimensions 0.145 m x 0.145 m x 1.176 m. The total LiLS volume is 1.176 m wide x 2.045 m long x 1.607 m tall consisting of 3760 liters or 3.68 metric tons. The center of the detector is situated 5.09 m above and 5.97 m to the side from the center of the reactor core. See figure 4.2 for a representation of the detector relative to the reactor core.

The LiLS is contained within an acrylic vessel. A layer of nitrogen gas is filled inside the acrylic vessel to allow for the expansion of the LiLS due to temperature changes. Several layers of shielding surround the acrylic vessel to create a nearly hermetic enclosure. The acrylic wall is 0.063 m thick, surrounded by a mixed layer of 0.025 m thick water bricks or 0.025 m thick borated polyethylene, then a 0.025 m to 0.075 m thick layer of borated polyethylene follows and finally an aluminum tank outer wall of 0.025 m thick. Outside of the aluminum enclosure is 0.025 m thick of lead and 0.10 m thick structural polyethylene blocks, then another 0.025 m thick layer of borated polyethylene and then an outer aluminum covering. The materials are similar below and above the detector with more material placed above to shield from cosmic radiation. See figure 4.3 for a schematic depicting the detector and shielding dimensions.

4.3.1 Optical Segmentation

The PROSPECT optical segmentation grid is designed to contain the scintillation light emitted inside the segment and guide the light to the PMTs at the cell ends [216]. For this reason, the panels are opaque so as to minimize cross talk between segments. This allows for a position resolution along x and y to be the length of the segment. They must also have high specular reflectance to light in the 400-550 nm wavelength range which contains the majority of the emitted scintillation spectrum. Simulations

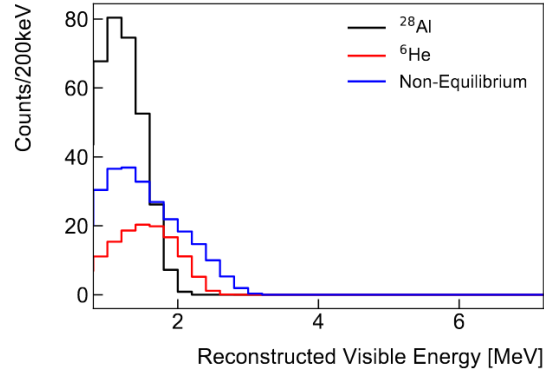


Figure 4.1: Pictured are corrections to the $\bar{\nu}_e$ spectrum at HFIR. Non-equilibrium contributions from beta decaying products with half lives on the order of hours to days are shown in blue. $\bar{\nu}_e$ from beta decaying ^{28}Al and ^6He produced from neutron captures near at the core are also shown. Source: [83].

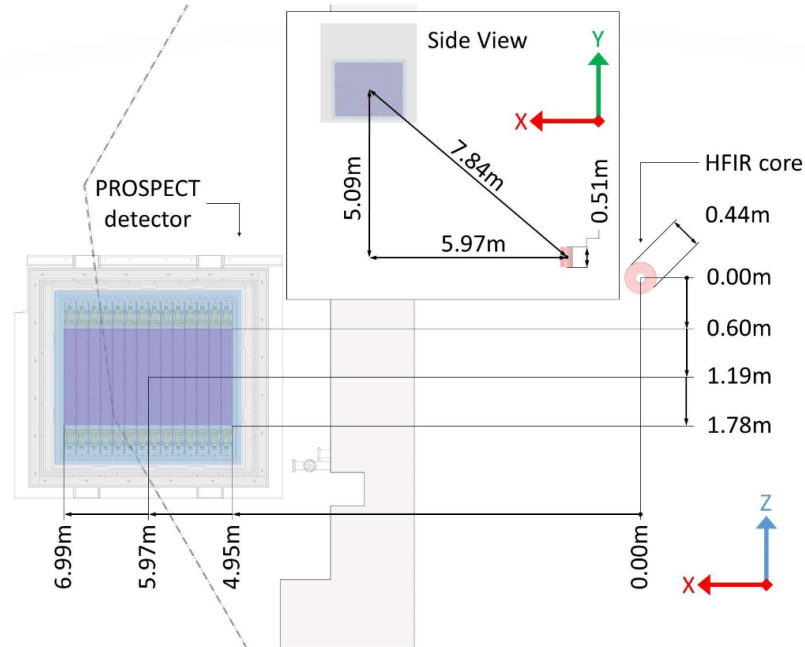


Figure 4.2: Diagram depicting the location of the PROSPECT detector relative to the reactor core. Top down view is shown with dashed line representing the concrete monolith boundary and grey region representing the reactor pool wall. Side view shown in box above. Coordinate system has z along the segment axis and x perpendicular to z toward the reactor with y being the height above ground. Source: [83].

determined that specular reflectance is preferred over diffuse reflectance for the purpose of optimizing light collection at the cell ends, so the organic reflecting film DF2000MA was chosen (see figure 4.4 for the reflectance as a function of wavelength for this material).

The optical grid must also satisfy the requirements that it is low mass in order to minimize energy loss of the positron due to interactions in non-scintillating components, it must be structurally stable, it must not interact with the scintillator, and it must be able to contain pathways for deployment of radioactive calibration sources. For structural stability, a base of 0.6 mm thick sheets of carbon fiber was used. The carbon fiber layer was sandwiched between layers of DF2000MA, an optically clear adhesive, and layers of fluorinated ethylene propylene (FEP). The FEP was chosen to protect the reflective material from the liquid scintillator. The FEP is heat sealed onto the reflective layer with excess amounts around each of the 4 edges in order to ensure total protection of the reflective layer from the scintillator.

The separators were held in place by 3D printed polylactic acid (PLA) rods with a rectangular cross-section shape. At certain points along the length of the rod, segments of the PLA were printed in a pinwheel design which allows the panels to be held together with minimal light leakage. The rectangular cross section allows a pathway for calibration source tubes to be fed through the central axis of the rod. The PLA rods were 3D printed using Fused Deposit Modeling. There were 9 different types of rods depending on the location. Each rod is no longer than 6 inches in length which was a requirement determined for structural stability. The rods are strung together on thin 1.8 m long Polytetrafluoroethylene (PTFE) rods prior to assembly within the detector. The 9 types correspond to standard rods which have 6 mm width pinwheel tabs at the ends and 13 mm width tabs in the middle, central rods which have 1 in tabs designed for inserting optical calibration components, and end rods which have various shaped pinwheel spacers designed to properly space the PMT housings and the separator panels.

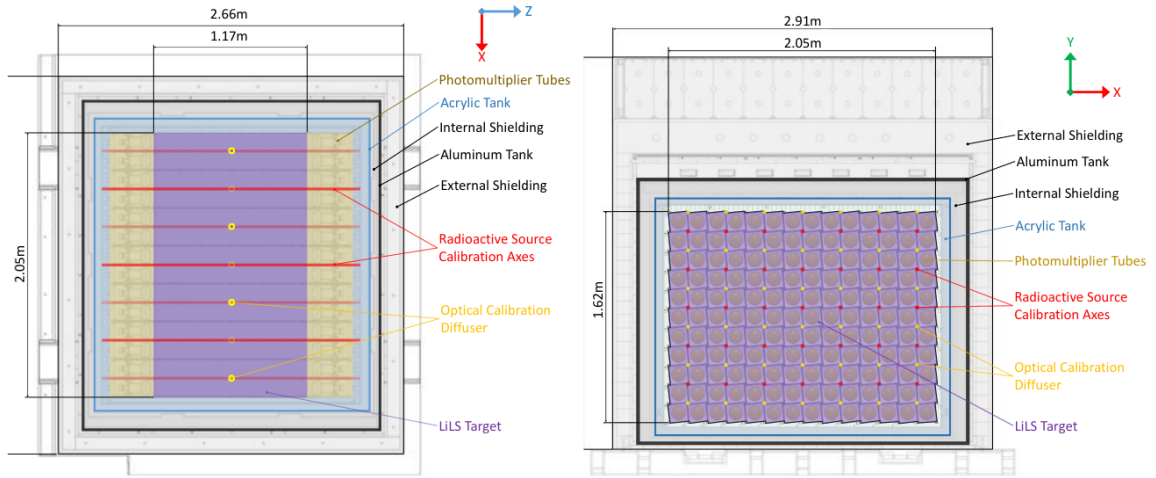


Figure 4.3: Schematic of the PROSPECT detector showing the 14 x 11 segments with reflector panel separators inside acrylic containment vessel. Internal shielding consists of borated polyethylene and water bricks, external shielding consists of lead, borated polyethylene, and water. Source: [83].

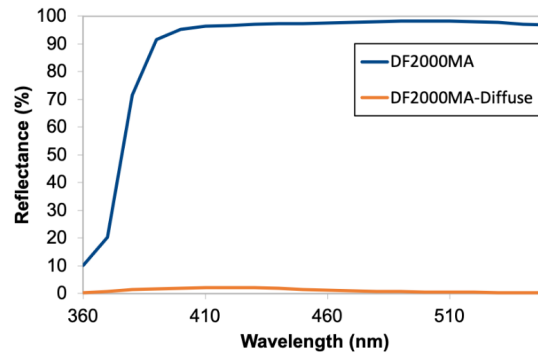


Figure 4.4: Reflectance and diffuse reflectance for DF2000MA as a function of light wavelength. Source: [216]

4.3.2 Photomultiplier Tubes and Housings

In order to obtain PMTs in a timely manner for the experiment start, two manufacturers were used. 240 Hamamatsu R6594SEL PMTs were used in the inner segments which constitute the entirety of the fiducial volume used. The remaining 68 PMTs were ADIT Electron Tubes 9372KB (ET) which were used for the outer left, right, and top layers.

The housing is a 350 mm length rectangular box constructed from acrylic and bonded using Acrifix. The front acrylic window is 13 mm thick and constructed using ultra-violet transmitting acrylic. The back flange is made from black acrylic with a 130 mm hole to allow the insertion of the PMT during assembly. The housings are supported by the pinwheel spacers in the front and the back plug in the back.

A conical light guide is constructed from the same reflective material as the separators on 1 mm thick acrylic. The remainder of the surface inside the housing not covered by the light guide is plastered with rectangular strips of the same reflective material. An acrylic plate at the back of the housing is used to press the round PMT face to the light guide. A conical section of Hitachi Finemet® magnetic shielding material surrounds the PMT. This protects from stray magnetic fields associated with beamline instruments operating in the floor below.

Uniform length (4.88 m) signal and high voltage cables are attached to custom PMT bases. These run to bulkhead connectors mounted on the outer aluminum tank. The housing was filled with mineral oil. See figure 4.5 for a diagram showing the described components in the PMT housing.

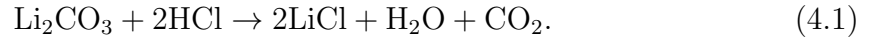
4.3.3 Liquid Scintillator

The base of the liquid scintillator was chosen to be EJ-309 produced by Eljen Technologies [217]. It was chosen to provide excellent pulse-shape discrimination (PSD) capabilities for distinguishing electron-like recoils from nuclear recoils. Additionally, it provides a light yield that meets performance specifications, achieving an energy

resolution of 4.5% RMS at 1 MeV. Note that the reflector panels discussed in the previous section were designed to match the emission spectrum of the scintillator displayed in figure 4.6.

In order to detect the neutron from the IBD reaction, ${}^6\text{Li}$ was infused into the LiLS via a LiCl solution. This was done via the mixture of a nonionic surfactant (an ether-based glycol from DOW chemical) along with a 9.98 mol/L aqueous solution of LiCl [218]. The Li had an enrichment of 95% by atom. These were mixed with 2,5-diphenyloxazole (PPO) and 1,4-bis(2-methylstyryl) benzene (bis-MSB) from Research Product International in the EJ-309 liquid which is based on the scintillator diisopropylnaphthalene. The LiLS in the PROSPECT detector had a doping value of 0.08% ${}^6\text{Li}$ by mass. A combustion analysis of the LiLS found that carbon constituted $84.34 \pm 0.11\%$ by mass and hydrogen $9.69 \pm 0.21\%$. The LiLS density is 0.9781 ± 0.0008 g/cc.

The LiCl was created from enriched Lithium carbonate via the reaction with hydrochloric acid:



The LiCl solution was then filtered through an anion exchange chromatography column which filtered out iron impurities in the form of FeCl_4^- .

The LiLS degrades in air due to the absorbance of oxygen, the effect of which is displayed in figure 4.7. For this reason a cover gas of nitrogen is filled within the acrylic tank at all times.

4.4 Calibration System

Energy and timing calibration was achieved with a combination of optical and radioactive sources deployed via source tubes inside the separator rods, and radioactivity intrinsic to the detector.

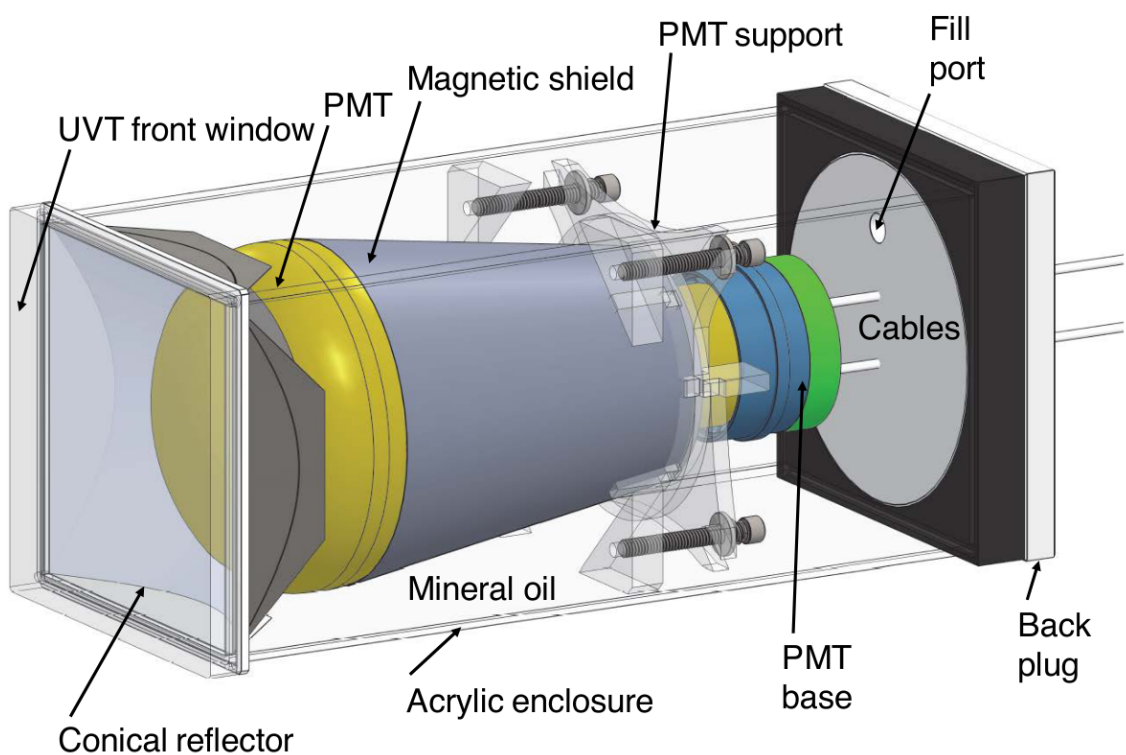


Figure 4.5: PMT housing schematic. Source: [113]

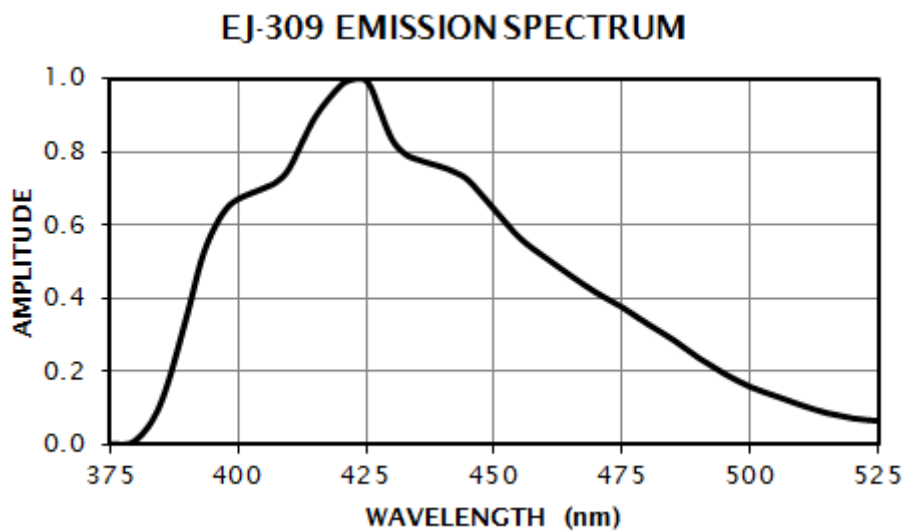


Figure 4.6: EJ-309 emission spectrum. Source: [217]

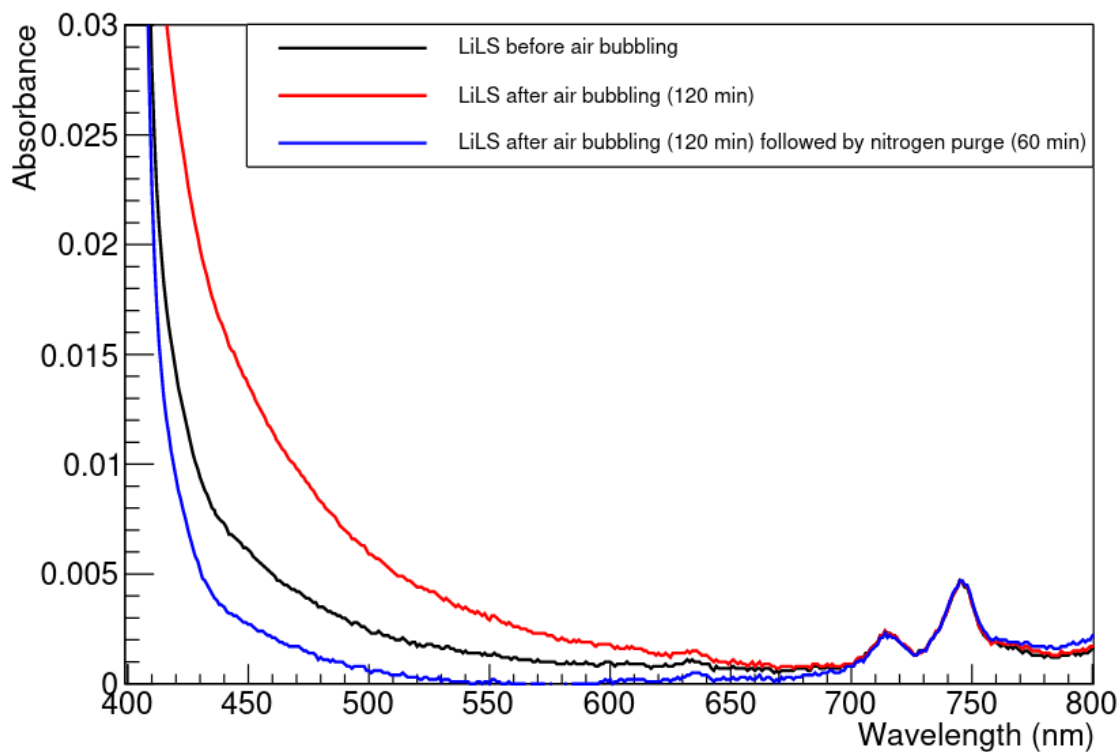


Figure 4.7: Relative absorbance of the LiLS measured after production. Different curves represent the measurement before (black) and after (red) exposure to air, with the blue curve showing the effect of sparging with nitrogen. This shows the effect of scintillator light yield degradation over time due to oxygen contamination. Source: [218]

The optical calibration system (OCS) is used to calibrate the timing differences between segments, the timing difference between West and East PMTs, and the single photon response of each PMT. A Thorlabs LP450-SF15 15 mW fiber pigtail laser pulser shines light into 42 light guides which deliver the light into the pinwheel rod holders. The laser is driven by an AVTECH model AVO-9A4-B-P0-N-DRXA-VXI-R5 driver, which supplies up to 800 mA pulses with 10 ns width and 0.5 ns rise time. The light is split 48 ways with a Thorlabs splitter and 2 of the extra ports are used for monitoring the light output via Thorlabs models PDA10A and PDA8 photodiodes.

A 3.0 m fiber optic cable, model IF 181L-3-0 from Industrial Fiber Optics, runs from each of the splitter ports to a bulkhead outside the detector. Then a set of 5.5 m fiber connected via Icotek fittings run through the openings in the pinwheel rods allowing illumination throughout the detector. A diagram showing the rods which contain the optical fiber and the source calibration tubes is displayed in figure 4.3. Openings within the pinwheel rod shine light into the four surrounding segments of that rod allowing for illumination of all 154 segments.

Varying the laser driver current allows for a single photon mode which is used to monitor the gain of the detector and 100s of photons per pulse which is used to track other properties of the detectors including relative timing offsets, PMT nonlinearities, and scintillator attenuation length.

Radioactive sources are delivered via dedicated source tubes in the other pinwheel rods not being used for the OCS. Toothed drive belts (timing belts) are used to push in and retract radioactive sources through the source tubes. A custom-made 3D printed pulley set on a NEMA 23 stepper motor via a spring-loaded jockey drives the belts. A 3D printed structure guides the belt from the source tube to a storage tube on top of the detector. Microswitches keep the pulley from retracting too far, allowing storage in a home position while also preventing the pulley from extending the track too far along the detector length.

Four sources are deployed along the source tubes. ^{137}Cs and ^{60}Co are used for energy response to gammas rays at energies of 0.662 MeV, 1.173 MeV, and 1.332 MeV. A ^{22}Na source which is a β^+ decaying isotope, is used for the positron energy response at 1.274 MeV and for the 511 keV annihilation gamma energy. Finally, a ^{252}Cf source which decays via fission provides the neutron response.

Intrinsic radioactivity within the detector comes from actinium chloride dissolved within the scintillator. ^{227}Ac was obtained from a commercial vendor and used to produce the solution which was placed in the detector at about 0.5 Bq uniformly dispersed throughout the volume. The decay chain includes a fast double alpha coincident decay from ^{219}Rn and ^{215}Po ($t_{1/2}=1.78$ ms). This allows for understanding the alpha response in the detector which is important in the neutron capture of ^6Li which results in an alpha and triton pair.

Additional useful radioactivity within the scintillator volume comes from β -decays of ^{212}Bi and ^{214}Bi which coincide with subsequent alpha decays of ^{212}Po and ^{214}Po respectively. These sources of bismuth arise from natural radioactivity in the form of ^{232}Th ($t_{1/2} = 14$ Gyr) and ^{238}U ($t_{1/2} = 4.5$ Gyr) respectively. The detector can also measure the well known beta decay spectrum of ^{12}B which arises from the reaction $^{12}\text{C}(\text{n,p})^{12}\text{B}$ within the scintillator due to fast neutrons produced from cosmic ray interactions in the surrounding shielding and building materials. This allows for electron energies up to 13.4 MeV which creates a useful check of the energy scale at the upper end of the energy spectrum. For each of these different intrinsic source decays, a set of analysis cuts can be used to isolate the events based on the energies and particles involved. More details on the analysis cuts used for each source used for calibration is described in section 5.3.2.

4.5 Detector Monitoring

Temperature is monitored with 11 resistance temperature detectors placed throughout the detector. Another temperature monitor is placed between the acrylic and

aluminum tanks to monitor the water. The LiLS and water levels are monitored by ultrasonic sensors placed on top of the aluminum and acrylic tanks.

A liquid nitrogen cover gas is placed above the liquid scintillator in order to prevent oxygen from dissolving into it. A mass flow controller sets the amount of nitrogen into the detector and another mass flow detector monitors nitrogen flow out. A oil filled bubbler monitors the outflow of nitrogen, ensuring that air cannot flow into the system if nitrogen flow were to cease. A combination pressure/temperature/humidity sensor monitors the amount of oxygen and water in the gas outlet. Tubes placed around the perimeter of the LiLS volume allow for the flow of nitrogen gas through the liquid if needed.

4.6 Data Acquisition System

The PMTs are biased by indepent high voltage (HV) supply from several sixteen channel ISEG EH161030n modules. These are housed in two MPOD crates from Weiner. Current and voltage values are monitored and logged via custom software.

Waveform Digitizer Modules (WFDs) are used to digitize the signal coming directly out of the PMT base. 21 CAEN V1725 digitizers were used to process the analog signals from the 308 PMTs. They are operated from Weiner 6023 VME crates. The digitizer have a sample rate of 250 MHz with 14 bits per sample which was determined to be adequate for sampling the timing distribution of the scintillation light in order to achieve a position resolution along the length of the cell that is comparable to the cell width (0.15 m). Optical fiber ran to two CAEN 3818 Optical Controller PCI Express Cards for readout and control of the digitizers. These DAQ computers send data to a 20 TB RAID-6 disk array via Ethernet cable, and to a process which generates plots for live analysis via display on a detector status webpage. The local array transmits data to storage arrays at Oak Ridge and Lawrence Livermore National Laboratory for archiving. The acquisition processes

were coordinated by a run control PC. A schematic showing the data acquisition (DAQ) system is displayed in figure [4.8](#).

4.6.1 Triggering

Most events within the detector will only occur within $< 5\%$ of the segments, therefore it is important to only record signals that contain voltages above a predefined threshold to minimize data storage used. In order to accomplish this, two triggers are used. First, a primary trigger signals if both PMTs of any segment contain a sample exceeding a voltage corresponding to about 5 photoelectrons within a 64 ns coincidence window. This primary trigger causes acquisition of waveforms set to a predefined length of 148 samples from every PMT. Firmware on the DAQ PC will examine the waveforms and compare to a secondary threshold. Samples are only recorded from a single WFD if the signal exceeds a threshold equivalent to roughly 2 photoelectrons. This sample along with the 24 samples before and 32 samples after are recorded.

Times are recorded for each waveform based on the number of digitizer clock ticks from the start of a run. Clock ticks are obtained from daisy-chained PLL-synchronized clocks embedded on the WFD. Timing offsets are calibrated using muon events; this process is described in more detail in section [5.2.2](#).

4.7 Data Processing

Raw waveform data from the digitizers is stored to disk by the two DAQ computers. The data is written in a proprietary CAEN format which was modified to include additional header information and remove data blocks with no waveforms. This process generates 8 different files written in parallel each containing data from two or three WFDs, allowing for the readout of all data from the DAQ without any data loss due to buffer overflows of the on-board memory on each WFD. The data files are then

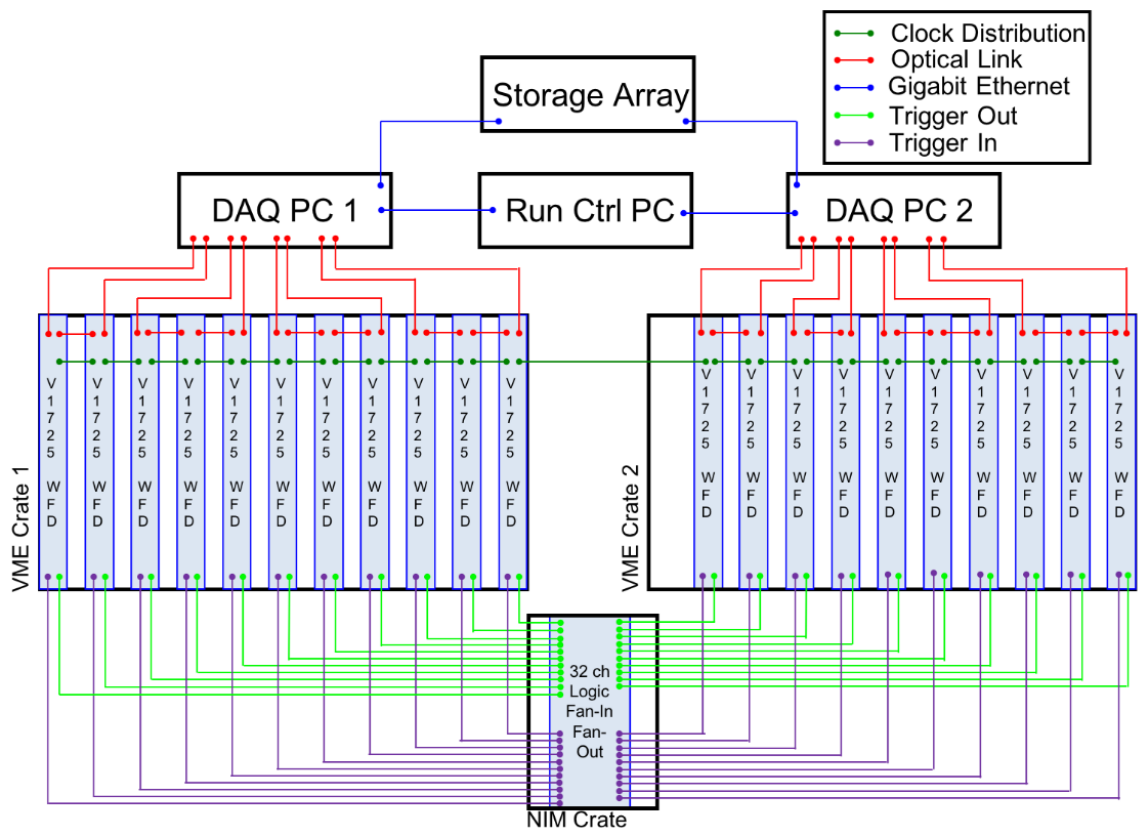


Figure 4.8: DAQ schematic. Source: [113]

collated and time ordered into a ROOT [219] binary file format. Additionally, the mapping between the physical channel numbers of each PMT and the logical channel number relating their position is stored.

Unpacked ROOT files are then processed into uncalibrated waveform data. This is accomplished by analyzing the local maxima within the waveform and generating summaries of information for well separated pulses within a given acquisition window. Timing, pulse area, and PSD are extracted for each pulse. This information is stored in an HDF5 format called a “DetPulse” file. Details on this pulse-level analysis is found in section 5.2.1.

The pulse summaries for each detector are then clustered based on a 20 ns clustering window. Signals within a cluster that match within a segment are paired and physics measurables such as timing, position, energy, and PSD are calculated. This information along with timing differences between PMTs, individual pulse areas, and identified particle type are stored in an HDF5 formatted “PhysPulse” file.

PhysPulse data is scanned for time correlations allowing for various analysis tasks such as IBD selection, Bi-Po correlated signal extraction, ^{12}B beta decay selection, etc.

4.8 Detector Performance Over Time

The data taking period used in the IBD analysis ran from March to October of 2018. Throughout this period there were several PMTs that were turned off due to current instabilities. This was a result of LiLS ingress into the housing of the PMTs. Not all of the seals between the housings and the LiLS volume were robust enough to hold for the several month duration of data taking. This caused leakage into the housing and subsequent seepage into the PMT electronics causing current failures. The working hypothesis consistent with the data is that LiLS which becomes conductive at high voltages due to the LiCl, came into contact with the PMT dividers. Bench tests performed at Yale after the conclusion of the experiment found that LiLS contact

with the high potential step resistors at the top of the divider chain of the divider created a short. This increased current draw. Eventually the solder joints corroded and the entire chip failed.

Due to this issue of LiLS ingress, several PMTs were turned off throughout the run. Only segments with two healthy PMTs could contribute to the IBD statistics, so this directly reduced the possible statistics of the experiment. By October, 46 segments had only 1 active PMT and 9 had no active PMTs. This meant 36% of the segments were unusable for IBD statistics purposes. However, the single-ended (SE) segments (segments with 1 PMT working) were able to aid in background rejection, which is important for maximizing the statistics of the experiment. More information on how this impacted the analysis can be found in section [5.5.2](#).

An additional issue that degraded the detector performance over time was the reduction in overall light collected per energy deposited in the scintillator. By the end of the data taking period, light collection was reduced by 30%. This is depicted in figure [4.9](#).

In order to unify the energy response of the detector over the entire data collection time period, an energy smearing was applied before usage in the IBD analysis. This smearing was set so that every segment would have an effective light collection of 325 photons/MeV. This corresponds to an energy resolution of 5.5% at 1 MeV.

4.8.1 PSD Performance

The ability to distinguish nuclear recoils from electronic recoils is critical in distinguishing the positron-neutron coincidence required for an IBD event. Figure [4.10](#) shows a good separation between ${}^6\text{Li}$ neutron capture events and electron-like recoils.

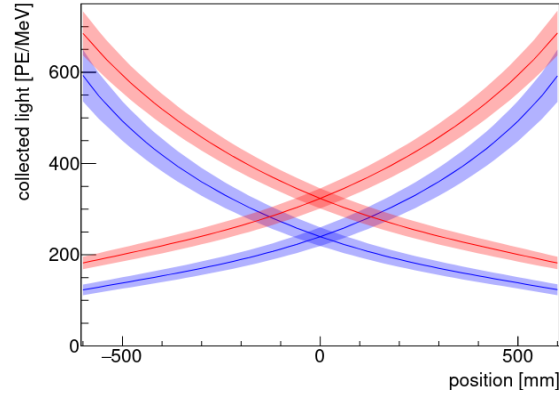


Figure 4.9: Variation in light collection as a function of position along the cell. Error band represents the RMS spread for all PMTs. For a single PMT, the light collection varies by a factor of 5 between events close to the PMT face and events at the opposite end of the segment. Red lines are from data taken in March, blue in September. A 30% reduction in light collection was observed from start to end of the data taking period. Source: [83].

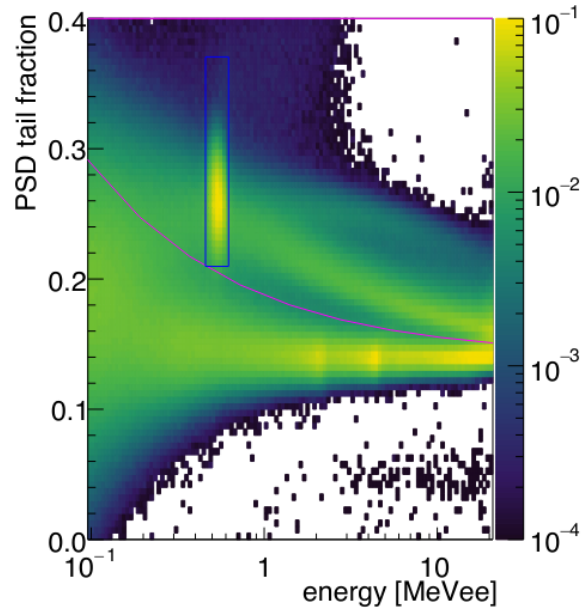


Figure 4.10: Histogram of prompt events selected requiring a delayed neutron capture on ${}^6\text{Li}$. Y axis is tail fraction of the pulse, X axis is reconstructed visible energy. Blue box indicates region of ${}^6\text{Li}$ neutron captures, well separated from electron-like recoils which are events below the red curve.

4.9 IBD Backgrounds

Backgrounds for IBD interactions are those in which an event falling in the electron-like PSD band occurs closely in space and tens of microseconds before a ${}^6\text{Li}$ neutron capture event. It is possible for recoiling protons and for a very small percentage of high PSD gammas in the 0.526 MeV_{ee} energy region of the neutron capture window to mimic the capture signal. This means reactor gamma backgrounds can accidentally coincide with a true or false positive neutron capture signal. These are called accidental backgrounds and are discussed in detail in section 4.9.2.

The other primary source of backgrounds come from events correlated with cosmic ray showers that can produce multiple neutrons sufficient to mimic the topology of the IBD signal within the detector. This is discussed in detail in the following section.

4.9.1 Cosmic Ray Induced Backgrounds

Due to the small amount of overburden at HFIR (~ 1 mwe), the cosmic ray background is intense. In order to mitigate these backgrounds, veto cuts are applied to the data sample as described in section 5.4.1. Backgrounds that sufficiently mimic the IBD signal passing all cuts will then be subtracted off with reactor off collected data sampled before and after then reactor on cycle. A depiction of the prompt energy spectrum for events passing all IBD requirements and cuts is seen in figure 4.11. The peak at 2 MeV corresponds to multi-neutron showers which cause a capture on Hydrogen emitting a gamma ray around 2 MeV, then a second neutron capturing on ${}^6\text{Li}$. The peak at 4.5 MeV is due to an inelastic scattering of a neutron on ${}^{12}\text{C}$ which causes the emission of a 4.43 MeV gamma, followed by a neutron capture on ${}^6\text{Li}$. Both events are typical cosmic ray events that can mimic the IBD signal.

Cosmic background rates scale with atmospheric pressure. As pressure increases, the rates of correlated IBD backgrounds decrease in the detector due to fewer cosmic rays reaching the surface. This relationship is seen in the reactor off measured IBD candidates as a function of atmospheric pressure seen in figure 4.12. A linear fit is

applied in order to correct for pressure differences between reactor on and off so as to properly subtract the reactor off sample. This fit turned out to show a correlation of -0.70 ± 0.01 %/mBar. The scaling between reactor off and on based on the measured rate scaling and pressure differences was found to be $1.00 \pm 0.03\%$.

The rates of other cosmogenic event classes such as muons, neutron captures on ${}^6\text{Li}$ (n-Li), (n-Li, n-Li) coincident events, and (n-p, n-Li) events were also observed as a function of atmospheric pressure. These all showed scaling offsets between reactor on and off within 0.1 % of unity. In order to conservatively estimate the on-off subtraction scaling effects due to atmospheric changes, a 0.5% uncertainty in the atmospheric scaling factor is applied.

4.9.2 Accidental Backgrounds

Reactor related gamma fluxes drive accidental backgrounds due to their high rate. The spatial variation and origin of these gamma backgrounds are explored in detail in chapter 3. Gamma rays cannot be distinguished from positrons based on their pulse shape. This is the primary prompt-like signal in the detector. As the scintillator degraded, the ability to reject gamma backgrounds from the n-Li capture region decreased, causing a larger amount of neutron capture-like signals over time. This is illustrated in figure 4.13.

The spatial distribution of the reactor on prompt-like signals is shown in figure 4.14. The orientation is facing the detector from the East, so that the reactor would be below and to the left of the diagram. Rates are higher in the bottom right segments due to neutrons scattering from beamline HB4 as discussed in section 3.4.

In order to properly subtract accidental backgrounds, a 10 ms window between -12 ms and -2 ms of a candidate n-Li event is scanned for prompt-like signals. For the IBD analysis, the window is between -120 us and -1 us for the prompt signal; the accidental window was chosen so that only events uncorrelated with the neutron capture are included. This allows for a high statistics sampling of random accidentals with the

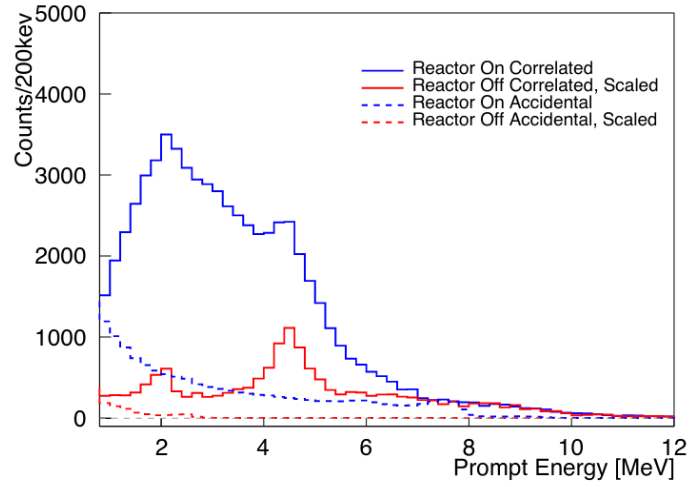


Figure 4.11: Energy distribution of prompt IBD-like signals over the entire data taking after all cuts are applied to both reactor on and reactor off data. The reactor off data (red) is scaled based on live time to match the reactor on data. Correlated signals shown are accidental subtracted.

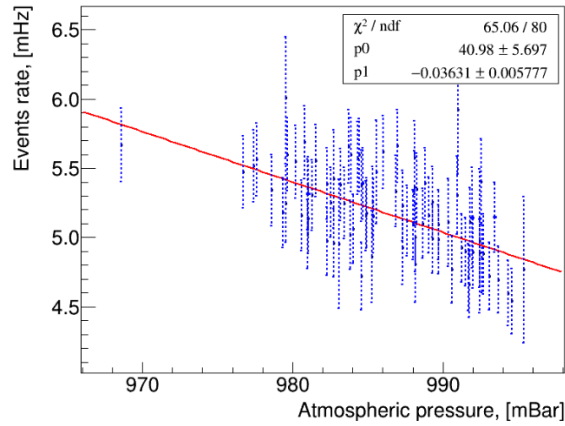


Figure 4.12: Reactor off IBD candidates rates vs atmospheric pressure. Linear fit applied to the data for correcting cosmogenic background rates between reactor off and on measurements. Source: [83]

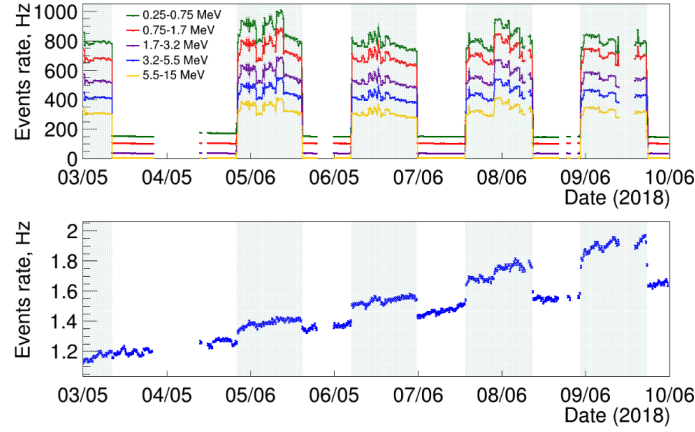


Figure 4.13: Top figure are IBD prompt-like signal rates over time in the detector. Bottom are delayed-like signal rates over time. Variation within the reactor on period occurs due to neutron beam experiment activities causing changing gamma fluxes. The increase over time in delayed-like signals is due to degraded light output over time causing more gammas to fall within the high PSD portion of the n-Li capture region. Source: [83]

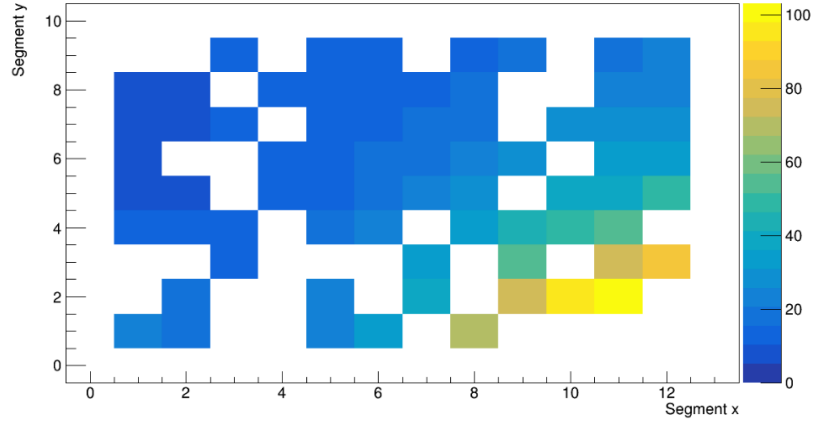


Figure 4.14: Reactor on prompt-like signal rates for each active segment used in the 2020 analysis. Reactor is closest to the bottom left. Rates in the bottom rate are higher due to neutron activation of materials surrounding the neutron beamline 4 beam splitter. Source: [83]

n-Li signal. After scaling for differences in window lengths, the accidental sample is subtracted directly from the IBD candidates. Accidentals are shown alongside cosmic backgrounds in figure 4.11. It can be seen that the accidental rate during reactor off is very close to 0.

4.10 Conclusion

This chapter overviewed the materials and methods of the PROSPECT experiment. It also discussed the data processing flow along with particle identification performance. Finally, the backgrounds for IBD detection were displayed. The next chapter will go into depth regarding the analysis procedure for both the energy spectrum and the sterile neutrino search.

Chapter 5

PROSPECT Data Analysis and Simulation

5.1 Introduction

In this chapter the details of the analysis for the PROSPECT experiment are described. We begin with a description of the types of PMT signals that are acquired and how those are processed. We discuss the clustering procedure of these signals to correlate signals across segments that have a common origin. Timing, position, energy, and pulse shape calibration techniques are detailed.

Next we discuss the issue of the changing detector configuration over time due to issues with scintillator leaking into PMT housings with caused PMT failure throughout the run. We discuss how the dataset was split into different periods each with their own detector response matrix in order to handle the changing list of active PMTs. We also show that segments with single live PMTs can be used for background rejection.

Finally, we outline the analysis cuts based on the calibrated physics quantities used to select IBD events and reject backgrounds. The uncertainties in this procedure are enumerated and the final spectrum and sterile neutrino search results are presented.

5.2 Low Level Signal Processing

This section describes the acquisition of pulse shape, timing, position, and energy information from the digitized PMT signals.

5.2.1 Pulse Analysis

A detector waveform consists of 148 14-bit samples representing 4 ns width digitization intervals. The PMT signal has a negative polarity so the waveform is first inverted so that larger signals correspond to larger energy depositions. This is scanned for local maxima separated by at least 20 samples. The global maxima is set as a default candidate for a “pulse” while the other local maxima are ordered from largest to smallest. The baseline is calculated from the samples between 5 and 30 before the global maximum sample. The average of the median 8 samples is used as the baseline. This baseline value is then subtracted from every sample in the waveform.

After baseline subtraction, local maxima that are at least 30 ADC units are considered pulses along with the global maximum. Each pulse area is calculated with the 3 samples before and 25 samples after the maximum. Pulse arrival time is calculated by scanning backwards from the maximum to where the sample first crosses 50% of the maximum. The arrival time is calculated via a linear interpolation between the two samples at the threshold. The pulse shape parameter is calculated as the ratio between the tail of the pulse and the full area; the tail consisting of the samples between 11 and 50 after the maximum and the full area consisting of samples 3 before and 50 after the maximum. This specific interval was chosen to maximize the separation between neutron capture on ${}^6\text{Li}$ signals and electron-like recoils in the 0.5 MeV_{ee} region (see figure 4.10 for a sample performance using this algorithm). A sample pulse with the baseline window, integration window, and PSD windows is shown in figure 5.1.

The time ordered pulses for a given run are written into an HDF5 file for further analysis. The next step is to calibrate a set of files so that physics quantities can be extracted and an IBD analysis can be performed.

5.2.2 Timing Calibration

Before being able to extract calibration constants, pulses are clustered in a 20 ns window and pulses from the same segment are paired as described in section 4.7.

Segment timing is characterized by the two variables: the segment time $t^i = \frac{1}{2}(t_0^i + t_1^i)$ and the time difference $\delta t^i = t_1^i - t_0^i$ where t_0^i and t_1^i are the West and East PMTs respectively for segment i . The time difference correlates with position along the cell axis (z position) due to shorter light transit lengths to one end or another depending on the energy deposition location.

In order to determine relative time offsets between PMTs due to cable lengths, PMT electronics, and WFD board clock offsets, clusters are scanned for candidate muon tracks. Muons transiting the detector will deposit energy at roughly the same times minus the muon transit times, thus enough statistics can be used to extract timing offsets. Candidate muons are chosen that contain total signals $> 10^5$ ADC counts and at least 4 paired segment hits. Muons that transit the full width of a segment will deposit $> 10\text{MeV}_{\text{ee}}$ of energy which will create clipped signals due to the gain settings which were optimized for a range up to $14\text{ MeV}_{\text{ee}}$. However, signal from muons crossing through the corners of the segments will produce a wide range of signals within the dynamic range of the PMTs. It turns out that the muon event rate for corner-clipping signals is large enough to gather enough statistics for a full timing calibration within 5 minutes of data taking, meaning each hour run has plenty of statistics for precise timing calibration.

Once enough muon statistics are aggregated, a principle component analysis (PCA) is performed in order to estimate the direction of the muon and the spread of the energy deposited. This PCA analysis is used to further narrow down candidate

events to eliminate multi-component electron showers from cosmic ray interactions. It was found that good muon candidates fell within the region of an RMS spread in track width between 0.2 and 0.4 cell widths and a track length > 4 cell widths.

Once the muon candidates are selected, the hits that are “corner-clipping” are selected by requiring the geometric mean of the two PMT signals to be between 4×10^3 and 5×10^4 ADC counts. Additionally, the distance from the event to the PCA predicted axis in the x-y plane must fall between 0.25 and 0.5 cell widths. This prevents secondary particles from the muon event from being included in the analysis. The final requirement is that the overall trajectory must be downward directed. With this secondary event selection, t_i and δt_i are tallied. The estimated muon transit time dl/c is subtracted from the segment times t_i where dl is the distance between subsequent segment hits projected onto the PCA axis.

The timing differentials between the average event time $\bar{t}_i - \bar{t}_j$ and the average time delta $\overline{\delta t}_i - \overline{\delta t}_j$ forms a set of linear equations with a common offset. The offset for the segment timing is effectively meaningless and can be chosen to be 0. The offset for the differential timing sets the differential timing at the center of the detector. The center of the detector is estimated using the average of the muon paths. This average times are solved using the method of least squares, yielding the segment timing offset $\bar{t}^i$ and differential timing offset $\overline{\delta t}^i$. The reconstructed event timing is then $t_{rec}^i = t^i - \bar{t}^i$ and the corrected time difference is $\Delta t^i \equiv \delta t_i - \overline{\delta t}^i$.

Typical timing differences for segments and PMT pairs are between 10 and -10 ns. The ET and Hamamatsu PMTs have different timing characteristics, with the ET displaying larger variance in timing. Board offsets are in 8 ns increments which largely account for the remaining timing differences. Overall the stability of the timing calibration is such that timing offsets only change for a given segment by less than 1 ns over the course of the data taking period, with ~ 20 ps variations between runs.

5.2.3 Position Corrected PSD Parameter

The PSD parameter varies depending on the location of the energy deposition along the length of the segment. This is due to photon collection effects where more light will reach the PMT face during the tail of the pulse if the deposition is farther away. To correct for this, the same event selection of corner-clipping muons is plotted as a function of Δt . The resulting curve roughly fits the parameterized function $p(1 + d[1 - e^{k\Delta t}])$ where p , d , and k are the constants to be fit for each PMT.

The position corrected PSD value is obtained by subtracting the measured position dependent $pd[1 - e^{k\Delta t}]$ factor. The parameter p represents the center of the PSD distribution for electron-like energy depositions. Proton-like recoils will have a PSD centered at a value larger than p which allows for particle identification. The combined PSD parameter is then the area-weighted average of the two position corrected PSD values for the PMT signals for a given segment.

The long term variation in p , d and k are due to changes in the optical properties of the scintillator. The position dependent terms d and k are always subtracted out, however the long term trend of p sets the center of the electron-like distribution which must be used for PSD cuts. In addition to these parameters, the center of the neutron capture on ${}^6\text{Li}$ PSD distribution is tracked over time. This also gradually lowers, and the neutron capture PSD acceptance bounds changes in correspondence with the gradual shift in its central value.

5.2.4 Position Calibration

As previously mentioned, the Δt parameter contains information on the location that the event occurred within the segment. Additionally, the relative number of photoelectrons collected by each PMT also gives information on the position.

The distribution of these two quantities for a subset of cosmogenic events that are identified as corner-clipping muons are plotted in figure 5.2. The fine scale oscillation in Δt seen is due to light collection decreasing near the pinwheel support

rod clips which are more specularly diffuse than the reflective panels that they hold in place. The pinwheel holders and reflective paneling is described in more detail in section 4.3.1. Because the corner-clipped muon events occur close to these tabs, this light collection effect is more prominently displayed in this dataset than in any other dataset with events homogeneously distributed throughout the detector. The position of the tabs are well known, so the variations in the Δt distribution along with the edges of the distribution corresponding to the 1176 mm cell lengths can be fit to a parameterized model in order to generate “calibration curves” for each segment.

A simple linear plus cubic polynomial was found to be sufficient for fitting the Δt versus true position from the corner-clipped muon events, $z = a\Delta t + b(\Delta t)^3$. This position calibration was able to reproduce radioactive source positions with the calibration tubes described in section 4.4 to within 1 cm. It was also found that relating the log ratio of the two PMT signal areas ($R = \ln \frac{S_1}{S_0}$) with a cubic polynomial of the form $z = a + bR + cR^3$ was sufficient for similar position accuracy.

Approximately two weeks worth of data is sufficient to build enough corner-clipped muon statistics to resolve the fine scale variations due to the pinwheel tabs for each segment. For this reason, the data taking period was divided into 11 different calibration periods for position calibration purposes. The constants for the parameterized fit to the Δt and R distributions are stored in the calibration database for use in the analysis code. It was found that both timing based and signal amplitude based z reconstruction was needed for the highest level of accuracy across all event types. For this reason the event-level position reconstruction metric z_{rec} is computed with a statistically weighted average of the two z estimates from R and Δt .

5.2.5 Visible Energy Calibration

The visible energy metric E_{vis} is a quantity that approximates the visible light produced after scintillator nonlinearity effects but before light transport and PMT electronics effects. This is done by understanding the position dependent light

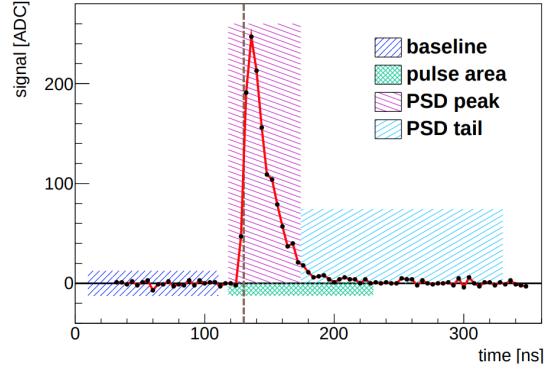


Figure 5.1: Sample baseline-subtracted pulse from an electron-like signal. Source: [83].

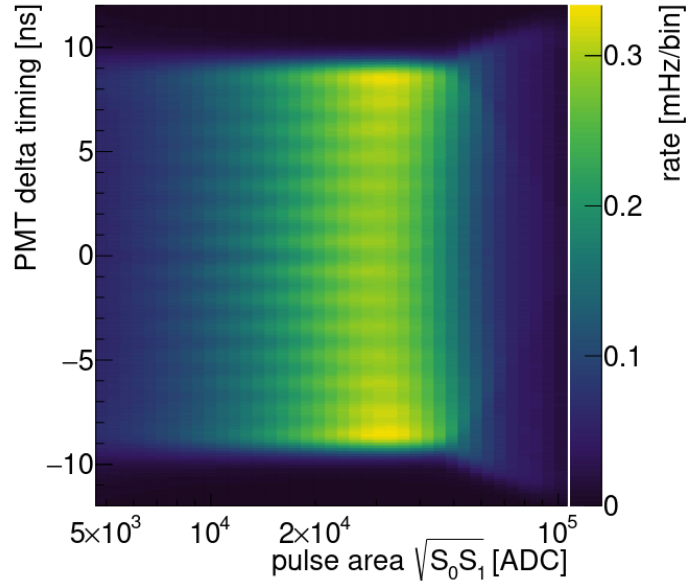


Figure 5.2: Histogram of timing differential between PMTs in a segment and geometric mean of pulse areas for corner-clipped muon events in a calibration run. Approximately two weeks of statistics are used for each position calibration run in order to get enough statistics for dips in spectra correlated with pinwheel tabs. Source: [83]

collection variation which can be calculated from distributions of signal amplitude for well characterized energy sources and the reconstructed position along the cell, z_{rec} . With such a source one can calculate the average pulse area per E_{vis} for each PMT of the event at the segment center which we will label g_i and the position dependent light collection efficiency normalized to 1 at the segment center which we label $\eta_i(z_{rec})$. A third parameter needed is the number of photoelectrons collected per MeV_{ee} of E_{vis} at the cell center which relates to the g_0 by the gain of the PMT. From these we can calculate the visible energy as

$$E_{vis} = \frac{S_0 n_0 / g_0 + S_1 n_1 / g_1}{n_0 \eta_0(z_{rec}) + n_1 \eta_1(z_{rec})}. \quad (5.1)$$

For such a calibration it was found that neutron captures on ${}^6\text{Li}$ were suitable for semiweekly calibrations needed to track PMT gains and light transport effects over time. This is because cosmic interactions generating neutrons produce a steady amount of captures over time with sufficient statistics. Utilizing PSD and time correlations one can cleanly separate this population of events from reactor correlated gamma backgrounds. The light yield from the alpha and triton in the ${}^6\text{Li}$ neutron capture reaction will be quenched due to nonlinear scintillator light production effects and therefor cannot be calculated. Instead, we relate the observed distribution to known calibration sources. This is done by matching the detector response simulation to the calibration sources and using the parameterized fit to determine an absolute energy scale. The detector response simulation is described in more detail in section 5.3. From this procedure we find that the center of the neutron capture peak visible energy distribution corresponds to 0.526 MeV_{ee} .

The center of the neutron capture peak for signals at the center of the cell are used to determine g_i for each calibration period. The full segment-wide distribution of the neutron peak is used to fit the $\eta_i(z_{rec})$ parameter. Meanwhile n_i which relates the number of photons to the visible energy is estimated from the width of the neutron capture peak in S_i space.

As previously mentioned, the scintillator light production properties degraded over the course of the run. In order to avoid complicated time-dependent uncertainties in the calculated IBD energy spectrum due to varying energy resolution, a quantity E_{smear} is used for the IBD analysis instead of the predicted E_{vis} . E_{smear} is simply the E_{vis} with added Gaussian smearing to approximate an energy resolution equal to the lowest resolution segment at the end of the data taking period. This corresponds to an energy resolution of 325 photoelectrons/MeV_{ee}. An illustration of the detector averaged energy resolution over time using E_{vis} and E_{smear} is shown in figure 5.3. This plot was produced by tracking the energy resolution for ^{215}Po produced from naturally ^{227}Ac that was dissolved in the scintillator as described in section 4.3.3.

Another complication related to understanding the energy response of the detector is the varying low energy thresholds across segments and over time. In order to unify this across segments for all periods a 90 keV threshold for the cluster energy (clustering is described in section 5.2.1) is applied in the analysis process. A 5 keV uncertainty for this threshold is used for uncertainty in the energy response.

Calibrated cluster variables are used for the IBD analysis. These are the total visible energy within the cluster, the median timing based on the observed t_{rec} , the z_{rec} and segment of the maximum energy hit detected in the cluster, and the energy weighted PSD of the cluster.

5.3 Energy Response Simulation

In order to relate the $\bar{\nu}_e$ energy $E_{\bar{\nu}}$ to the visible energy seen by the positron in the IBD reaction, a Monte Carlo simulation that accurately reproduces the energy response of the detector to radioactive source calibration and intrinsic background radiation data is used. Geant4 [181] is the simulation package chosen for this task. The simulation code used by PROSPECT is called PG4. This approach is utilized so that energy losses due to energy depositions in the reflective panels, support rods,

and losses to the edges of the detector as a function of energy are accurately reflected in the energy response of the detector.

PG4 uses a fairly accurate model of the detector geometry plus the surrounding shielding. This includes modeling of the panels, support rods, calibration tubes and source enclosures, LiLS volume, acrylic and steel containers, PMT housings and openings, and shielding geometries. Geant4 accurately models radiation transport through the detector and energy depositions within the scintillator are tabulated in an HDF5 file. The scintillation process along with the transport of the produced optical photons from said process are not simulated. This is a very time consuming process to simulate; to simplify this a parameterized model is used to estimate the light production and particle quenching effects.

Geant4 splits each particles track into individual steps in which interactions can occur. The length of these steps is determined by the energy of the particle. The energy deposited in the form of ionization of the medium is tracked at each step and the scintillation energy output at each step is calculated using Birk's empirical model for quenching [220]

$$\frac{dE_{scint}}{dx} = \frac{\frac{dE}{dx}}{1 + k_B \frac{dE}{dx}}. \quad (5.2)$$

At each step i energy deposited in the form of ionization is divided by the distance travelled for that step. The constant k_B is the first-order Birk's constant which is fit to the data.

Additionally, high energy electrons produced from gamma and cosmic interactions will generate Cherenkov radiation in the scintillator. This radiation will subsequently ionize the medium causing scintillation light which is also modelled at the step level with the formula

$$E_c = k_c \sum_{\lambda} N_{\lambda} E_{\lambda}, \quad (5.3)$$

where E_c is the amount of scintillation light energy due to Cherenkov radiation, k_c is a normalization parameter tuned to data set based on the refractive index of the scintillator, N_λ is the number of photon produced at wavelength λ and E_λ is the energy of those photons.

Thus the total energy produced in the form of scintillation light for a given particle track will consist of the summation over all steps i of the Cherenkov and ionization energy produced,

$$E_{MC} = A \sum_i (E_{scint,i} + E_{c,i}), \quad (5.4)$$

where A is an additional constant that is used to scale the overall percentage of energy being converted to scintillation light. This summation is performed for each segment that the particle track deposits energy in.

5.3.1 Detector Waveform Simulation

Using the energy weighted position of the simulated energy depositions along with E_{MC} , simulated waveforms are produced from templates gathered on individual pulses sampled from background data. Templates are averaged pulses for two different PSD values, one low PSD within the electron-like recoil band and one high PSD in the nuclear recoil band. Two template pulses are randomly assigned to each simulated PMT, one at low PSD and one at high PSD.

The PSD for a simulated energy deposition will be calculated based on the $\frac{dE}{dx}$ value in simulation. Larger quenching will result in higher PSD. The PSD values are tuned to match observed cosmic backgrounds and gamma backgrounds.

Once a PSD is assigned based on the simulated $\frac{dE}{dx}$, the position dependent signal area, timing, and PSD values are calculated from inverting the segment's calibration curves described in sections 5.2.5, 5.2.2 and 5.2.3 to obtain the PSD and signal area for each PMT. The high and low PSD template waveforms assigned to each PMT are linearly combined to match this PSD, and scaled and time shifted to match the area and timing calculated. Overlapping energy depositions in time and segment

are summed in the same waveform channel so that pileup is properly simulated. Subsequent analysis of the simulated waveforms proceeds identically to the analysis of real data.

5.3.2 Simulated Energy Response Calibration

In order to find the best set of simulation parameters (k_B, k_c, A in equation 5.4, a grid search was performed to minimize the total chi-squared value of a fit to the observed energy spectra from calibration source deployments of ^{22}Na ($2 \times 0.511 + 1.27$ MeV), ^{137}Cs (0.66 MeV) and ^{60}Co ($1.17 + 1.33$ MeV) at the center of the detector. The multiplicity spectra for each of these gamma sources is also included in the total chi-square minimization. Additionally, the chi-squared value for neutron capture on Hydrogen which produces a 2.22 MeV gamma from a ^{252}Cf source deployed at the center of the detector was also used. Finally, the electron spectrum of ^{12}B which is produced from cosmic radiation was also compared with simulation. The chi-square value is calculated for each histogram with

$$\chi^2 = \sum_{i=1}^n \frac{(W_E w_{Si} - W_S w_{Ei})^2}{W_E^2 \sigma_{Si}^2 + W_S^2 \sigma_{Ei}^2}, \quad (5.5)$$

where the bin values are labelled w , uncertainties σ , and the full sum of bin values W . E labels experiment and S labels simulation variables.

After the minimum χ^2 value is found for the datasets described, the uncertainty in the best-fit parameters is estimated by calculating the variation in the parameters for parameter sets yielding a difference in χ^2 within 30 units of the minimum. For this work the only the points in the k_B, k_c space were varied simultaneously, A was then scaled to best fit the data for each k_B, k_c pair chosen. The choice of 30 units of $\Delta\chi^2$ is conservative to compensate for this simplification. Half the width of the largest variation in these parameters with values yielding a $\Delta\chi^2$ smaller than $\Delta\chi_{min}^2$ is used as the uncertainty in the best fit parameters.

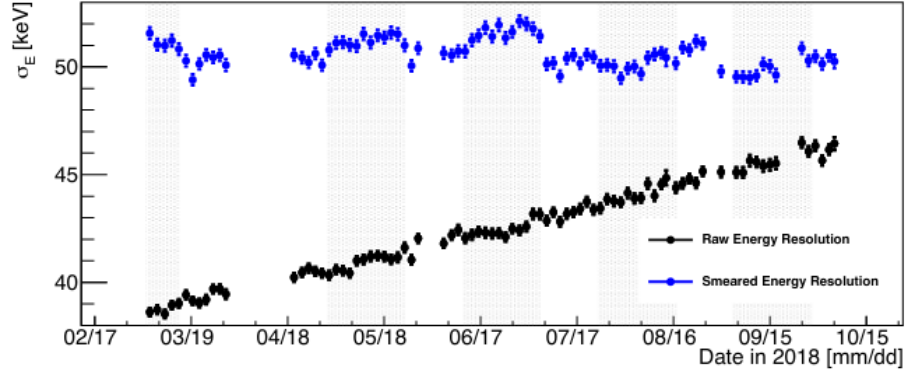


Figure 5.3: Energy resolution σ_E over time for ^{215}Po interaction from $^{219}\text{Rn} - ^{215}\text{Po}$ $\alpha - \alpha$ decays. Blue points indicate resolution after smearing has been applied to make the resolution uniform over time. Source: [83]

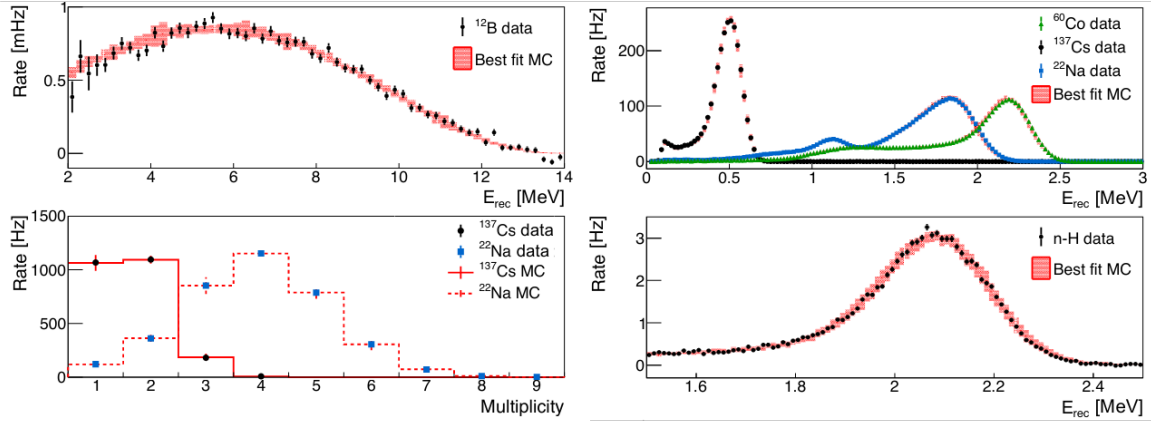


Figure 5.4: Best fit simulation energy and multiplicity spectra compared to data. Source: [83]

The energy response uncertainties are propagated by varying the values within their uncertainties in a number of toy MC simulations. The covariance matrix indicating the uncertainties and cross correlated uncertainties for each energy bin are computed from the variances measured across toy simulations. This does not capture other energy uncertainties such as the dead mass fraction of the scintillator panels which decrease overall energy deposited in the form of detectable light. This is propagated into the energy uncertainty covariance matrix with toy simulations varying the thickness of the reflector panels by 0.3 mm. Additionally, the 5 keV uncertainty in the 90 keV segment energy threshold is also propagated separately with toy simulations. Each of these individual covariance matrices are added together for the final covariance matrix representing the systematic uncertainties for the energy spectrum. This process is described in detail in section 5.6.

5.3.3 Energy Resolution

Energy resolution is simulated based on a parameterized model fit to the deployed radioactive gamma sources:

$$\frac{\sigma_E}{E_{rec}} = \sqrt{a^2 + \frac{b^2}{E_{rec}} + \frac{c^2}{E_{rec}^2}}. \quad (5.6)$$

Figure 5.5 shows the best fit line to the calibration source data. This corresponds to parameters $a = 1.15\% \pm 0.47\%$, $b = 4.61\% \pm 0.24\%$, $c = 0.0 \pm 1.3\%$.

Because the simulation is processed through the same analysis chain as the real data, the resolution is artificially reduced to 325 PE/MeV_{ee}. The uncertainty in this energy resolution is estimated by changing the magnitude of this smearing parameter randomly within 5% of the nominal value and re-doing the analysis repeatedly.

5.3.4 IBD Simulation

IBD interactions are simulated by generating particles at random vertices chosen within the detector given a $1/r^2$ probability distribution where r is the distance from the center of the reactor core to the point chosen within the detector. The vertices are chosen in all regions of the detector simulation that might produce detectable signals including PMT faces, optical grid, and support structures.

For producing IBD detection efficiencies, a simple point-like model of the core is used. For producing realistic IBD distributions for the oscillation analysis, a cylindrical reactor core as described in section 4.2 is used as the source.

The angular distribution in terms of $\cos\theta$ where θ is the angle between the incoming antineutrino and outgoing positron is calculated in reference [221]. The relation to first order in $(1/M)$ is

$$\frac{d\sigma}{d\cos\theta} = \frac{\sigma_0}{2}[(g_V^2 + 3g_A^2) + (g_V^2 - g_A^2)v_e^{(1)}\cos\theta]E_e^{(1)}p_e^{(1)} - \frac{\sigma_0}{2}\left[\frac{\Gamma}{M}\right]E_e^{(0)}p_e^{(0)}. \quad (5.7)$$

Here σ_0 is a normalizing constant, G_V and G_A are the vector and weak axial vector coupling constants, v_e is the positron velocity in units of c , the superscript (1) and (0) represent first and zeroth order in $1/M$, E_e is the positron energy, p_e is the positron momentum, M is the average nucleon mass, and Γ is a kinematic term defined in the reference.

Once the positron angle is chosen, the positron and neutron energies along with the positron angle is used to determine the neutron angle with four-momenta conservation. The distribution in equation 5.7 is mostly oriented reverse of the motion of the incoming neutron for reactor $\bar{\nu}_e$ energies, so positrons will mostly be directed back towards the reactor while neutrons are mostly directed away.

The simulation utilizes two of Geant4’s neutron scattering libraries. G4NeutronHPElastic is used for energies above 4 eV, below 4 eV the G4NeutronHPThermalScattering library is used. Positrons are propagated with the Geant4 default library for electromagnetic interactions, emstandard.

The energy response matrix for antineutrino energy and visible energy as described in section 5.2.5 is constructed by generating random IBD vertices for antineutrinos with energies between the detection threshold of 1.806 MeV and 10.0 MeV. Simulation parameters are tuned as described in the simulation energy scale calibration section, 5.3.2. The events are paired, calibrated and clustered as described in section 5.2.1 and the resulting E_{vis} is histogrammed for each $E_{\bar{\nu}}$ thrown. The energy response matrix used is shown in figure 5.6.

5.3.5 IBD Efficiency Simulation

IBD detection efficiency varies across position in the detector and over time due to degrading optical properties and failing PMTs. Detection efficiency will be lower at the edges of the detector due to neutrons from the origin of the IBD interaction will be more likely to migrate outside of the detectable region. For this same reason, segments with larger numbers of neighboring blind or single-ended segments will also have a lower IBD detection efficiency.

Simulations were performed for ^{252}Cf source deployments within the detector in order to verify the neutron mobility for thermal energies. In order to select ^{252}Cf fission events, a prompt electron-like signal for the resulting gammas and a delayed ^6Li neutron capture event is used. The resulting capture rates for segments containing the neutron capture event as a function of distance from the source was compared to simulation using a custom ^{252}Cf fission generator. Good agreement between simulation and data as pictured in figure 5.7 gives confidence that the simulation can accurately model position dependent efficiency variations due to neutron mobility.

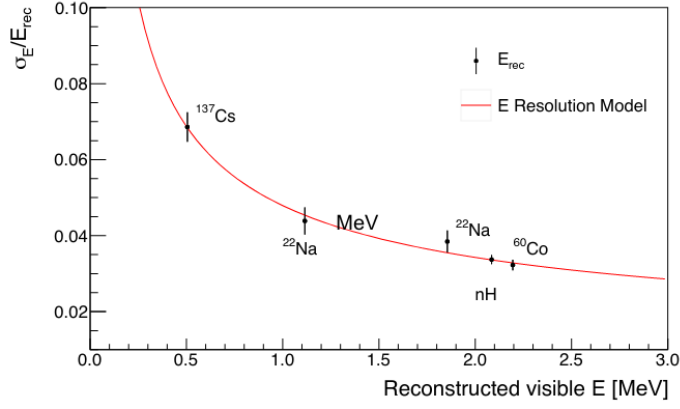


Figure 5.5: Measured energy resolution for different labelled radioactive source deployments at the center of the detector. Line is from parameterized model (equation 5.6) fit. Error bars include systematic and statistical uncertainties.

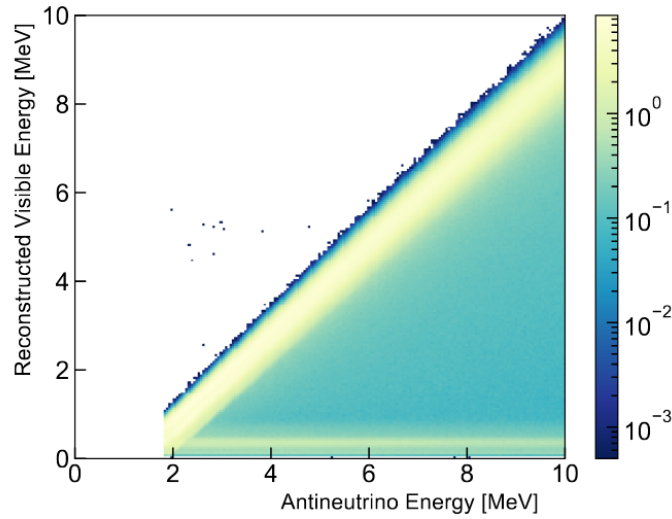


Figure 5.6: Energy response matrix used to translate detected energy into antineutrino energy. The diagonal line corresponds to energies with mostly full positron energy deposition in the LiLS corresponding to positron energy roughly 0.8 MeV below the antineutrino energy. Nonzero values below this line correspond to varying amounts of energy loss possible.

From the IBD simulation generated as described in section 5.3.4, the total number of detected IBD events in each segment after analysis cuts are applied to the simulated data represents the relative segment detection efficiency. The relative IBD detection efficiency for each segment is pictured in figure 5.8. Absolute IBD efficiency is not estimated for this analysis because a measurement of the absolute flux was not a goal of the PROSPECT experiment. However, this is one of the goals of a planned upgrade, PROSPECT2.

Other causes of efficiency variation include uncertainties in relative segment volumes and differences in segment fiducialization. Rather than propagating these uncertainties through the MC simulation, a conservative upper bound on the uncertainties and their impact on the relative efficiencies is instead estimated based on studies. For example, measurements of the optical grid show that segments vary in volume less than 1% of each other. Differences in Z resolution from detected (^{219}Rn , ^{215}Po) events are less than 1 cm across segments which corresponds to less than 2% z fiducialization variance per segment. There is also expected to be small segment to segment variation in PSD performance, which would lead to sub-1% level variations in efficiency. In order to address all of these uncertainties a 5% segment uncorrelated uncertainty is added to the efficiency.

5.4 IBD Selection and Uncertainties

Selection of IBD events requires the detection of a positron energy deposition shortly followed by its annihilation gammas and within a time window of approximately 100 μs a neutron capture signal on ^6Li . The majority of positron events will be confined to 3 segments in the light that they produce. The gammas will deposit their energy within 10s of centimeters of their production location. The positron and gamma events will occur within nanoseconds of each other, which is a similar order of magnitude of the light propagation within a segment. Thus, the positron event will be contained in a single event cluster.

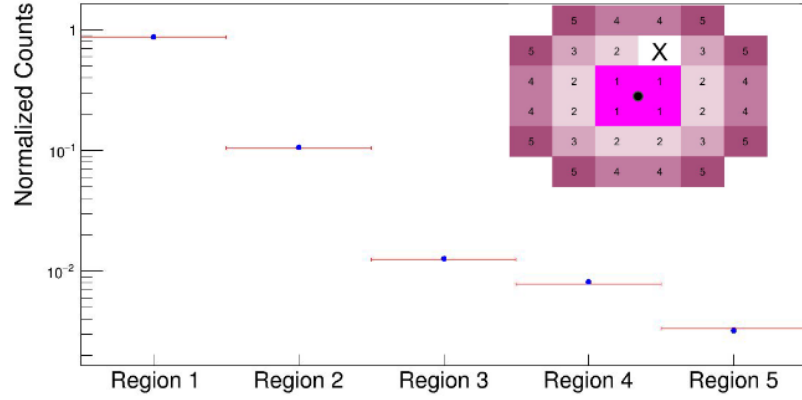


Figure 5.7: Data bins and associated statistical uncertainties pictured for normalized neutron capture event rate from ^{252}Cf source deployment for events selected with a prompt gamma-like event followed by a delayed ^6Li neutron capture signal. Horizontal axis represents the distance from the source deployment, with the diagram in the upper left depicting the segment location for each distance value. Points are corresponding simulated rates. Source: [83]

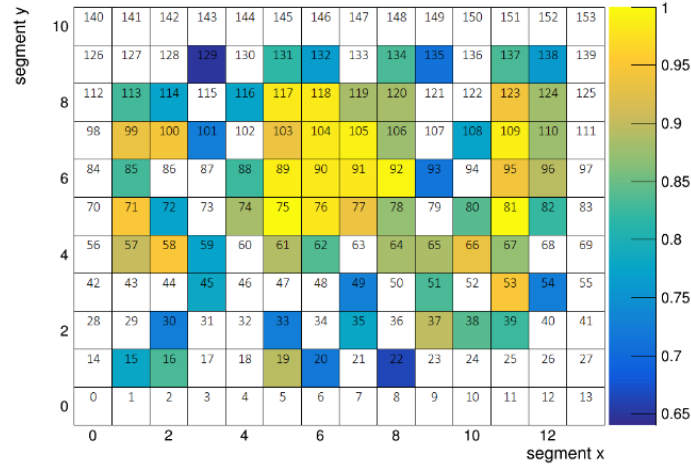


Figure 5.8: Simulated relative detection efficiency for IBD events based on 2020 analysis of PROSPECT data. Segments with no values represent segments turned off for this analysis. Source: [83]

The IBD selection is based on identifying a prompt positron cluster followed by a delayed neutron capture signal. This signal can be mimicked by cosmic backgrounds and accidentals as described in the backgrounds section of the previous chapter, section 4.9. In order to eliminate these backgrounds, a series of vetos are applied to the data. The details of IBD identification and background rejection vetos are described in the following section. The uncertainties associated with the relative efficiencies of this event selection will then be detailed.

5.4.1 IBD Selection

A requirement for a positron event cluster is that all segment PSD values must be within 2.0σ of the energy dependent electron-like PSD band. Additionally, the cluster energy E_{rec} must be between 0.8 and 7.4 MeV_{ee}.

The neutron produced in the IBD interaction will thermalize over the course of tens of microseconds. This thermalization produces a low amount of scintillation light that falls below detection thresholds. MC estimations find that roughly 75% of neutrons produced from IBDs within the detector volume will capture on ⁶Li. This capture reaction produces an alpha-triton pair which will result in an average of 0.526 MeV_{ee} of energy detected in the segment. Thus, the requirements for a cluster considered as a neutron capture signal must have an energy within 2.0σ of 0.526 MeV_{ee}. Additionally, the PSD must lie within 2.2σ of the mean value. In order to ensure the majority of cluster pairs that could be IBDs are considered, a time window between prompt positron and delayed neutron events is chosen to be between 1 and 120 μ s.

The neutron tends to migrate 10s of centimeters before capturing. Thus, an additional requirement between prompt-cluster pairs is that the highest E_{smear} segment must be within the same segment or a horizontally or vertically adjacent segment as the neutron capture. If within the same segment, the neutron capture must occur within 140 mm in z . If adjacent, they must occur within 60 mm in z .

High gamma fluxes from the reactor cause too many accidental signals at the edges of the detector. For this reason, the cluster is ignored if the highest energy segment in the positron candidate cluster is contained within one of the outer segments. Additionally, if the event occurs near the edge of the segment (near one of the PMT faces), it will be thrown out for the same reason. Because of the additional gamma background component from the neutron beamline HB3 which causes larger backgrounds in the southwest region of the detector (see the gamma rates in figure 3.10), events with maximum E_{smear} within segments 24, 25, 26, and 40 were also removed from the analysis. This rejection is called fiducialization. The fiducial z cut accepts events within ± 484 mm of the segment center (recall that the segment length is 1176 mm).

Finally, events that contain energy depositions within single-ended (SE) segments must have SE energy less than 0.8 MeV and a SE PSD within 3.5σ of the SE PSD band. The energy cut attempts to remove events that cannot be 511 keV gammas and the PSD cut removes nuclear recoil-like events. More details on the SE analysis is found in section 5.5.2.

5.4.2 Background Vetoes

As described in section 4.9, cosmic ray showers can mimic the event topology of the IBD reaction. Muons are often present during these showers. Muons can be simply identified by considering any event cluster with at least 15 MeV_{ee} of visible energy, since muons dominate the background in this energy range due to the long tracks of ionization created through the detector. All IBD candidates with a delayed neutron capture time within 200 us after a muon detection are rejected. This removes interaction secondaries from the cosmic ray that may drift into the detector to produce a ${}^6\text{Li}$ capture.

Similarly, events with neutron capture candidates within 300 us of another neutron capture signal are rejected. This rejects multi-neutron showers from cosmic ray

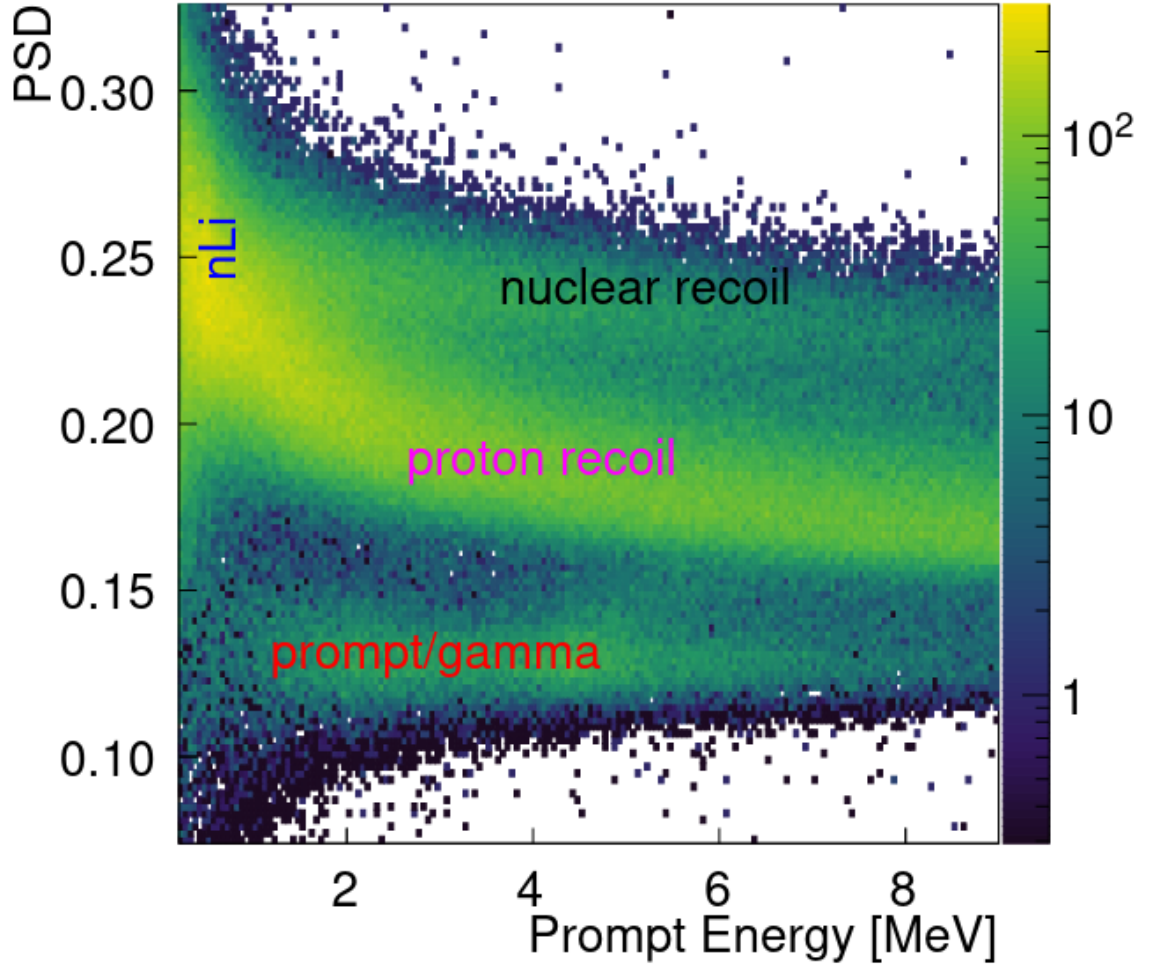


Figure 5.9: Energy PSD distribution of the highest energy segment for prompt clusters within 200 μ s before a ^6Li neutron capture signal. Cosmic ray interactions produce multi-neutron showers which can cause neutron elastic scattering on protons and heavier nuclei in coincidence with a capture event, or two neutron capture events. Regions are labelled based on the types of reactions producing signals there. Source: [83]

interactions in the materials surrounding the detector. Finally, in order to reject cosmic ray interactions that produce heavy secondaries, any nuclear recoil-like signal above $0.25 \text{ MeV}_{\text{ee}}$ in one or more segments will trigger a veto of IBD delay candidates within 200 μs after the recoil event. Recoil events are identified as events with a PSD greater than 2σ of the peak of the electron-like PSD distribution. These three cuts are called “muon”, “neutron”, and “recoil” vetoes respectively. Together, they are called the “cosmic veto”. The energy PSD distribution of prompt clusters for IBD candidates before cuts and vetoes are applied is shown in figure 5.9.

In order to further reduce backgrounds, one can utilize the SE segments to veto recoil-like events in a manner similar to the recoil veto. Using the SE PSD variable, any IBD candidate delay event within 170 μs of a SE segment with a SE PSD greater than 3.5σ above the center of the SE PSD electron-like distribution will be vetoed. This removes cosmic-related background that produce secondaries that only interact in SE segments.

5.5 Analysis Strategy for Time Varying Detector

5.5.1 Data Splitting

Due to scintillator ingress into PMT housings, several PMTs failed throughout the data taking period. Over the course of the production data taking (five reactor on periods), approximately 1/3 of the segments had one or both PMTs fail. In order to maximize the IBD statistics, one must determine the usable segments for each reactor on period. In order to perform a proper background subtraction using the same list of live PMTs for each period, the background data taken before and after each cycle is utilized. This imposes the requirement that in order to consider a PMT live for that reactor on period analysis, the PMT must be alive for both the reactor off periods before and after that on period. The exception is period 1 for which there was no reactor off data before it was taken. In the middle of the reactor off periods

between reactor on periods 1 and 2, 2 and 3, and 4 and 5 there was a calibration data taking campaign. These campaigns form a natural boundary for deciding which PMTs should be considered alive for each period. For the reactor off cycle between period 3 and 4, the boundary was chosen such that the maximum amount of live segment data taking time was found. Based on these criteria, the collaboration came up with the "period splitting" analysis as shown in figure 5.10. One can see that in general the number of dead PMTs grew over time, with the exception of period 1 to 2 in which extra caution was taken when the unstable PMTs first was noticed and more were turned off than necessary.

By splitting the dataset into 5 periods one maximizes the IBD statistics retrieved at the expense of complicating the analysis. Because each period uses a different list of live segments, the efficiency of those segments will be different across periods due to the varying amount of dead material around them. For similar reasons, the energy response and associated uncertainties for the oscillation and spectrum analyses will also be different across periods. Thus, a separate detector response matrix and associated uncertainties for each of the five periods must be calculated. The detector configuration used for each period is shown in figure 5.11.

5.5.2 Single Ended Event Reconstruction

As outlined in section 5.2.1, the timing difference and relative signal amplitudes between PMTs in a segment are critical for reconstructing the position along the segment. With only one PMT operational, the ability to reconstruct z diminishes greatly. This significantly affects the energy estimation of the event due to the fact that a factor of 3 difference is seen in light collected between PMTs for events occurring near the PMT face (recall figure 4.9). On the other hand, the z correction to the PSD parameter is significantly smaller than its correction to energy, making the SE PSD a useful quantity for determining electron-like vs heavier recoiling particles. This is illustrated in figure 5.12 in which detector events are split up based on the three

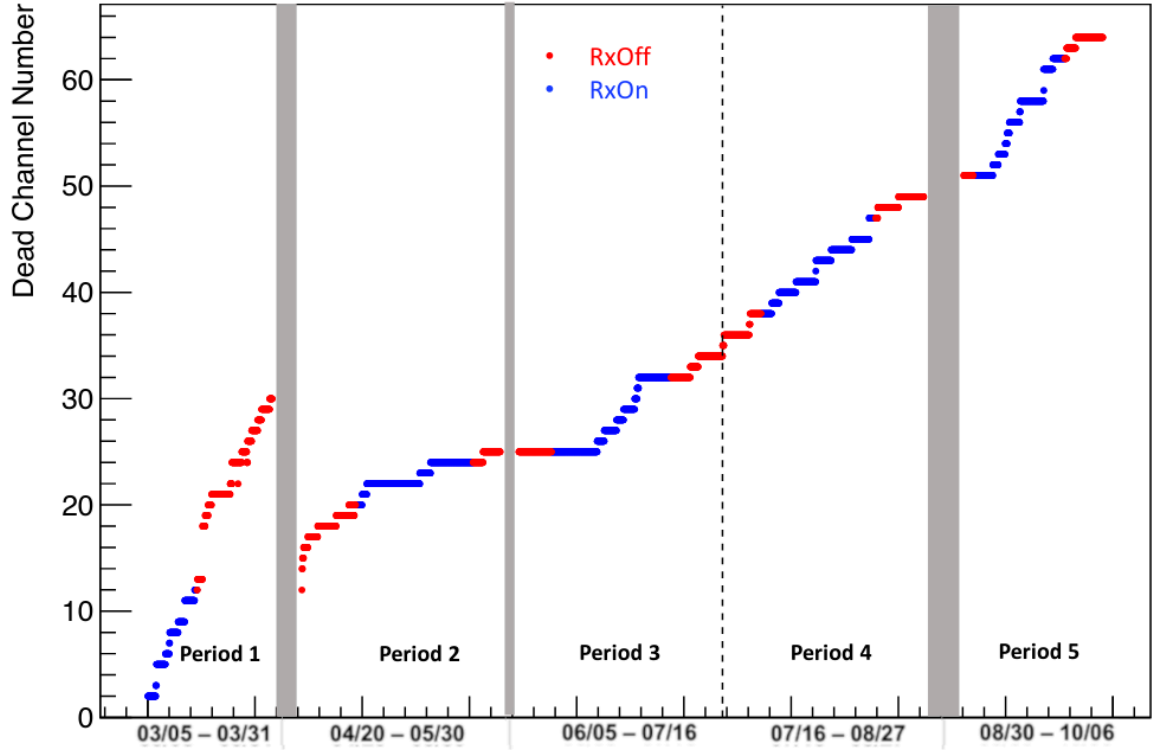


Figure 5.10: Number of dead PMTs over time. Grey regions represent calibration periods which also form boundaries for analysis periods. Dotted line represents the period boundary between 3 and 4 where no calibration campaign took place. Note that for each period the maximum number of dead segments is what was used across the entire period in order to ensure a proper background subtraction. Source: [222]

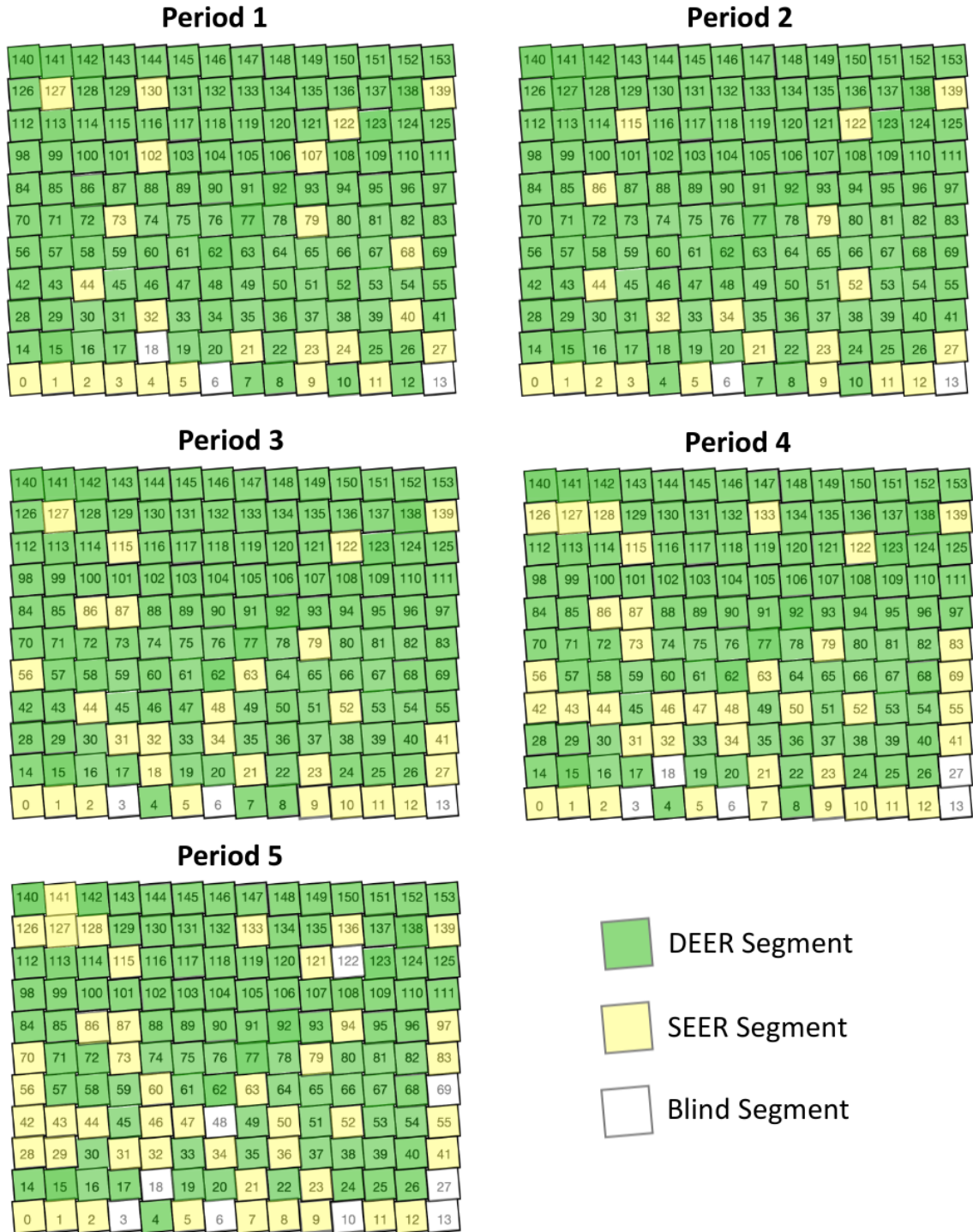


Figure 5.11: Detector configuration used for the 5 period analysis. Each period corresponds to a reactor on data taking period, see figure 5.10 for the reactor on and off data used for each period. Source: [222]

primary classifications of ionization (electron-like recoil band and below), neutron captures on ${}^6\text{Li}$, and heavier recoiling particles. The cuts for these event classes are the same as used in the IBD analysis described in section 5.4.1.

Energy smearing in the SE space makes neutron capture identification impossible as is apparent from the large overlap between neutron captures and recoils seen in figure 5.12. The poor energy resolution makes event reconstruction for IBD interactions occurring within SE segments too unreliable to be useful for additional statistics. On the other hand, since the SE PSD has a degraded ability to separate electron-like and nuclear recoils, a cut rejecting backgrounds based on this variable can be utilized for improved background rejection.

The cut utilized is a two parameter exponential function fit to each SE segment's SE PSD distribution. For seven energy ranges between 90 keV and 10.0 MeV, a Gaussian was fit to the electron-like PSD band. The mean (μ) and standard deviation (σ) of the fits are recorded. The average of the means is stored in the calibration database for each segment. A two parameter function is fit to the σ distribution as a function of energy, $\sqrt{a^2 + b^2/E}$. The best fit across all SE segments is used for the "SE PSD" cut, which checks if the SE PSD is above $\mu_i + n_\sigma \sqrt{a^2 + b^2/E}$, where μ_i is the segment i mean SE PSD and n_σ is the number of sigma above the mean for the cut threshold. It was found that an n_σ of 3.5 was best for determining maximizing the effective statistics of the dataset.

A veto window is also constructed around events containing any segment with SE PSD above the electron-like band. A window length of 170 us after the detected electron-like SE hit was found to optimize effective statistics of the dataset. Any neutron capture-like delay candidates in this window are rejected from the analysis. This is called the "SE recoil veto".

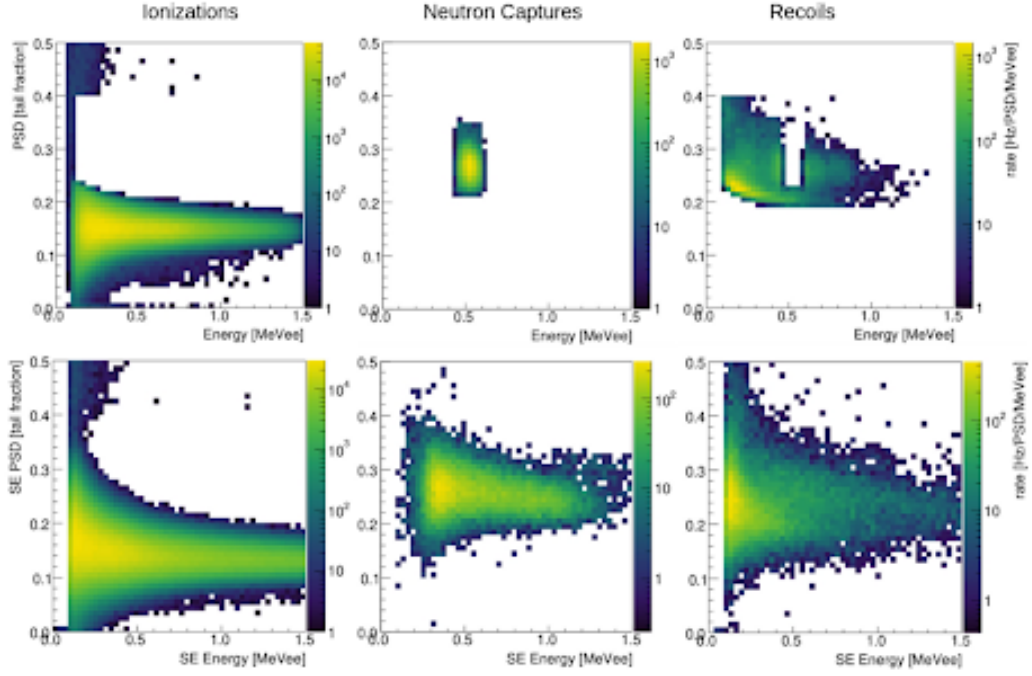


Figure 5.12: Events from a day of reactor on split into ionization, recoil, and neutron capture event classes as described in 5.4.1. Top row are segment reconstructed E and PSD distributions, bottom are SE E and SE PSD distributions. Note the large increase in the spread in energy between the DE and SE variables for neutron captures, making neutron capture identification impossible. Electron-like and nuclear recoil-like bands are still separated, albeit less so.

5.6 Spectrum Analysis

In order to convert detectable visible energy into antineutrino energy, the energy response matrix discussed in section 5.3.2 is used to convert the measured antineutrino energy spectrum. This is performed for each of the five detector configuration periods as described in section 5.5.1.

Because each configuration has a different detector response matrix, a proper treatment of the statistical uncertainties correlated across periods is necessary. This is done with the Wiener-SVD unfolding technique [223]. This smooths out noise amplification effects that are induced when inverting a detector response with its associated uncertainties. The final antineutrino spectrum, Φ is found via:

$$\Phi = C^{-1} \cdot V_C \cdot W_C \cdot V_C^T \cdot C \cdot (\tilde{R}^T \tilde{R})^{-1} \cdot \tilde{R}^T \cdot \tilde{D} \quad (5.8)$$

where C is the 2nd derivative curvature matrix, V_C is the right matrix from a singular value decomposition of $\tilde{R} \cdot C$ and W_C is the Wiener filter. The response matrix $\tilde{R}$ is the stacked responses of the separate periods, and the data matrix $\tilde{D}$ is the stacked data for each period (1-5):

$$\tilde{R} = \begin{pmatrix} \tilde{R}^1 \\ \vdots \\ \tilde{R}^5 \end{pmatrix}, \quad \tilde{D} = \begin{pmatrix} D^1 \\ \vdots \\ D^5 \end{pmatrix} \quad (5.9)$$

The Wiener-SVD method requires an estimate of the true spectrum, which we will denote S . This is used to construct the Wiener filter,

$$W_C = \frac{\overline{R^2 \cdot S^2}}{R^2 \cdot S^2 + \overline{N^2}}. \quad (5.10)$$

N is the expected noise for the measurement. This is taken to be the reactor off subtracted signal. The purpose of supplying the expected signal and noise is so that the unfolding minimizes the unfolded signal to noise across the spectrum.

In the analysis presented here, the expected signal is using the Huber-Mueller model [108] in conjunction with the modelling of the neutrino background sources as described in section 4.2. In order to propagate an associated uncertainty due to our lack of knowledge of the true spectrum, an additional 3% bin-to-bin model uncertainty is added to the toys used in generating the covariance matrix. This follows the method used by Daya Bay’s analysis [224].

In order to calculate a covariance matrix for each period, the detector configuration as shown in figure 5.11 is used for simulations when generating toys that are dependent on the spatial and detector effects of varying dead and SE segments. The Huber-Mueller model IBD spectrum is simulated for each toy while varying the parameter of interest within $\pm 1\sigma$ of the nominal value. The covariance for each toy with respect to the reference model (which is the simulation using the nominal values for all measured parameters) is calculated as $Cov_{ij} = (\hat{S}_i - \hat{S}'_i)(\hat{S}_j - \hat{S}'_j)$, where $\hat{S}(\hat{S}')$ is the visible reconstructed energy spectrum for the nominal (toy) simulation. The index runs over the 5*N energy bins, representing the output histogram for each period PMT active PMT configuration. The visible reconstructed energy is measured between 0.8 and 7.4 MeV in 33 bins. The table of parameters varied is shown in 5.1. Typically parameters were varied several hundred times to produce the final covariance matrix which is an average of the covariances of each toy. The covariance matrix used in the spectrum analysis is the summation of each covariance matrix for the individual parameters listed in the table. The diagonals of the covariance matrices for the various systematic uncertainties is shown in figure 5.13.

The final spectrum after taking into account the full SEER based analysis is shown in figure 5.14. As of the writing of this dissertation, this final result is only available in preprint on the arxiv [222]. In this analysis, we show an improvement over the single period non-SEER analysis of a factor of two increase in effective statistics and a signal to correlated background ratio of 3.81 vs 1.37. The comparison to the Huber-Mueller model is also shown in the figure. The χ^2/ndf value for the comparison between Huber-Mueller model is 28/25 which results in a single-sided P value of 0.31. By

Table 5.1: Systematic uncertainties for which covariance matrices were generated.

Parameter	Uncertainty	Description
Background Norm.	1%	Background variations between reactor off and on periods
n -H Peak	3%	Accounts for uncertainty in background subtraction in n -H peak region
Detector Non-linearity	0.002	Uncertainty in Birks non-linearity energy deposition
Cherenkov Contribution	0.41	Uncertainty on Cherenkov contribution to collected photons
Energy Scale	0.004	Uncertainty on linear energy scale
Energy Resolution	5%	Uncertainty in photostatistics contribution to energy-dependent resolution
Energy Loss	8 keV	Uncertainty in energy lost by escaping 511 γ -rays
^{28}Al Activation	25%	Uncertainty in the ^{28}Al contribution to the spectrum
Non-equilibrium Corr.	25%	Uncertainty in extrapolating $\bar{\nu}_e$ contribution from long-lived fission daughters
Panel Thickness	0.03 mm	Uncertainty in the mass of scintillator separator panels
Z Fiducial Cut	25 mm	Uncertainty in the position of events near edge of fiducial volume
Energy Threshold	5 keV	Uncertainty in the segment-by-segment energy threshold cut

comparison, the χ^2/ndf value when comparing to the Daya Bay measurement [224] is 21.7/23 ($P = 0.55$).

In order to quantify the 5-7 MeV excess, a gaussian was fit to the data/prediction ratio for the Daya Bay measurement with the amplitude, mean, and sigma allowed to float to minimize the χ^2 difference with the HM model. This results in a gaussian with a mean of 5.98 MeV a standard deviation of 0.63 MeV, and a relative height of 13.8%. This Gaussian is then added to the PROSPECT measured data with its amplitude free to vary along with the total normalization, and a minimum χ^2 difference is found with an amplitude of $8.9\% \pm 2.9\%$. This fit is performed in prompt energy E_{vis} space which consists of the 33 energy bins for each period, resulting in a χ^2/ndf of 151.1/163 ($P = 0.77$). A similar fit with the Gaussian mean and sigma allowed to vary to minimize the χ^2 difference directly with the prompt data yields a χ^2/ndf of 148.3/161 ($P = 0.80$), indicating that the shape of the excess is statistically compatible between experiments.

5.7 Sterile Neutrino Search

In order to test for neutrino oscillations, the data was split into 16 energy bins denoted e and 10 baseline bins denoted l for a total of 160 l/e bins. The baseline assignment scheme is shown in figure 5.15. This configuration was chosen so that roughly the same number of events were detected for each baseline.

The background subtracted $\bar{\nu}_e$ spectrum for each baseline bin along with the prediction based on the Huber model with no oscillations as described in section 5.6 is shown in figure 5.16.

In order to test the presence of neutrino oscillations, a χ^2 metric is constructed using the relative difference between prediction and measurement for a given $\sin^2 \theta_{14}$, Δm_{41}^2 pair. The predictions are constructed using a PG4 model which constructs IBD events according to the Huber-Mueller model spectrum and with a $\bar{\nu}_e$ survival probability governed by equation 1.15. Predictions are denoted $P_{l,e}$, measurements

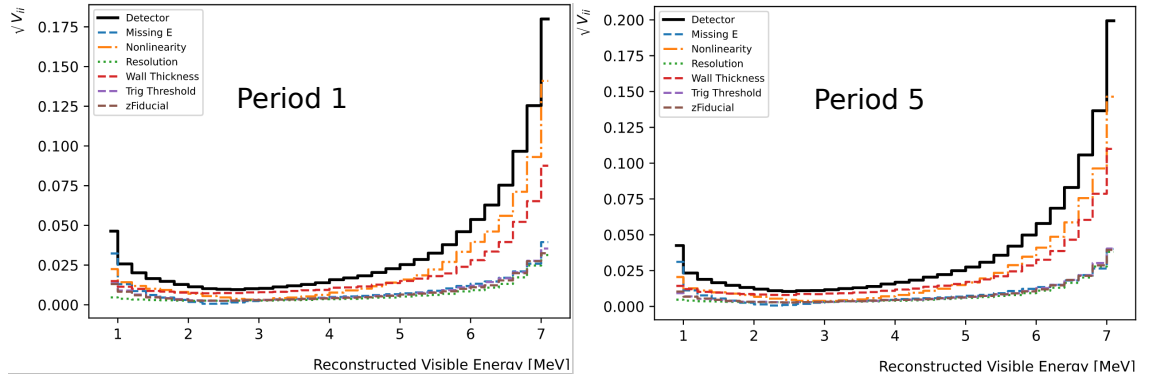


Figure 5.13: Square root of the covariance matrix diagonals for each systematic uncertainty relating to the energy reconstruction. Uncertainties for period 1 and 5 are shown to demonstrate the varying detector response over time.

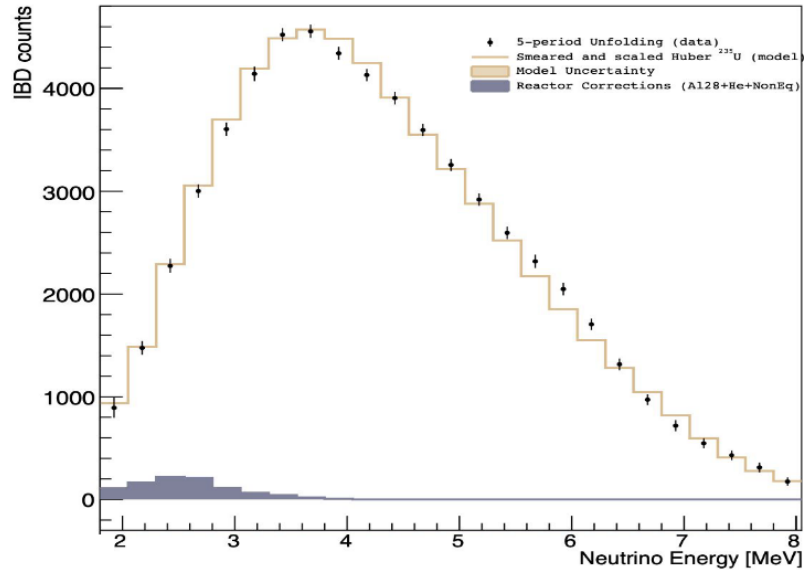


Figure 5.14: Spectrum after 5 period unfolding is performed. The Huber-Mueller model is also shown after being passed through the detector response. The non-equilibrium corrections and contributions from ${}^6\text{He}$ and ${}^{28}\text{Al}$ are shown in grey. A χ^2/ndf of 28/25 (P value = 0.31) is found. The Gaussian-like excess in 6 MeV region is compatible with other ${}^{235}\text{U}$ measurements. Source: [222]

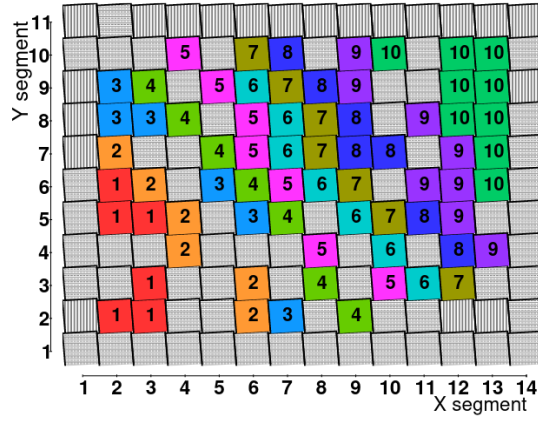


Figure 5.15: Baseline bin assignments for each segment.

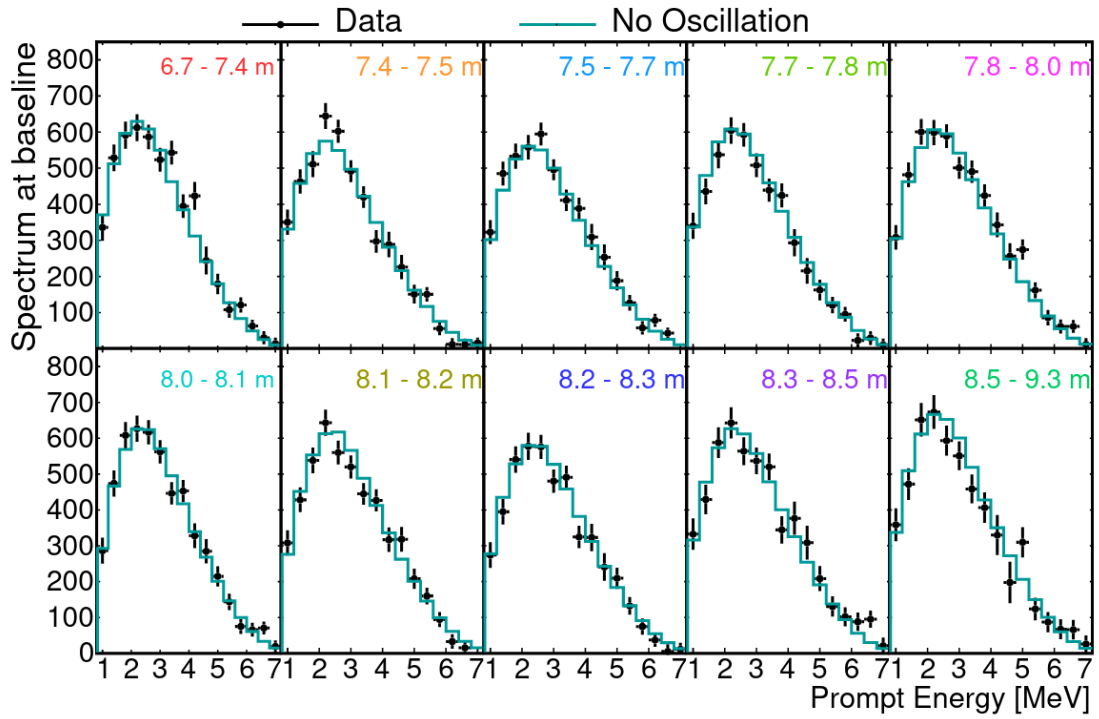


Figure 5.16: Measured $\bar{\nu}_e$ reconstructed energy spectrum for each baseline bin, also depicted are PG4 predictions using the unoscillated Huber-Mueller model.

$M_{l,e}$. The quantity $M_{l,e} - \frac{M_e}{P_e} P_{l,e}$ is used for the comparison, using a relative difference scaled by the total counts in the energy bin e . Here $P_e = \sum_l P_{l,e}$ and $M_e = \sum_l M_{l,e}$. The test statistic χ^2 is then defined as

$$\chi^2 = \Delta^T V_{\text{tot}}^{-1} \Delta, \quad (5.11)$$

where Δ is a 160 element vector composed of the relative differences for each l, e bin and V_{tot} is the covariance matrix consisting of addition of all systematic uncertainty covariance matrices and the systematic uncertainties. V_{tot} is constructed in an analogous manner as for the spectrum analysis described in section 5.6. A table of systematic uncertainties factored into this matrix is shown in table 5.2.

In order to test the statistical compatibility between null hypothesis (no sterile oscillations) and different possible parameters of Δm_{41}^2 and $\sin^2 \theta_{14}$ the Feldman-Cousins and Gaussian-CLS methods for determining exclusion contours in the Δm_{41}^2 - $\sin^2 \theta_{14}$ plane were generated as described in sections 1.7.1 and 1.7.2. This plot is shown in figure 5.17.

The point that minimized the χ^2 is $(\sin^2 \theta_{14}, \Delta m_{41}^2) = (0.11, 1.78 \text{ eV}^2)$ with a χ^2/NDF of 119.3/142. For comparison, the no-oscillation possibility results in a χ^2/NDF of 123.3/144 and the value for the best-fit point of $(0.165, 2.39 \text{ eV}^2)$ in the Mueller RAA paper [108] is 135.1. Using the the Feldman-Cousins approach to test the statistical compatibility of the null oscillation possibility, the $\Delta\chi^2$ between the best-fit point and the no-oscillation model yields a p-value of 0.57 while the $\Delta\chi^2$ for the RAA best-fit point yields a p-value of 0.015, indicating that it is disfavored at the level of 2.5σ .

5.8 Conclusion

This section detailed the various aspects of the analysis of the PROSPECT experiment. A particularly challenging element of this analysis is the detection of neutrinos

Table 5.2: Systematic uncertainties used for the covariance matrix generation in the oscillation analysis. PG4 fluctuated toy simulations are used to determine matrix elements across 16 baseline and 10 energy bins.

Parameter	Value	Uncertainty
Abs Bkg Norm	—	1.0%
Abs n-H peak norm	—	3.0%
Rel. signal norm	—	5%
Baseline Unc	—	10 cm
1st-order Birks	0.132 MeV/cm	0.004 MeV/cm
2nd-order Birks	0.023 MeV/cm	0.004 MeV/cm
Cherenkov contrib	37%	2%
Abs Energy Scale	—	0.6%
Abs photostats res	—	5%
Abs energy leakage	—	8 keV
Abs energy thresh	—	5 keV
Rel energy scale	—	0.6%
Rel photostats res	—	5%
Rel energy leakage	—	8 keV
Rel energy thresh	—	5 keV
Refl. panel thickness	1.18 mm	0.03 mm

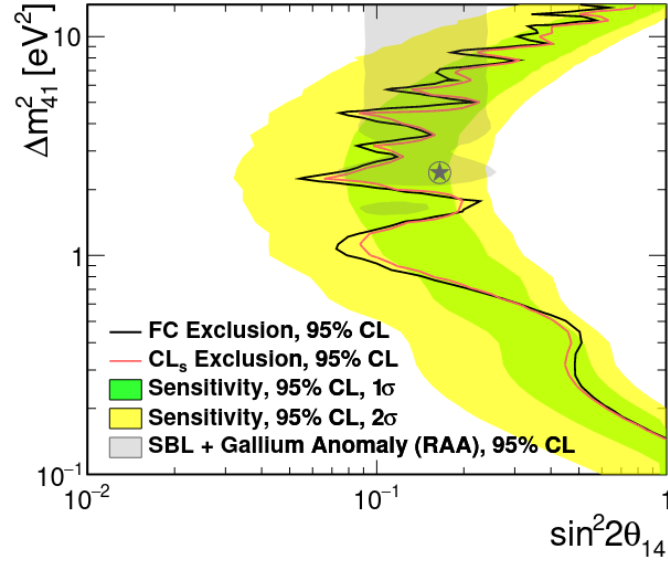


Figure 5.17: 95% exclusion contours generated using both the Feldman-Cousins method and the Gaussian-CLS method. Both show good agreement with one another. Grey region along with stared point are best fit point and allowed regions from short baseline reactor experiments and the Gallium anomaly as depicted in [108]. Also pictured are the exclusion ranges at 1σ (green) and 2σ (yellow) produced by toy MC datasets. Source: [83]

at the surface of the earth amidst a large background of cosmic ray interactions. The ability to distinguish neutron captures from gamma rays and the time correlation between the positron energy deposition and the neutron capture from the IBD is the key to successfully selecting $\bar{\nu}_e$ events.

Because of the issue of PMT failure over time, a five period analysis was performed. Additionally, information regarding the pulse shape of single ended events was shown to have use in background rejection. By incorporating the information of single ended segments and by splitting the data analysis into five periods, significant improvements in the effective statistics and the signal:background over the initial analysis that only utilized the live segments at the end of the full data taking period.

One possibility that was not explored in this analysis is that of reconstructing the position and energy of events that occur in SE segments. This sets the stage for the next chapter which details the work done to try to reconstruct these quantities using machine learning (ML) techniques. It will also describe how ML can be used to aid in particle identification.

Chapter 6

Machine learning techniques for event reconstruction in PROSPECT

6.1 Introduction

Neutrino experiments at a reactor and at sea level with minimal overburden must rely on sophisticated background rejection techniques to achieve requisite levels of signal:background. The details of the methods used by PROSPECT were discussed in chapter 5. What follows is a description of a new technique developed for processing detector signals by utilizing various neural network (NN) architectures.

In this chapter a brief summary of some use cases of machine learning in neutrino physics is given. Then, the two data analysis tasks using ML are described - positron identification and single-ended event reconstruction. Next, a description of each of the neural networks is provided along with the methods of preparing the PROSPECT data for them. This involves regularizing the PMT signals (henceforth referred to as waveforms) before processing them through the network.

The final portion of the chapter details the results from the positron identification study and the single ended event reconstruction (SEER) study. In the case of the SEER analysis, improvements in background rejection over the analysis described in section 5.5.2 are demonstrated.

6.1.1 Machine Learning in Neutrino Physics

With the increase in availability of high performance computing resources [225] and the increase in accessibility of machine learning (ML) algorithms, there has been more interest in applying ML to neutrino physics analysis tasks. For a review of the subject, check out Psihas, et al. [226] ISMRAN [227] is an antineutrino experiment utilizing plastic scintillator for antineutrino detection at a 100 MW reactor in India was able to utilize a multiperceptron layer (MLP) implementation for signal classification [228]. The ANTARES [229] collaboration has utilized a variety of ML classification techniques, including boosted trees and random forest, on extracted features from their acoustic based detector signals.

ORCA, NEOS, DUNE, MicroBoone, and others have successfully used sparse convolutional neural networks (CNN) for event classification and image segmentation. [230, 231, 232, 233, 234] In general, a number of particle physics experiments have found convolutional neural networks useful for signal extraction tasks [235]. For this reason we have decided to investigate the use of CNNs for particle identification and event classification in PROSPECT.

6.1.2 ML Based Particle Identification in PROSPECT

Two major analysis tasks were attempted using machine learning. The first was a look at the possibility of positron identification. In general, particle identification is done using the PSD of the event and comparing to measured distributions for known particle types. In the PROSPECT detector, 5 major event classes were assigned for the purpose of IBD selection. These were labelled electron-like (ionization),

proton-like (recoil), neutron capture on ${}^6\text{Li}$ (ncap), muon, and ingress. Electron-like and proton-like are characterized by their energy-PSD distributions as described in section 4.8.1. Neutron capture events will always fall in the recoil band and will cluster around a mean PSD of ~ 0.26 and a mean energy of ~ 0.5 MeV. Ingress events are those which occurred within scintillator that leaked into the PMT housings. These have very high PSD, destroying the ability to reconstruct the particle type and must be thrown out of the analysis. Muon events are classified simply by energy considerations, since anything above ~ 15 MeV will very likely be a muon passing through several segments of the detector.

Because an IBD consists of a positron and a neutron energy deposition, identifying positrons would be extremely helpful in signal selection given the lack of positrons in background interactions. However, this is not possible with PSD alone due to positrons and electrons depositing roughly the same energy density. The distinguishing portion of the event is the annihilation of the positron which results in two 511 keV gammas. Gammas also have similar PSD as electrons and positrons, and are therefore not possible to distinguish with PSD alone. However, the topology for these events will change due to difference in path lengths for gamma rays versus positrons and electrons. Positrons and electrons will nearly always deposit all of their energy in a single segment, whereas gammas will often scatter in multiple segments. Thus, a neural network may be able to use the event topology to distinguish from these three event classes. This is explored in detail in section 6.5.

Another use case of particle identification for ML is the classification of SE signals. As shown in section 5.5.2, the PSD from a single PMT is still useful for distinguishing ionizations from recoils. ML is also used to perform this task, as described in section 6.2.3.

6.1.3 ML Based SEER Analysis

The other primary use case of ML is for SEER. As just described, one can use ML to predict the PID of the SE segment for a given event. One can also predict the energy and the position along the cell (z coordinate) of the SE event. These can also aid in event selection, as positron events will tend to have low energy gammas in neighboring SE segments due to the 511 keV annihilation gammas scattering. By getting a better estimate of the energy using ML, one can better reject backgrounds that do not follow this pattern. The following section will detail the different ML architectures used in these analysis tasks.

6.2 Machine Learning Architectures Applied

A number of different machine learning architectures were applied to the problems of background rejection and SE reconstruction. These include a fully connected neural network (FCNN) applied to the PMT waveform, a 1-D convolutional neural network (CNN) applied to the waveform, and 2D CNNs and graph convolutional networks (GCN) applied to full detector events (i.e. clusters of detector signals). The following section will go into detail on the implementation of each of these models.

For this work, all models are implemented in the python package pytorch [236]. The sparse convolutional neural network package used is spconv [237] and the graph neural networks are implemented using the pytorch geometric package [238].

6.2.1 Fully Connected Networks for Waveform Analysis

A fully connected neural network (FCNN) is one in which each input is connected to every output. Each layer in this type of network can be described as a linear transformation,

$$y = Ax + b. \tag{6.1}$$

Here y is the output of the layer, x is the input, A is a matrix of trainable weights and b is a trainable constant. These will be referred to as linear layers. It was found through experimentation that the best models were those in which a number of linear layers are chained together, first expanding the input waveform into a size roughly twice that of the number of samples fed into the network. This is followed by a number of layers that shrink the number of outputs to a single output which is the prediction. FCNN were approximately as successful at predicting the Z position for events that have a multiplicity of one, or those in which energy is only deposited in a single cell. For higher multiplicity events, CNNs and GCNs that take in all data from neighboring cells to predict the single cell perform better than FCNN models. For this reason the bulk of this section will focus on the implementation of both CNNs and GCNs.

6.2.2 Convolutional Neural Networks

Convolutional neural networks (CNNs) as first introduced by [239] are deep neural networks that are ideal for learning translationally invariant features of spatial data. CNNs consist of several convolutional layers chained together. The output of this series of layers can then be fed into a linear network as described in section 6.2.1 in order to output a classification score or some other metric. The convolutional layer for the 2D case can be described as a convolution between the input data denoted x which is a tensor of size $W_1 \times H_1 \times D_1$ and a rectangular filter window of size $F_1 \times F_2 \times D_1$ that moves across the spatial extent of the inputs. Here W and H represents the spatial width and height of the input feature set, D represents the number of features, or channels, and F_1 , F_2 are the width and height of the filter window. The filter window will cover all possible locations in which the spatial extent of the window can completely fit inside the space of the inputs. The input of a convolutional layer can be padded with zeros in any spatial dimension in order to increase the spatial extent of the output layer. We will denote the padding in each

dimension P_n . The output at a given coordinate i, j is the result of the i th, j th convolution. In addition to padding the inputs, one can also change the stride of the filter, which is the number of spaces the filter moves between each convolution. We will denote this as S . One can also choose to perform this operation any number of times in order to produce an output layer with more than one channel. The k th filter used for such an operation will be denoted $\mathcal{F}^k$, and the number of filters K . Thus, the output of a 2D convolutional layer, $\hat{x}$, will be a tensor of dimension $W_2 \times H_2 \times D_2$ given input x where

$$\hat{x}_{i,j,k} = \sum_{f=1}^{F_1} \sum_{g=1}^{F_2} \mathcal{F}_{f,g}^k y_{f,g}^{i,j}, \quad (6.2)$$

$$W_2 = (W_1 - F_1 + 2P_1) / S + 1, \quad (6.3)$$

$$H_2 = (H_1 - F_2 + 2P_2) / S + 1, \quad (6.4)$$

$$D_2 = K. \quad (6.5)$$

Here $y^{i,j}$ is the subset of x that is covered by the filter on the (i th, j th) convolution operation along dimension (1, 2).

In a typical CNN, the output of each convolutional layer is then passed through a batch normalization layer then an activation layer. The batch normalization layer [240] transforms the value at each channel in the output of the convolutional layer, $\hat{x}_k$, into the number of standard deviations from the mean for that channel, $\bar{x}_k$:

$$\bar{x}_k = \frac{\hat{x}_k - \mu_k}{\sqrt{\sigma_k^2 + \epsilon}} * \gamma_k + \beta_k. \quad (6.6)$$

The calculations of the mean, μ_k , and variance, σ_k , are performed over a single batch of samples rather than the entire dataset. ϵ is a small number used to avoid division by zero. γ_k and β_k are learnable parameters designed to scale and shift the output of the normalization.

For this work, the activation layer used is always the ReLU layer which sets negative values of the input to 0.

$$\text{ReLU}(x) = \max(0, x). \quad (6.7)$$

Convolutional Neural Networks with PROSPECT Data

In order to utilize CNNs with PROSPECT data, one must choose the how to map the PMT data to the inputs of the CNN. The natural choice given the spatial arrangement of the detector segments is to assign the features of each of the 14x11 segments to a spatial input. In this scenario, the features fed into the model are either the waveforms of each of the two PMTs concatenated together as described in section 6.4.1 or the extracted quantities as described in section 6.4.2. Signals are clustered according to the algorithm described in section 5.2.1, and each segment containing PMTs firing above threshold into the cluster corresponds to the inputs to the CNN. All segments that did not fire in a given cluster are assigned zeros to their input features. Because the typical event occurring in the PROSPECT detector only contains 2 to 4 segments with signals above threshold, the input to the neural network is very sparse. This makes the PROSPECT data ideal for sparse convolutional networks which utilize sparse matrix algebra to calculate the output of each convolutional layer. For this reason, the sparse CNN library `spconv` [237] was chosen. The `spconv` library allows one to use submanifold sparse convolutional layers as first described in [241] which only transfers information from nonzero segments to the next layer. This significantly reduces the computational burden of the network without any loss of information relevant for segment level predictions. All of the CNN networks utilized for SE reconstruction utilize these submanifold convolutions for every convolutional layer.

Position Reconstruction Using Convolutional Neural Networks

Position reconstruction is a difficult problem for single PMT readouts due to the fact that the existing position reconstruction algorithm relies on both the light ratio between PMTs and the differential timing between PMTs. Any single PMT reconstruction method must rely solely on the timing distribution of the light collected. Without any knowledge beforehand of the type of CNN architecture that would best suit this problem, an experimental approach was taken to determine what works. Both full waveforms and extracted quantities were used as inputs to the CNN. The results were benchmarked against a simple "nearest neighbors average" approach in which we simply average the z position reconstructed from neighboring double-ended segments.

For any segment level predictions, the output must have the same shape as the inputs, i.e. a 14×11 array of numbers representing the z predictions for each segment. Generic convolutional layers will typically shrink the feature space, but when a padding of $P = (F - 1)/2$ is used, the output size will remain the same as the input. Note that F must be an odd number for this to work. For this reason, convolutional layers were varied with filter sizes of 1, 3, and 5. The total number of layers were varied up to 12 and a parameter representing the number of $F = 1$ or pointwise convolutional layers was also used. Finally, a parameter representing the expansion (or contraction) of features is used to set the number of output features, and thus the number of filters used at each layer. Since the output needs to be 1 feature, the number of output channels at each layer is calculated by a linear change in features from the previous layer, with the number of expansion layers being another tunable hyperparameter. The remaining layers linearly shrink the outputs to 1. These hyperparameters, or parameters describing the architecture of the network, were varied using a gradient free optimization method as described in section 6.3.3. Through experimentation it was found that layers with larger numbers of intermediate layers outperformed smaller numbers up to around 10 layers, beyond

which there didn't seem to have any additional improvement. The architecture of the best network found on a dataset containing all types of events that could be seen in an IBD analysis and the full relevant energy range (.05 - 10.0 MeVee SE energy) can be found in figure [6.1](#).

Energy Reconstruction

Single ended energy reconstruction with CNNs can be treated very similarly to segment-level Z reconstruction as described in the previous section. However, the major difference is the fact that energy is not physically restricted to a specific set of possible values like the position along the cell length is. The Z distribution of events is roughly linear, with larger amounts favoring one side due to ambient gamma backgrounds in the experiment hall whereas the energy distribution exponentially decays at higher energies due to the increasing rarity of processes producing higher energy gammas.

An alternative method to using the network to directly predict the true energy is to use the Z prediction from the neural network and calculate what the energy would be given that position. Calibration curves are used that fit the ratio in light received between PMTs to positions, this ratio at the predicted position is used to predict the light that would have been seen by the other PMT if it were working, then the combined light output is used to calculate the position-corrected energy prediction.

What was found through the best hyperparameter optimization was that the error in energy predicted as a function of true energy tended to match the best predictions based on inverse-calibration using the best Z prediction models at energies greater than 0.5, but for lower energies the Z prediction based model outperformed. For this reason, we chose to utilize the Z prediction model to predict the energy rather than having a dedicated neural network model for energy prediction on single ended cells.

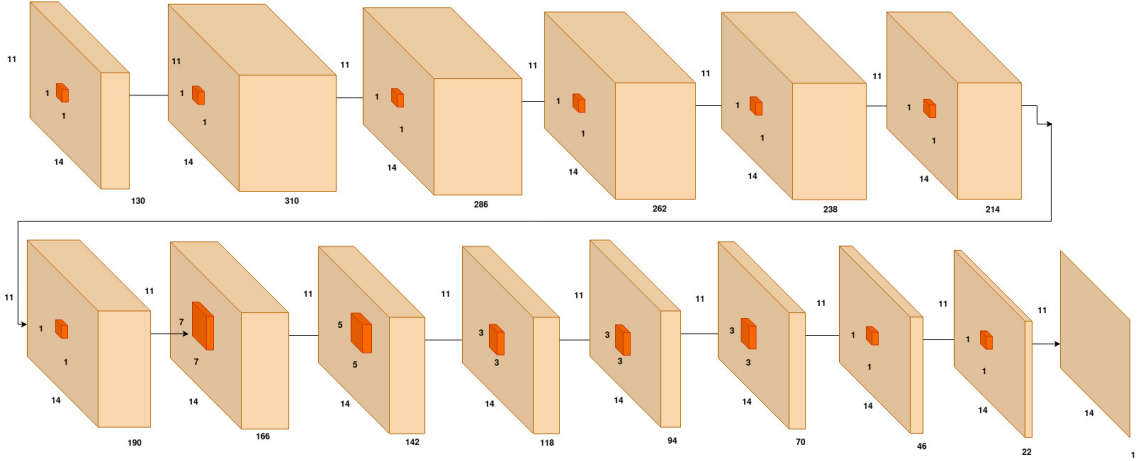


Figure 6.1: Best Z Reconstruction CNN Model Pictured is a diagram of the convolutional neural network architecture used for the best performing Z reconstruction. Each brown block represents the size of the feature space at each layer. Orange blocks represent the size of the convolutional filters. The padding for each layer is set such that the spatial size of the output features is preserved. Each convolutional layer consists of a submanifold sparse CNN block followed by a batch normalization layer then a ReLU layer. It was found that mixing 1×1 (pointwise) convolution layers with larger sized filter layers was best for z prediction. The pointwise layers capture information from the timing of the pulse while the larger filters add in information from neighboring segments.

Segment PID Reconstruction

PID is reconstructed in a similar manner as described in previous sections for energy and Z values. The major difference is that the output contains 5 quantities rather than 1 for each segment, where each value represents the likelihood of the sample being a member of each of the respective PID classes described in section 6.1.2. These values are referred to as class scores. The truth value that the model is trained on is based on the label given for the dual ended analysis. The cross entropy loss is minimized. Cross entropy loss is commonly used for classification problems. For a problem containing C classes, It is defined for each sample as

$$\text{loss}(x) = -\log \left(\frac{\exp(x_j)}{\sum_{i=0}^{C-1} \exp\{x_i\}} \right). \quad (6.8)$$

where j is the index of the correct class and x is the vector of class scores for the sample.

Event PID Reconstruction

Sometimes one only needs PID information for a whole cluster rather than individual segments within a cluster. For example, for neutron capture identification one only cares that a single segment contains a neutron capture-like deposition. In this case, PID labels are given to each event and the output of the network is a single set of class scores representing the aggregation of all information for the event. For a CNN based classifier, the typical strategy is to flatten all of the spatial outputs of the final convolutional layer into a single vector that is fed into a fully connected network that results in the class scores for the event.

In this scenario, the original spatial information of the inputs are not needed to be preserved at each stage, therefor there are no restrictions on the amount of padding or stride used when performing hyperparameter searches for the best network for the given problem. Otherwise, the structure typical to the Z reconstruction networks previously mentioned in section 6.2.2 is still used - the number of layers and the

size of the output feature space is varied in a similar fashion. Here an additional two hyperparameters are used in the search, one representing the number of features output by the final convolutional layer before feeding into the FCNN, and another representing the number of linear layers in the FCNN.

Table 6.1 is the best network found for the purpose of classifying neutron captures, ionizations, and recoils for a subset of events in the SE energy range for possible neutron captures.

6.2.3 Graph Convolutional Networks

GCNs have already been shown to be useful in a variety of particle physics experiments [242] and several neutrino physics experiments including Ice Cube [243], liquid Argon-based time projection chambers [244] such as DUNE [245], and scintillator-based neutrino experiments [246]. GCNs are an ideal candidate for PROSPECT data due to its effectiveness at representing sparse datasets. Graphs can be arbitrarily large and therefore code written for training on graphs implement sparse matrix algebra [238]. Implementation of the GCN on PROSPECT data follows the architecture modelled by the CNNs as described in section 6.2.2. Graphs are composed of nodes and edges. Similar to the CNN construction, we utilize event clusters as defined in section 5.2.1 as individual graphs. The “nodes” of the graph are segments that had one or more PMTs signaling above threshold. The features of each node are then either the two PMT waveforms concatenated together or the extracted waveform features. The “edges” of the graph are defined using a “k nearest neighbors” approach. Here k is a parameter of the network that represents the maximum number of connections a segment can have. If an event contains more segments signaling above-threshold then the segment will be connected to the segments in closest proximity. Through experimentation, it was found that a k value of 4 or greater was optimal. Since most of the events contain a multiplicity of 4 or less, this means that for most events each segment is connected to every other segment.

Table 6.1: Architecture used for best performing neutron capture classifier. Note that each Conv layer is followed by a batch normalization and then a ReLU layer. See section 6.8 for more information on this model.

Layer	Input Size	Output Size	Filter Size	Padding	Stride
Conv1	$14 \times 11 \times 130$	$14 \times 11 \times 145$	3×3	1	1
Conv2	$14 \times 11 \times 145$	$14 \times 11 \times 160$	3×3	1	1
Conv3	$14 \times 11 \times 160$	$13 \times 10 \times 175$	2×2	0	1
Conv4	$13 \times 10 \times 175$	$12 \times 9 \times 190$	2×2	0	1
Conv5	$12 \times 9 \times 190$	$6 \times 4 \times 50$	2×2	0	2
flatten	$6 \times 4 \times 50$	1200			
linear1	1200	442			
linear2	442	163			
linear3	163	60			
linear4	60	22			
linear5	22	8			
linear6	8	3			

Nodes connected by edges are convoluted together when propagating weights in a single layer. This is analogous to a CNN where segments within the filter window are convoluted together. When the neural network weights are convoluted with the node itself, this is known as a self-loop. As Kipf and Welling [247] showed that one can represent a single graph convolutional layer as

$$H^{(l+1)} = \sigma \left(\tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{(l)} W^{(l)} \right). \quad (6.9)$$

Here σ represents a nonlinear activation function, H represents the features of the graph at layer l , W are the weights used for convolution, A is the adjacency matrix, $\tilde{A} = A + I_N$ is the adjacency matrix with added self connections via the identity matrix I_N , and $\tilde{D}_{ii} = \sum_j \tilde{A}_{ij}$. The adjacency matrix is defined by the choice of edges; it is a matrix of 1s and 0s with a 1 at position i, j indicating that the node at position i is connected to the node at position j .

Types of Graph Networks Tested

While equation 6.9 shows the basic idea behind a graph convolutional layer, there are a number of ways this can be implemented and a number of variations on the idea can be used to enhance training speed and model performance. The python package pytorch geometric [238] is utilized for the implementation and as of this writing has 42 different graph neural network (GNN) layer operators implemented. Rather than completing a detailed study of each one of these operators to choose one that best fits our use case, a brute force approach was used where the easiest ones to implement were tested in a hyperparameter search. This search used a fixed architecture other than the specific GNN layer which was randomly varied over about 100 trials. The problem these were tested on was the single ended Z prediction. The top performing operators were then subjected to further hyperparameter testing to determine which one worked best for Z prediction.

Of the 42 operators available in pytorch geometric, 18 different operators were implemented. Of these 18, the 5 top performers were GCNConv [247], FeaStConv [248], SuperGATConv [249], PointConv [250], GMMConv [251], and ARMAConv [252]. Of these, GMMConv was chosen due to it outperforming the others by a slim margin on a hyperparameter search. For this reason we will focus on GMMConv in the remainder of this paper.

Gaussian Mixture Model Layer

GMMConv utilizes a gaussian mixture model in its weights used in the convolutional layers. The exact form of a specific layer is

$$\mathbf{x}'_i = \frac{1}{|\mathcal{N}(i)|} \sum_{j \in \mathcal{N}(i)} \frac{1}{K} \sum_{k=1}^K \mathbf{w}_k(\mathbf{e}_{i,j}) \odot \mathbf{\Theta}_k \mathbf{x}_j, \quad (6.10)$$

where

$$\mathbf{w}_k(\mathbf{e}) = \exp \left(-\frac{1}{2} (\mathbf{e} - \mu_k)^\top \Sigma_k^{-1} (\mathbf{e} - \mu_k) \right). \quad (6.11)$$

denotes a weight matrix with trainable mean vector μ_k and trainable diagonal covariance matrix σ_k . $\mathbf{x}_i$ denotes the features of the network at node i , $\mathbf{x}'_i$ denotes the outputs of the network at node i , $\mathcal{N}(i)$ denotes the neighborhood (connected nodes) of node i , K denotes the number of gaussian kernels used, and $\mathbf{\Theta}_k$ represents the set of trainable weights convoluted with the inputs for kernel k . The number of kernels used is configurable by the user. We allow this to vary between 1 and 6 for hyperparameter searches.

The parameter $\mathbf{e}_{ij}$ denotes the edge attribute between node i and j which can be configured by the user; in our case we set them to the Cartesian distance between segments: $\mathbf{e}_{ij} = \mathbf{p}_j - \mathbf{p}_i$, where $\mathbf{p}_i$ denotes the position of node i .

The exact details of the architecture depend on the type of problem. We applied the GCN architecture to both Z prediction and PID classifier problems, which are detailed in the following sections.

PID Classification with Graph Convolutional Networks

For PID classification (see table 6.2 for list of PIDs), we require 5 floating point numbers representing the log-likelihood of each class. This is straightforward in a GCN because each sample is represented with a different number of nodes, one for each segment that contained above-threshold signals. Thus, the output of a GCN layer will preserve the multiplicity of each event. This is unlike the CNN layer as described in 6.2.2 which requires special care to retrieve outputs for the relevant segments firing in a given event.

The architecture for PID classification is conceptually very similar to the CNN architecture. The inputs are fed through a GCN layer, then a batch normalization layer is applied to the outputs which then feed into a ReLU layer acting as our nonlinear activation function. Note the graph batch normalization layer is equivalent to CNN batch normalization layer described in equation 6.6. GMMConv was found to be the best GNN layer operator for PID classification purposes.

The primary difference between the graph architecture and the equivalent CNN architecture is the choice of adjacency matrix which determines which segment features are convoluted together. For PID classification, the “k-nearest neighbors” approach was utilized. This means for each segment in the cluster, the k nearest segments that also signalled above threshold in the cluster are connected to it. Self loops can also be included, meaning the segments own features can be convoluted with the layer weights for that segments output. The choice to use self loops along with the parameter k were varied in the hyperparameter search, and it was found that self loops are optimal along with k values of greater than or equal to 4. Because most events have a multiplicity of 4 or fewer, it was optimal to connect all of the segment features with each other segment in the event.

Similar to the CNN architecture, we optimize the architecture using a parameter that represents the expansion of the feature size, the number of expansion layers, and the number of contraction layers. These parameters are all varied for a

hyperparameter search as described in section 6.3.3. The best model found for PID classification is shown in table 6.3.

Position Reconstruction with Graph Convolutional Networks

Z predictions using graph convolutional layers follows the same pattern as is used for PID predictions as described in section 6.2.3, except that there is only a single output representing the position along the cell axis rather than the 5 class outputs. It was found through several dozen trials of a hyperparameter search that the GCN does not perform as well as the CNN for Z predictions. This is in contrast to PID prediction, which the GCN outperforms the equivalent CNN model.

In order to try and match the performance of the CNN Z prediction described in section 6.2.2, an adjacency matrix was chosen that was identical to a square filter running over each of the segments. This was done by choosing connections that are 1, 2 or 3 segments apart in x and y (corresponding to a filter size of 3×3 , 5×5 , and 7×7). The pattern of changing between pointwise convolutions, which are graphs consisting of a single segment with self-loops, and 7, 5 or 3 sized filters was copied. Using this approach, roughly the same results as using the k-nearest neighbors approach were achieved, indicating that the choice of adjacency matrix was not the reason for the reduced performance compared to the CNN approach. See table 6.4 for a full comparison of neural network architectures used for Z prediction.

6.2.4 Other Network Architectures Tested

In addition to GCNs, CNNs, and FCNNs, there were some architectures attempted. Because the waveform is a time series, it was initially thought that utilizing architectures designed for processing time series data could help capture additional information to improve upon the naive approach used in the GCNs or CNNs which was to simply feed each sample of the waveform as features of the network. To this end, recurrent neural networks (RNNs), temporal convolutional networks [253] (TCNs)

Table 6.2: Table of different particle identification types and their descriptions.

Class	Description
Ionization	Events inside the fit ionization PSD band
Recoil	Events inside the nuclear recoil band
Neutron Capture	events within the neutron capture PSD and Energy range
Muon	High energy events (total visible energy > 15 MeVee)
Ingress	Events with PSD above the neutron capture band

Table 6.3: Architecture used for best performing GCN PID classifier. Each GMMConv layer is followed by a batch normalization and then a ReLU layer. A kernel size of 2 is used for every GMMConv layer.

Layer	Input Size	Output Size
GMMConv1	130	191
GMMConv2	191	252
GMMConv3	252	313
GMMConv4	313	374
GMMConv5	374	435
GMMConv6	435	364
GMMConv7	364	293
GMMConv8	293	222
GMMConv9	222	151
GMMConv10	151	80
GMMConv11	80	5

were used to process the waveforms before feeding them into a CNN architecture. In the case of the TCN, the outcome was identical to no TCN being applied. In the case of the RNN, the gradient descent algorithm was unable to converge and no useful predictions were able to be made. From these failures we can glean that the changes in sample heights over time was less important for feature prediction than simply knowing the heights at specific times.

Another architecture tried in the same vein was 3D convolutional networks where the 3rd axis used is the temporal axis of the waveform. In this construction we use the two samples from both PMTs as the two features fed into the network at each time and spatial location. The difficulty with this approach was the enormous amount of time it takes to perform 3D convolutional layers. To decrease the computational complexity, we factorized the time and spatial dimensions by first performing pointwise convolutions in space and length N convolutions in time to reduce the size of the temporal dimension before performing spatial convolutions with a filter of length 1 in the time dimension. This still resulted in a factor of 6 increase in CPU time per epoch relative to 2D convolutions so we did not perform detailed tests of the algorithm.

6.3 Training and Optimizing the Neural Networks

6.3.1 Neural Network Training

Training is done using stochastic gradient descent (SGD) with Nesterov momentum as first described by [254]. Typical values used for the momentum are .90-.98 and learning rates around .01-.02. Pytorch's automatic differentiation algorithm is used to calculate gradients in batches that are around 10,000 to 20,000 samples in size. The Pytorch Lightning framework as detailed in [255] is used to structure the machine learning code in a way that leverages best-practices recommended by professionals in the machine learning community.

Separate subsets of the available data are used for training, validation, and testing. Typically the validation dataset is roughly $1/3$ to $1/5$ the size of the training dataset. Depending on the phase space sampled for the training set, the number of samples used for training is typically between 1 and 3 million events. It was found experimentally that training sets using less than 1 million events tended to perform worse, but using more than this gave negligible performance benefits.

The truth data used in training was either the simulation truth value extracted from the Geant4 simulation, or it is the calibrated physics quantity found for double ended readouts when training on real data. Because the PMTs gradually failed throughout the several month long data taking period, training and validation data sets were constructed from the first day of data in which all PMTs were operational, and calibrated physics quantities from the PMTs could be utilized to train the single ended prediction models. The dead PMTs were turned off by simply zeroing out their waveforms and re-aligning the waveforms via the procedure described in [section 6.4.1](#) when appropriate.

Training is split into epochs. One full pass of the training dataset in which the gradients of each batch are computed and model weights are updated until all batches in the dataset have been exhausted. At this point the model is tested on the validation dataset. This sequence constitutes a single epoch. The loss for the validation dataset in a given epoch is compared to the current best loss of all epochs. If the loss fails to improve by a certain amount for a number of epochs in a row, the training is automatically cancelled. This criterion varies from problem to problem, but typical values used in this work were 5 epochs failing to improve the loss by .01 resulted in cancellation of the training run. Model weights for the best validation loss are saved for later use. Splitting into separate training and validation datasets in this manner prevents “overtraining” in which the model finds patterns in the training dataset that don’t generalize to other data.

Typically, given the large size of the training sets, the training usually only needs to run for 30 or so epochs before reaching the limit of its loss reduction. The loss

function used is the mean absolute error (MAE) for scalar quantities like Z position or energy, and cross entropy loss for classification tasks. Cross entropy loss is defined in equation 6.8.

The models used will generate outputs for each segment, but we only care about the performance of the model for SE segments. It was found through experimentation that training only based on the loss for SE segments found optimal performance for these segments and faster convergence. Thus, for training we ignore the loss on DE segments.

6.3.2 Dataset Generation

In order to generate training and validation datasets for a given task, data was either simulated with the desired particle types or sampled from the first day of reactor on data when all PMTs were operational. Simulated datasets utilize the Monte Carlo truth values of position and energy deposited for the targeted values. When using real data, the double ended calibrated energy and position values are utilized as targets, then training is performed on the data with the “dead” PMT waveforms set to 0.

For real datasets, the full calibration procedure is performed on the first day of data assuming all PMTs are fully functioning. Then, the data is sampled in the energy range of interest for the problem at hand. For the finalized models used in this study, clusters with a total energy range of 0.05 to 10.0 MeVee were chosen. Training and validation datasets were constructed by creating two separate categories of sampled events, one with only ionization-like pulses and others with one or more non-ionization-like pulses. These two categories were then interwoven in the training and validation dataset so that there were an equal number of ionization-like and non-ionization-like clusters. This prevented bias in the model when training for classification purposes. It also ensured the Z reconstruction model was able to perform on all classes of interest.

For the purposes of training a Z prediction model it was found that the events also needed to be uniformly sampled in Z for each class. This was due to the fact that the ambient gamma backgrounds at the experiment location were higher on one side of the detector along the Z axis due to neutron activated material from a beamline shutter in the floor below. When trained using this distribution, the model gave more predictions on the negative Z side due to the fact that that the deposition had a statistically higher probability of occurring in that region of the detector. It was found that training on a uniformly sampled distribution in Z for each class alleviated this bias in the prediction. However, a bias inherent to the single ended Z prediction is still present in the model as is discussed in section 6.7.1.

Once the data was properly sampled, the data was then normalized and each class interleaved in order to create the training and validation datasets. The training set generally consisted of 2 million events and the subsequent 200,000 events were used for validation. This number was chosen due to the good statistical coverage for each event type, z position, and energies of interest.

6.3.3 Optimization

Optimization is performed using a gradient-free optimization library Optuna as described in [256]. Hyperparameters of the model are chosen and varied within bounds that are allowed given the memory constraints and CPU resources available. A typical set up for the hyperparameter search would be to set the number of trials to 100, vary around 4 hyperparameters, and set a flag to prune unpromising trials. It was found that the default hyperparameter sampler and trial pruner was sufficient for our needs. The default sampling algorithm is the Tree-structured Parzen Estimator algorithm [257]. The default pruner is the median pruner, which will prune the trial if the trial's best intermediate result is worse than median for previous trials at the same epoch.

A sqlite database was utilized for storing trial results. This allowed for easy parallelization of the hyperparameter optimization process. Multiple hyperparameter runs for a couple of days were set off on a process utilizing 2 threads, one thread reserved for data computations and one for data loading. Each thread references the same database for determining loss values for previous trials used for the next parameter selection and as a reference for when to prune unpromising trials.

Hyperparameter Searches Using a CPU Cluster

Note that when utilizing PyTorch in CPU mode, if one does not specify the number of CPU threads available, it will use all that are available. This caused problems running on the CPU based cluster at the Physics Division of ORNL until this behavior was recognized. Several tests were done to determine the optimal number of CPUs to utilize during a hyperparameter run. It was found that overwhelmingly the most efficient option was to only use a single thread per trial process, with only a single dataloader thread for a total of two threads.

To give a concrete example of this, one Z prediction model containing 48,000 parameters took about 29 seconds to run a single epoch on a training dataset of 1 million samples. When using 2 threads for computations and 2 threads for dataloading, this time only decreased to 21 seconds which is roughly a 30% improvement for double the computational resources. Using 4 threads for computations and 4 for dataloading resulted in 14 seconds per epoch, which is half the time of using 1 and 1, for 4 times the resources. Further increases in the number of CPUs utilized decreased incremental gains further. Thus, a single thread for both computations and dataloading was used for hyperparameter optimizations on the cluster. This allowed for a much larger number of threads to be utilized in parallel for hyperparameter searches which more than made up for the increase in time from only using a single CPU thread. Similarly, when bulk processing waveforms for the IBD dataset, the files were processed in parallel using a single thread per process.

6.4 Data Preparation for Machine Learning Models

There are two types of inputs for the machine learning models. One is feeding in the PMT waveforms after baseline subtraction, time alignment and value normalization is applied. The other is using extracted quantities from the waveforms and dual ended reconstructed quantities when applicable.

6.4.1 Waveform Preparation

Once waveforms are clustered using the procedure described in 5.2.1, the pulses are aligned using the calibrated arrival times relative to the event trigger. 65 samples are allocated for each waveform. This was determined from studies that found 54 samples were needed to best discriminate ionization-like pulses from nuclear-recoil-like pulses. An additional 5 samples were used for the purposes of this study and 6 samples were added for potential offsets between detectors in a given cluster. The first pulse that arrived is set so that the eighth sample is the arrival sample. All other pulses are offset such that their arrival sample is at sample n , where $n = (\text{round}((t_i - t_0)/4) + 8)$, t_i is the arrival time of the i th waveform in the cluster and t_0 is the arrival time of the first waveform.

Once the waveforms are time aligned, they are scaled to match the lowest gain of the PMTs. This ensures that all PMT signals fit within the normalized range from 0 to $2^{14} - 1$. Before feeding these values into a neural network they are scaled to 32-bit floating point numbers between 0 and 1 by dividing by $2^{14} - 1$.

6.4.2 Extracted Quantities Inputs

A natural choice for inputs into the neural network are the quantities extracted from the waveforms used for the physics analysis. These are the pulse area, PSD parameter and timing of each of the waveforms in a cluster. It is interesting to see how the

performance of a network trained on these variables compared to the full information of the waveforms. It is also interesting to see if the addition of other features of the waveform not used in the IBD analysis could improve the model.

In this work we chose to utilize the pulse area, timing relative to event start, and PSD for each live PMT. Data is grouped by segment, so each pair of PMT features are concatenated together. If both PMTs are alive in a segment, the reconstructed energy, position, cell axis position, and pulse shape are also included. Features not available for a given segment are set to 0. Normalization factors for each feature are chosen so that most signals fit between 0 and 1 which is important for stability of the gradient descent algorithms used when training the network.

A second model based on extracted features was also utilized that contains information not used for the IBD analysis. These additional features are the pulse width, rise time, fall time, and pulse height variables. It was found that the addition of these variables improved the model compared to using only features relevant to the IBD reconstruction analysis, although not to the point of being at parity with the full waveform model. A full model comparison is shown for SE Z reconstruction performance in section [6.7.1](#).

6.5 Positron Identification

In order to identify an IBD event, a correlated positron plus neutron signal is used to distinguish from backgrounds. In liquid scintillators one cannot distinguish a positron from a gamma or an electron deposition through the pulse shape alone. However, with a segmented detector one could potentially distinguish based on topological characteristics. An electron and a positron will rapidly deposit its energy in a liquid scintillator, making them unlikely to escape a segment in the PROSPECT detector. The positron will then annihilate and produce two 511 keV gamma rays which will be emitted in opposite directions. Meanwhile, single gamma rays will scatter

in potentially multiple segments if the energy is high enough before either fully depositing its energy or leaving the detector.

This section applies the CNN architecture described in section 6.2.2 for the purpose of distinguishing electron, gamma, and positron depositions in the PROSPECT detector. The events and waveforms were simulated as described in section 5.3. It will also discuss the possibility of identifying Positrons via identification of Ortho-Positronium formation.

6.5.1 Gammas, Electrons and Positrons (GEP) Classification

Gammas, electrons, and positrons were fired in Geant4 at random positions and momenta within the scintillator bulk. Energies varied on a uniform spectrum from 0 to 9 MeV. After hyperparameter optimization, the overall accuracy of the model classification on the test dataset was 0.80. The test dataset consists of 1e6 events per class separate from the events used for the training dataset. A confusion matrix, which quantifies the frequency each class is labelled, is shown in figure 6.2.

We can also look at a confusion matrix at specific ranges of deposited energies. This is displayed for energies ranging from 2-5 MeV in figure 6.3. This tells us that the network is achieving a precision of around 80% for positron identification within these energies.

In order to better understand this we can check the precision at various physical quantities such as the energy or PSD of the pulse. This can be visualized with a 2D contour plot of precision at various cuts on energy and PSD. This is displayed in figure 6.4. We can see the network is able to distinguish features in the dataset beyond the PSD distribution given its accuracy within the overlapping PSD bands of the particle distributions. Other metrics related to the statistical distributions of the pulse and the topology of the event can be explored to better understand how the network achieves such an accuracy.

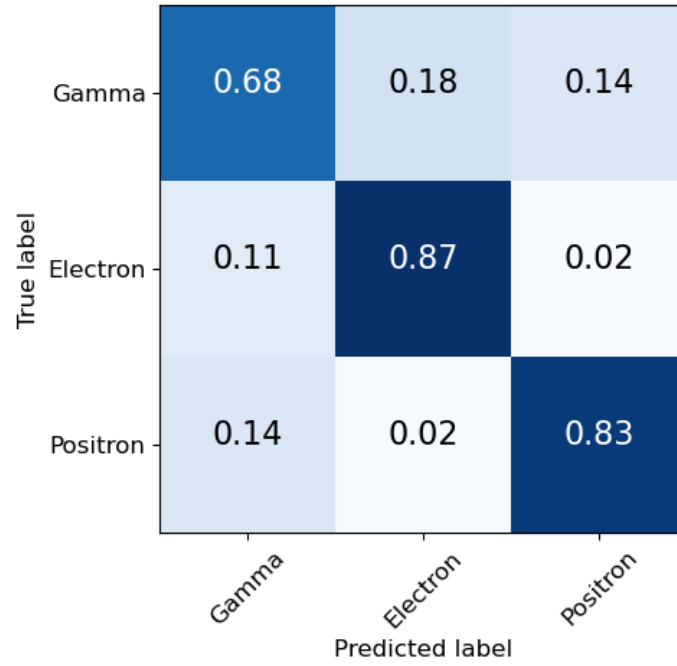


Figure 6.2: Confusion matrix for GEP study.

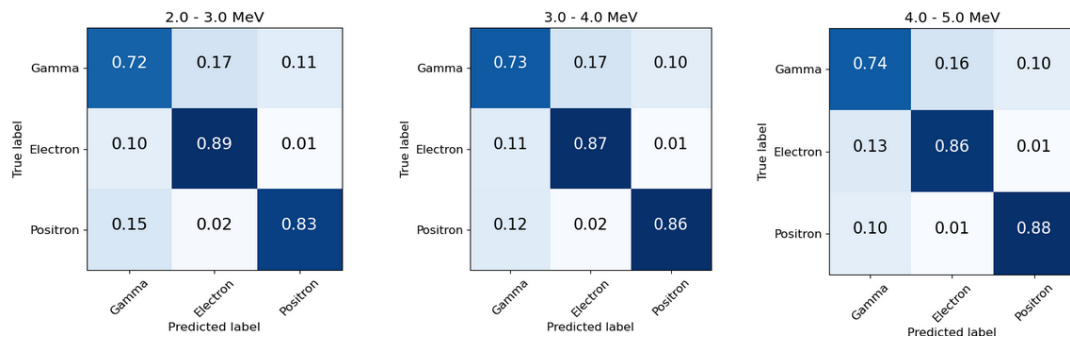


Figure 6.3: Three different confusion matrices, one for each 1 MeV increment between 2 and 5 MeV.

One such metric is the multiplicity of the event. We can clearly see from figure 6.5 that the multiplicity distributions are very different. For example, electrons tend to deposit their energy in one cell. We can see from the class precision at each multiplicity in figure 6.6 that electrons are often mistaken for other particles when they deposit energy in more than one cell.

6.5.2 GEP Using Extracted Features

One question is whether using the full waveforms allows for additional discrimination power compared to using extracted features of the waveforms. In current PROSPECT analysis, features such as the pulse area, PSD, and relative timing of the pulses (used for determining the location of the energy deposition along the length of the cell) are utilized for background rejection. For this analysis, we used the pulse height, area, total photoelectrons in each PMT, relative timing of the pulses, combined PSD, and the start time of the pulse relative to the event start as the features for each segment in the array instead of the two waveforms. This significantly reduces the size of the neural network, going from a 14x11x300 sized feature space to 14x11x7. While this significantly decreases the training time for the network (by roughly a factor of 10), it also results in a 12% decrease in total accuracy for the network using the same training and validation datasets previously described.

A total accuracy of 0.68 was achieved along with a precision of 0.75 for positron identification was found for the best model found using the extracted features. The confusion matrix for this model is pictured in figure 6.7. This indicates that there is utility in analyzing the full waveform data for background discrimination in PROSPECT. However, note that the CNN architecture used for this model was constructed based on knowledge gained from the hyperparameter optimization of the full waveform model; a full hyperparameter optimization has not yet been explored for the extracted feature model. Additionally, one could envision slight improvements to the accuracy of this model by using, for example, the PSD information for both

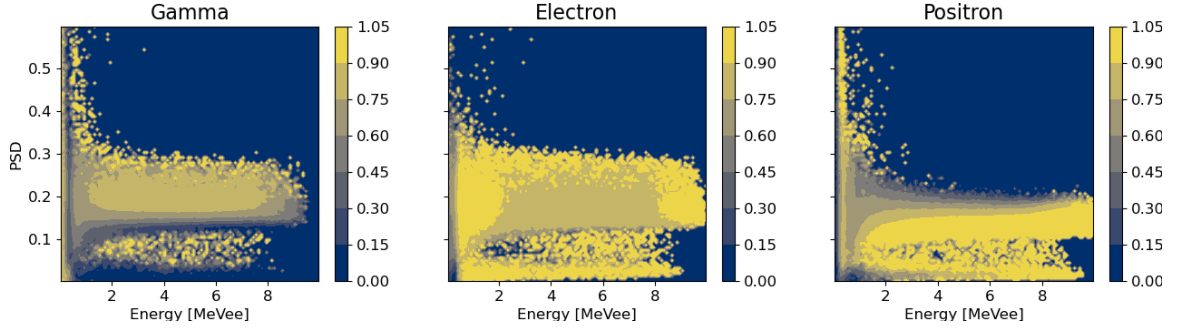


Figure 6.4: Precision for each class label is calculated over 100x100 energy - PSD bins.

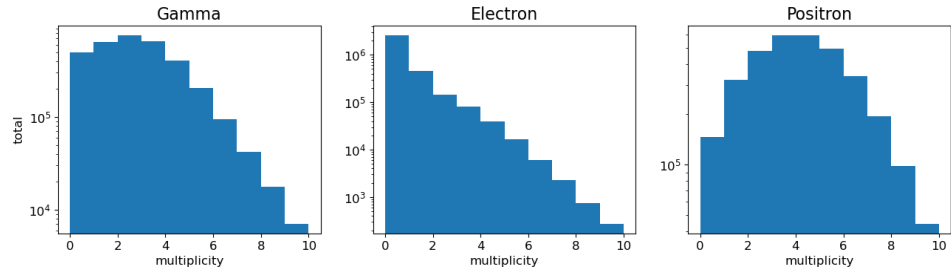


Figure 6.5: Multiplicity distribution for the different simulated particles.

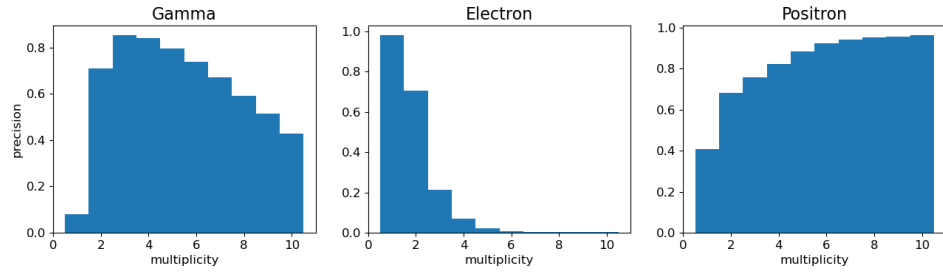


Figure 6.6: Precision at various values of multiplicity for events with each class label.

PMTs. Therefore, more work would be needed to determine how close one could come to the accuracy of the full waveform model.

6.5.3 Ortho-Positronium Formation for Positron Identification

An additional property that could distinguish positrons from electrons and gammas is the formation of Ortho-Positronium (O-Ps). Positronium [258] (Ps) is a bound state of an electron and positron. In liquid scintillator it has a lifetime of about 3ns [259]. Although simulations found that with the 4ns sample length of the digitizer used for the PROSPECT experiment was not sufficient to distinguish normal positron annihilation with OPs formation and decay, we found that with a lifetime of 20 ns our neural network algorithm (the same used for GEP) was able to distinguish the two with 68% accuracy. This indicates a potential use of OPs decay for positron identification in detectors with timing resolution smaller than the OPs lifetime.

6.6 Single Ended Event Reconstruction With Machine Learning

As discussed in section 4.8, scintillator ingress into PMT housings caused failures of PMTs at varying rates throughout the lifetime of the experiment. Section 5.5.2 describes in detail the procedures used to analyze the SE segment data in order to reject non-IBD events. The following will discuss machine learning methods to do the same. It will focus on two major developments, the first being a position reconstruction network and the second being an event classification network.

6.6.1 Machine Learning Methods

Machine learning can improve upon the basic analysis strategy by giving an estimate of the z position of the energy deposition along with an estimate of particle identification (PID). The z estimation is done via a neural network architecture that utilizes the detector information for the all segments in a given event and outputs a number representing the z position of the energy deposition in each segment. More details of this can be found in sections 6.2.2 and 6.2.3. Neural networks are also employed to estimate the PID of a given event as described in sections 6.2.3 and 6.2.2. The PID estimates come in the form of class scores which represent the likelihood of the segment being in each class.

Once a z estimate and PID class scores are obtained, a given IBD candidate can be rejected if the class score of any class other than ionization reaches beyond a threshold. The z estimate can be used to get an estimate of the energy of the single ended deposition so that events with energies too high to have come from the 511 keV gammas from the positron annihilation can be rejected.

In addition to rejecting non positron-like events, the class information can also be utilized to identify potential neutron captures occurring in SE segments for the delay portion of the IBD event identification. Previous studies showed that approximately 10% of neutrons from IBD interactions will migrate to a neighboring cell before capturing on ${}^6\text{Li}$, thus the ability to identify neutron captures via ML techniques will add events that would otherwise go unidentified.

6.7 ML SEER Performance

This section will describe the performance of the ML models used for Z reconstruction, energy reconstruction and particle identification. We will also show the Z reconstruction performance for a sample of calibration source deployments at known locations. When applicable, a comparison with conventional methods is also given.

6.7.1 Single Ended Position Reconstruction Performance

Figure 6.8 displays the mean absolute error as a function of visible energy, position, and multiplicity for the model described in 6.1. The events used for this plot are the first full day of measured data in the IBD dataset. The error on average is about 120 mm for ionizations, 80 mm for neutron captures, and 150 mm for recoils.

Table 6.4 shows the performance of different algorithms used for Z reconstruction. The different models displayed here are as follows: The CNN and GCN models with waveforms are described in sections 6.2.2 and 6.2.3. The single waveform CNN and FCNN only uses the waveform from the single alive PMT as input. FCNNs are described in section 6.2.1. The single waveform CNN utilizes a 1-D CNN with the different waveform samples acting as the dimension of the convolutions, with each sample representing the single feature. The extracted features model uses the same 2D CNN as the waveform model but with 7 features extracted from the waveform instead of the full waveform. The features+ model uses the additional features described in section 6.4.2 (pulse width, rise time, etc). Nearest neighbor average simply averages the positions of neighboring DE segments to create a prediction. This represents a worst case scenario to benchmark the other models against.

It is interesting to note that the GCN does not perform quite as well as the CNN for this problem, despite outperforming the CNN in particle identification which we will discuss in section 6.7.3. It is also interesting to note that when using extracted features such as pulse area and timing, the network performs significantly worse. This performance improves when adding more features, although it is still quite far behind the full waveform models.

The single waveform models tested only use information from the segment of the energy deposition of interest. The fact that this model performs better than the neighboring average method indicates that the pulse itself contains information about the position which is not being captured in the extracted features. Clearly given the gap in performance between the extracted features models and the full

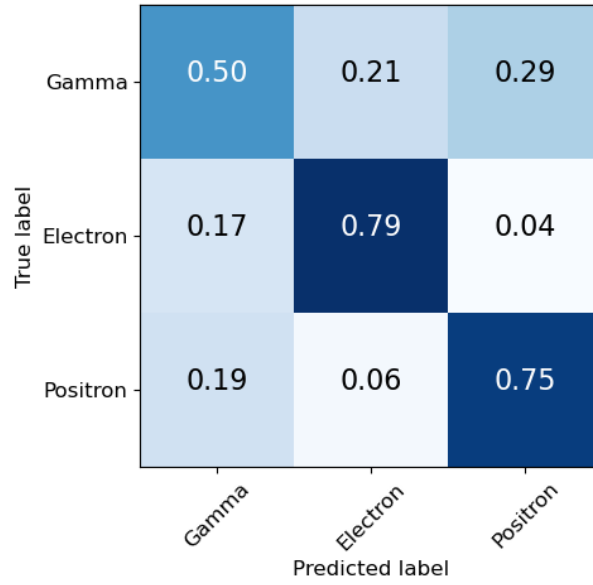


Figure 6.7: Confusion matrix for the GEP model using extracted features from the waveform.

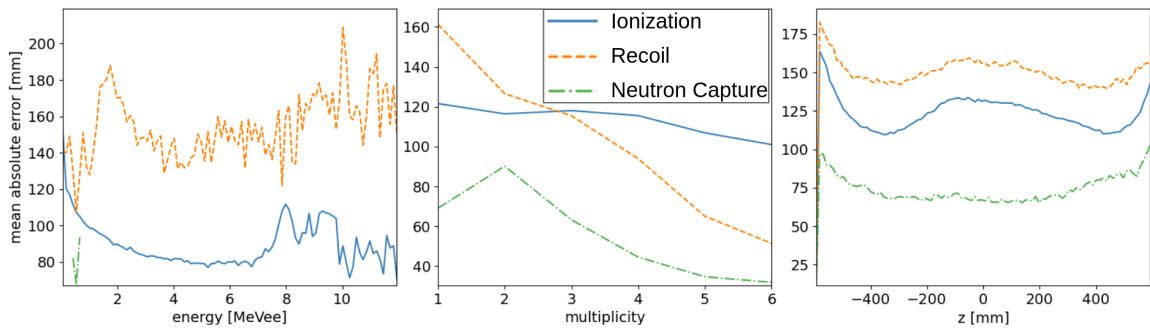


Figure 6.8: Z Reconstruction Performance From left to right: Mean absolute error as a function of energy, position, multiplicity for different event classes.

waveform models, more work is needed to determine if there are parameters that could be extracted to better predict the SE Z position.

Position Scan Calibration Data

In addition to testing on the first day of data, we tested the algorithm on position scan calibration data. The data shown is was taken with a ^{137}Cs source deployed at various locations along the length of the cell in one of the corner rod source deployment tubes as described in [83]. Two runs were selected for comparison, one in April which was about a month into the data taking campaign, and another 4 months later in August. Pictured in figure 6.9 is an example position reconstructed with the dual ended information and the ML SE reconstruction for a comparison. A gaussian plus a linear background was fit to the data and the centroid of the gaussian is compared to the actual known source position. This was done for each source location within each day of runs and the difference between fitted and real position is shown in table 6.5. The ML reconstruction performs about three times worse than the dual ended calibration reconstruction. Both methods lose accuracy over time due to degradation of the scintillator light yield as is described in [83].

6.7.2 Single Ended Energy Reconstruction Performance

From tests on simulated data, it was found that utilizing the best Z reconstruction model to estimate the missing photoelectrons from the dead PMT in order to estimate the energy works better than using a ML prediction directly for the energy. Figure 6.10 shows the mean absolute percentage error of the energy reconstruction algorithm as a function of visible deposited energy. The data utilized for this was all events occurring during the first hour of reactor-on data used for the IBD analysis. Energy reconstruction performance is found by using the calibrated energy prediction when both PMTs are working as the benchmark for comparison.

Table 6.4: Performance comparison between different NN architectures used for Z reconstruction. The error shown is for the best network found for the given architecture after a hyperparameter search. Typical hyperparameter searches explored at least 20 different trials, although more trials were performed for those that showed more promise such as the CNNs and GCNs. Note the nearest neighbor average technique is not a NN but a simple averaging of locations from hits in neighboring DE segments.

Architecture	Mean Absolute Error [mm]
CNN with Waveform	133
GCN with Waveform	147
Single Waveform CNN	211
CNN with Extracted Features+	212
Single Waveform FCNN	218
CNN with Extracted Features	238
Nearest neighbors average	306

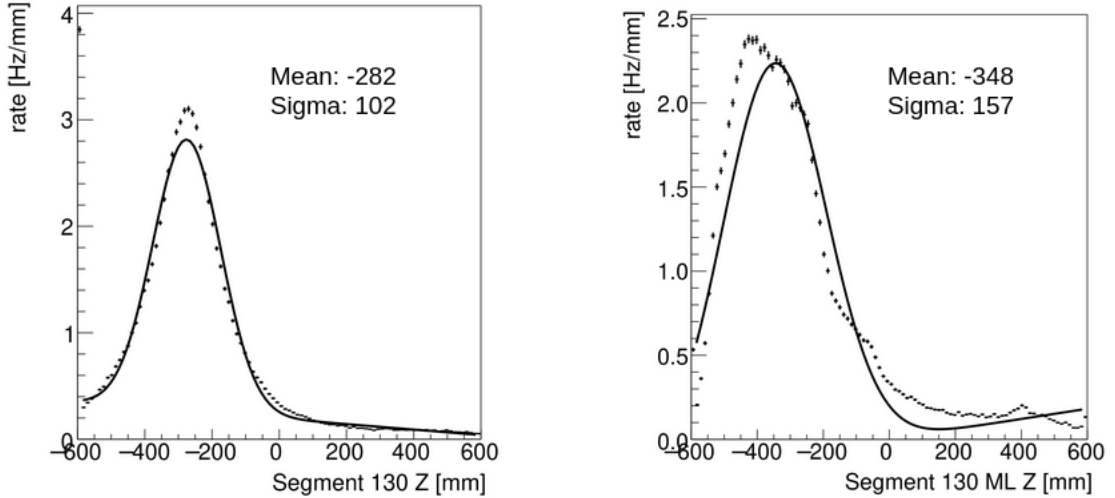


Figure 6.9: Example Z Calibration Reconstruction: Left is the dual ended calibration reconstruction method, right is the ML method using only the waveform from a single PMT along with neighboring PMT information treated as alive. In this run the source was placed at -300 mm. Solid line is the Gaussian plus linear background fit.

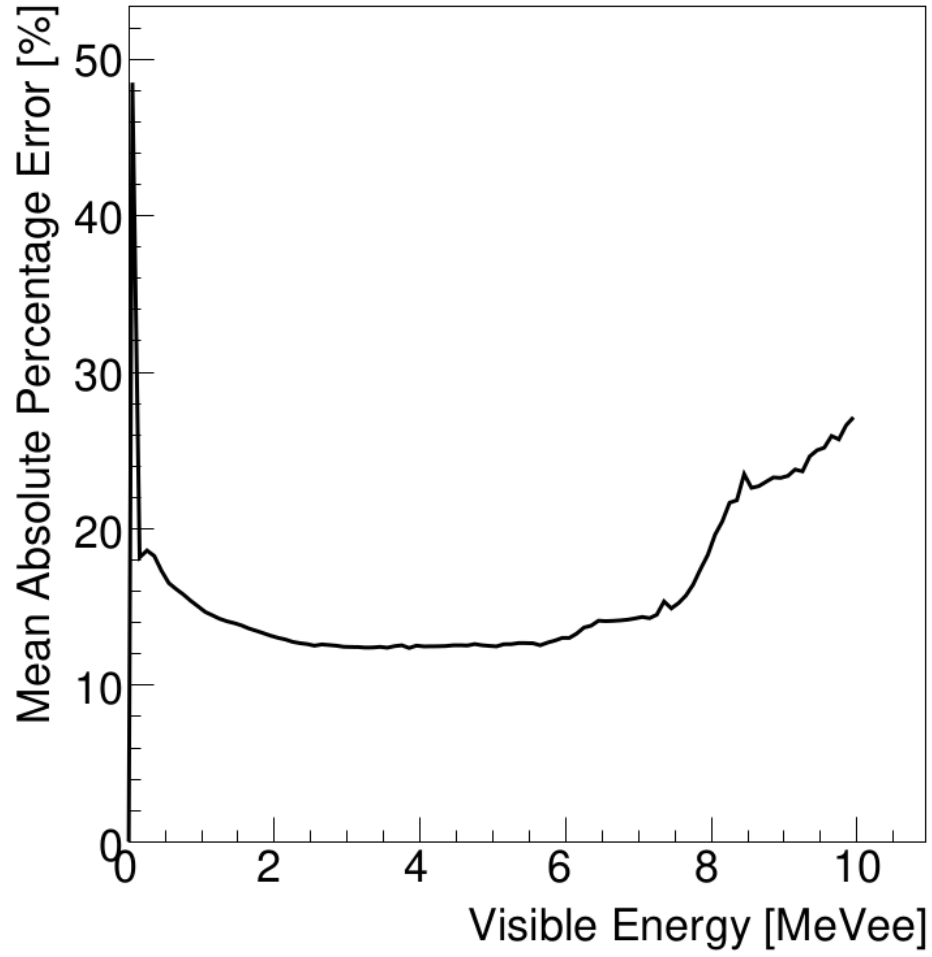


Figure 6.10: Energy Mean Absolute Percentage Error. Low energies (< 0.1 MeVee) perform poorly due to the algorithms poor z reconstruction ability at low light levels. Larger errors at high energies (> 7.8 MeVee) are due to less training data available at this region of the phase space.

6.7.3 Particle Identification Performance

Particle ID performance is shown in figure 6.11. This confusion matrix shows the percentage of single ended PIDs that were predicted for each category. The x axis is the predicted label and the y axis is the true label. The numbers are divided by the total number of true labels for each row. The predicted label for this plot is the one with the largest class score. The data displayed here comes from the first day of data collected for the IBD dataset, for all events with total visible energy between 0.05 and 10.0 MeVee.

6.8 SE Neutron Capture Identification

In order to determine the feasibility of identifying neutron capture-like signals occurring in SE segments, a study was performed comparing the usage of ML-reconstructed SE energy and PID to a basic non-ML energy and PSD cut on neutron capture identification power. For a comparative metric, the $F1$ score was used which is defined as the harmonic mean between precision and recall of neutron capture events. Recall is the number of correctly labelled neutron capture events divided by the total number of neutron capture events, and precision is the fraction of correctly labelled neutron capture events. The harmonic mean is given as $F1 = 2 \frac{PR}{P+R}$, which punishes low precision in favor of large recalls and vice-versa.

Since we are only interested in neutron capture events that occur as a single segment hit cluster, only single segment hits were used in this study. Additionally, since the energy region for neutron capture events occurs within a narrow 0.4 to 0.6 MeVee range, only events containing single ended visible energies between 0.1 and 1.5 MeVee were selected. See figure 6.12 for a visual representation of the energy-PSD distributions for dual ended calibrated variables and the equivalent single ended variable distributions.

Table 6.5: Results from a sample of the calibration data. The difference between calibration source position and reconstructed position is calculated with a gaussian fit to the reconstructed position histogram and the average absolute difference between source positions and centroid is displayed for each segment.

Calibration Run	Segment	Cal Difference [mm]	ML Difference [mm]
April	40	16	61
April	41	19	73
April	130	26	47
September	130	21	68

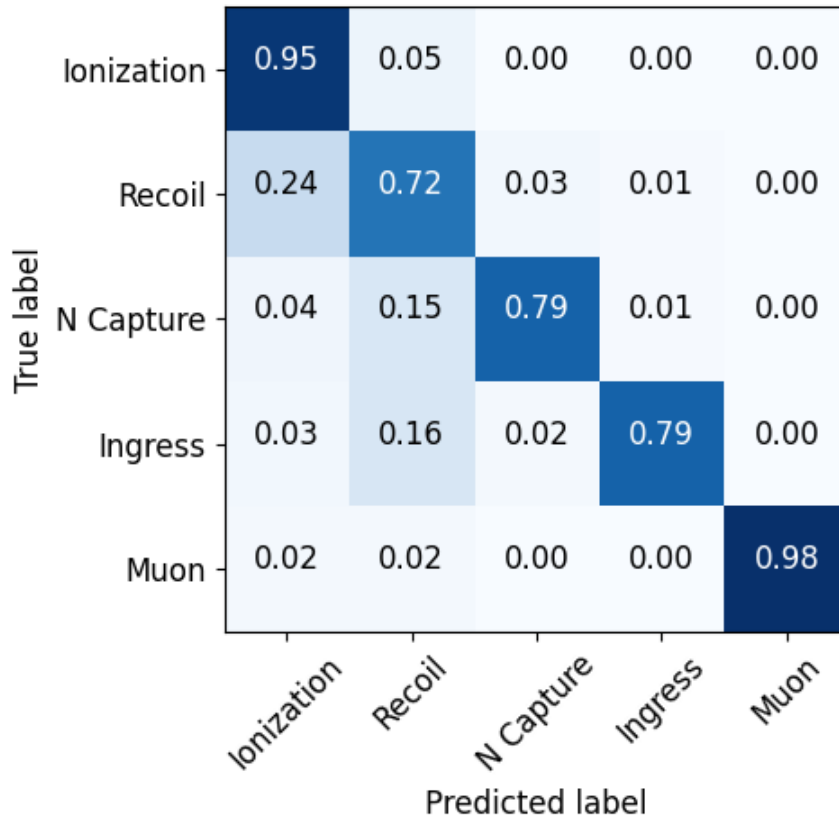


Figure 6.11: Confusion matrix for the best performing SE classifier. Most problematic for the IBD analysis are recoil events which are mislabelled ionizations.

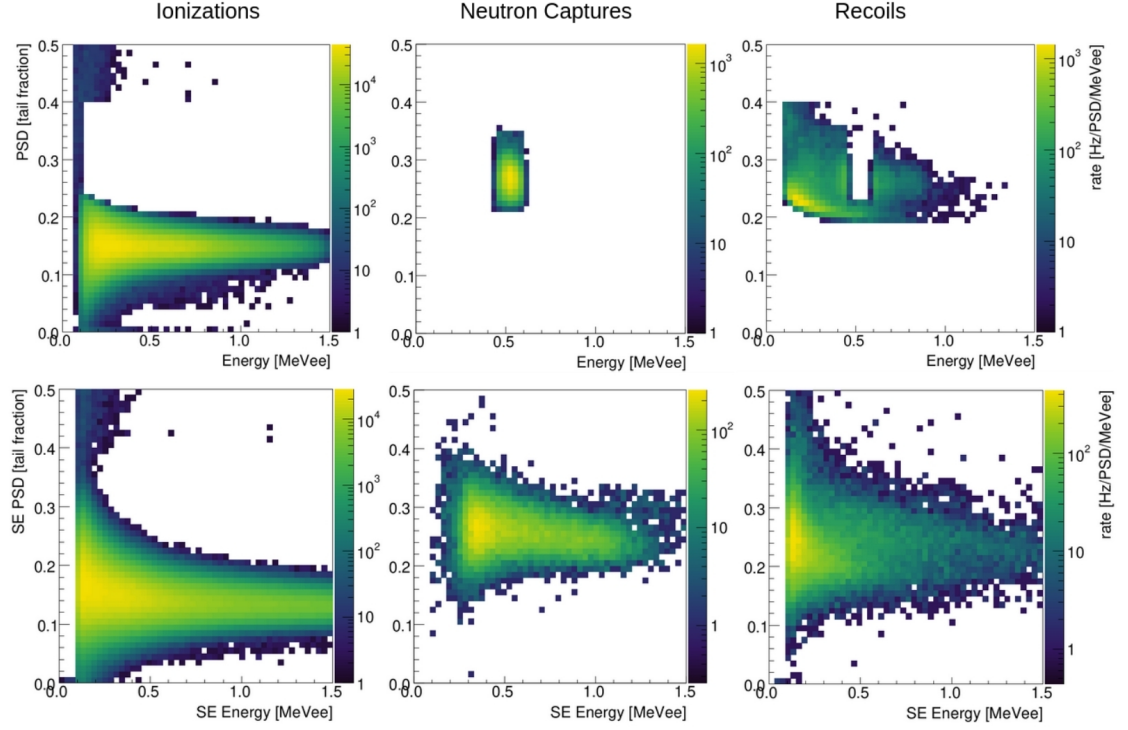


Figure 6.12: Top panel shows energy PSD distributions using dual ended calibrated quantities and bottom panel shows single ended quantities. Events displayed are the ones used for training a classifier for neutron captures, recoils and ionizations based on single site events in the 0.1 to 1.5 MeVee SE energy range. Events are labelled based on the dual ended PID designation described in table 6.2.

Techniques for Single Ended Neutron Capture Identification

A test dataset consisting of 1e6 events in each of the three classes was used for the purpose of comparing three different techniques for SE neutron capture identification. First, the SE energy and SE PSD distributions for the labelled neutron capture events were fit using gaussians and cuts based on the number of sigma from the center of the distribution were tuned to maximize F1 score on the test dataset. Four different parameters were utilized, the number of sigma above and below for both the SE energy and SE PSD value.

The second technique is the same as the first, except that the energy estimation is based on the ML Z prediction. As was discussed in section 6.2.2, the best method for reconstructing energy was found by using the ML Z estimate and using calibration curves of pulse amplitude vs Z to estimate the photoelectrons that would have been detected by the missing PMT. Thus, the Z prediction is used to get an energy prediction which will be called ML energy. In the same manner as technique 1, the ML energy and PSD distributions for neutron capture events are fit with gaussians and the number of sigma from the centroid of the distribution is used as a tunable parameter for optimizing the F1 score. Figure 6.13 shows the energy-PSD distributions for neutron capture events using dual ended calibration, SE variables, and ML variables.

The third technique utilizes a classifier which is trained on the three classes relevant to this problem - ionization, recoil, and neutron capture. The classifier for this study consisted of a convolutional neural network designed to output a single classification score for event. The confusion matrix for the classifier is shown in figure 6.14. For this technique, a threshold is chosen which represents the minimum neutron capture classification score to pass the cut. This threshold is varied.

Neutron Capture Identification Results

A comparison of all three techniques is shown in table 6.6. The cuts shown for each technique are the ones that resulted in the lowest F1 score. The improved energy

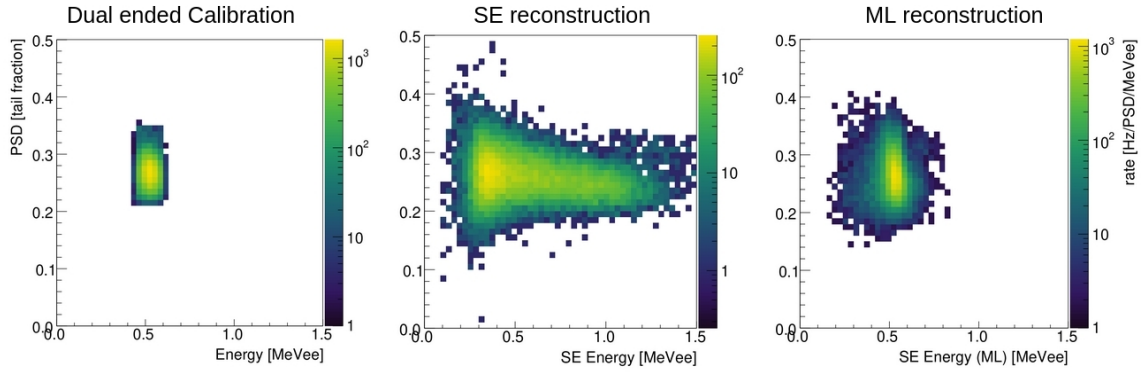


Figure 6.13: From left to right are the dual ended, single ended, and single ended ML reconstructed energy PSD distributions for neutron capture events. The ML Z estimation greatly improves energy reconstruction which leads to less overlap between neutron capture and recoil events.

True label	ionizations	0.8707	0.1262	0.0031
	recoils	0.1071	0.7180	0.1749
	ncapts	0.0093	0.0735	0.9171
		ionizations	recoils	ncapts
		Predicted label		

Figure 6.14: Neutron captures are most likely to be confused with recoils, with 17% of recoils being mislabelled as neutron captures and 7% of neutron captures being mislabelled as recoils.

estimation from the SE Z reconstruction improves the F1 score by 10%. However, the classifier outperforms both cut based methods, with a further 7% improvement in F1 score over the energy reconstruction method.

Despite these improvements over the traditional method, the cut turns out is not good enough for discriminating background events in a real event selection. When adding events containing a SE neutron-capture like signal as determined by setting a threshold at score t_{nc} , the effective statistic metric (which will be described in section 6.10.1) decreased for any value of t_{nc} . This indicates that a precision of 75% on the test dataset (which uses equal numbers of each event class) allows too many reactor gammas and electron-like cosmic backgrounds miscategorized as neutron captures for the cut to be useful in practice.

Table 6.6: Results from the neutron capture identification case study. The case study shows that a classifier is best for distinguishing neutron capture events from recoils and ionizations. $\sigma_{P,E}^{A,B}$ are the sigma widths of the cutoff above (A) or below (B) the mean for PSD (P) and energy (E). Thresh is the neutron capture classifier score threshold.

Method	σ_P^A	σ_P^B	σ_E^A	σ_E^B	Thresh	Prec	Rec	F1
E PSD Cut	0.80	4.00	1.50	5.00	n/a	0.668	0.704	0.686
ML E PSD Cut	0.83	4.67	2.33	5.00	n/a	0.714	0.769	0.740
ML Classifier	n/a	n/a	n/a	n/a	0.67	0.753	0.833	0.791

6.9 Ionization Identification

The nominal method for single ended reconstruction is to utilize the PSD and visible energy in the SE segment and determine if it is recoil-like via a fit to the ionization-like region of the PSD vs energy band. Any prompt candidate events outside of this band are determined recoil-like and are rejected. The fit is performed by finding the 1 sigma width of the best fit Gaussian to the SE PSD distribution for seven different energy ranges between 0 and 10 MeVee of visible SE energy. A functional form of

$w_i = \sqrt{A + \frac{B}{E_i}}$ is used fit to the sigma widths w_i at each energy midpoint E_i to derive a scaling function for any energy. The cut that is optimized is the number of sigma widths above the band to accept IBD candidates. The idea is that a prompt positron signal should not have any segments containing recoil-like signals. This is the same as what is done with the double ended analysis except that the differentiation between ionization and recoils is not as good for SE signals.

In order to determine if the improved energy estimation using the ML based SE Z reconstruction improves this cut, the same procedure is applied using the ML energy variable. Another method is to utilize the classifier output for reconstructing PID as described in 6.2.3. Here the a threshold for accepting the signal as ionization-like is applied; events containing SE hits below this threshold are rejected as prompt candidates.

Similar to the neutron capture ID case study, we varied the relevant parameters to optimize the F1 score for ionization selection in order to get a comparison between methods. The results of these three methods are shown in table 6.7.

6.9.1 Ionization Identification Results

After optimizing F1 scores, an n sigma of 1.82 and 2.06 were found for the nominal and ML based PSD cuts respectively. A low acceptance threshold of 0.21 was found for classifier method. The low threshold was likely due to the fact that any event falling with the 0.05 to 10.0 MeVee total visible energy range was considered for this study. This means that most of the events are going to be ionizations from reactor backgrounds, so the number of recoil-like events is relatively small. A larger threshold is likely to be found optimal when applying to a real IBD analysis because the prompt-delay candidate search will greatly increase the proportion of possible recoils in coincidence with a candidate neutron capture-like event.

As we can see from table 6.7, the classifier outperforms the cut based methods, while the improved SE energy information from the ML technique does not improve

this cut relative to the nominal method. This study shows that the classifier would be the proper choice for improving event rejection using SE segment information.

6.10 Inverse Beta Decay Selection Results

This section will describe the usage of the ML-based SEER for enhancing IBD background discrimination. The nominal SEER cuts based on Gaussian fits to the SE PSD band at different energies and the SE visible energy (no position correction) is described in detail in section 5.5.2. A comparison between the nominal SEER cuts and the ML-based method will be shown. A discussion on further possible improvements given more detailed waveform simulation development is given at the end of the section.

6.10.1 Method

The machine learning approach follows as described in section 6.6.1. Position reconstruction is used to estimate the energy which allows a tighter bound on the largest allowed energy hit in a SE segment. Ionization identification allows us to replace the SE PSD fit-based cut with a class score threshold. Events with any SE segments containing a ionization class score below the threshold are rejected. Additionally, a veto window is constructed identical to the “SE Recoil veto” as described in section 5.5.2 for events with an ionization class score below this threshold. The model used for energy reconstruction is shown in figure 6.1; the event classification model used is shown in table 6.3.

In order to optimize the energy threshold and class score threshold, first the nominal SEER cuts as shown in table 6.8 are used and the energy cut or the PSD cut are swapped out one at a time. Each cut is optimized individually, the metric used for maximization is the effective statistics N_{eff} which is defined as

$$N_{eff} = \sum_i n_i^2 / \sigma_i^2, \quad (6.12)$$

where n_i is the background subtracted IBD counts in energy bin i and σ_i is the statistical uncertainty based on counting statistics for the accidentals, and the reactor on and off signals. There is a tradeoff between increasing the total reactor on statistics which increases the effective statistics but also increases the reactor off total statistics which lowers the effective statistics due to the additional uncertainty in the background induced. Also, the reactor on and off signals are accidental subtracted so stricter cuts will also reduce accidentals which will reduce their respective uncertainties increasing effective statistics.

Once the value of the energy and classifier thresholds are chosen based on maximization of the effective statistics for 20% of the dataset sampled evenly across all 5 periods, the remaining cuts shown in table 6.8 are varied one at a time to maximize the effective statistics while the ML-based cuts are set in place. Finally, once the new values of the non-ML cuts are found, the ML cuts are then re-varied for the final maximum shown also in table 6.8.

6.10.2 Results

After the first round of optimization using the nominal values for all non-ML cuts and varying the cuts one at a time, it was found that using the ML energy estimator the cut could be moved from 0.8 SE MeV_{ee} to 0.6 ML MeV_{ee}. This resulted in a small 0.5% increase in the effective statistics of the dataset. The introduction of the ML classifier for ionizations resulted in a larger gain of 1.5% increase in effective statistics. A class score of 0.03 was found to optimize this which was much lower than the 0.21 found to optimize the F1 score in the test dataset. However, this test dataset was based on a uniform sampling of the background data which gave a much larger fraction of ionizations than the IBD candidates which require the delayed neutron

capture. So it is understandable that the optimal threshold for IBD selection is much lower.

Introducing both of these ML cuts with the nominal non-ML cut values, a 2% increase in effective statistics results along with a 8% increase in the signal to accidental background ratio and a 4% increase in signal to correlated background ratio.

This increase in signal to background allows us to relax the non-ML cuts to less restrictive values which allows more of both signal and background. Because the ML SEER cuts are more efficient than the non-ML SEER cuts, this increase in both signal and background brings about larger effective statistics. The final reoptimized cut values are shown in the last column of table 6.8. Ultimately the introduction of the ML SEER cuts results in a 4% increase in effective statistics albeit with a 2% (4%) reduction in signal to correlated (accidental) background ratio. The results are summarized in table 6.9.

6.10.3 Discussion

Modest improvements in the event selection were obtained using machine learning based SEER. It is possible that additional improvements could be found utilizing the positron classifier. This would require more detailed pulse simulations that capture the underlying timing correlations that the networks learn in order to perform as they do. This way one could be confident of the performance of the network that has been trained on simulated data when applied to real data. The SEER analysis was able to get around this issue by training with real data and using the dual ended reconstructed calibrated values as the target.

In addition to being able to train with simulated data, one could also utilize a realistic pulse simulation to estimate the efficiency of the ML-based event selection, which is needed for any IBD analysis. In the same manner as is done for the nominal event selection, IBD events with positron energies in the range of interest would be

simulated based on the inverse square law distribution within the detector and the ML selection would be applied to determine the energy dependent efficiencies.

One interesting finding in this study is that both graph and convolutional neural networks exhibit similar performance for tasks of interest related to event reconstruction. It is not entirely clear why the CNN outperforms the GNNs on Z reconstruction while the GNN outperforms the CNN on segment event classification. It was also found that different types of graph network implementations worked to varying degrees for different problems. The GMMConv that was chosen as the best classifier, for example, did not perform best at Z reconstruction. Thus, it is valuable to explore different implementations of these ML algorithms to find which ones best suit the problem at hand.

6.11 Conclusion

Convolutional neural networks and graph convolutional networks were applied to the PROSPECT dataset for the purpose of recovering information from single ended segments. It was found that utilizing the full waveform information from the digitized PMT signals were required to provide the best performance for SE reconstruction. CNNs were found to excel at reconstructing the position of the event in SE segments while GCNs performed best at classifying energy depositions in SE segments. With a position reconstruction one can better estimate the amount of energy deposited in a segment and use this to more powerfully reject IBD backgrounds. Similarly, the classification reconstruction can also help determine heavier recoiling particles in SE segments which allows further background rejection. It was shown that the GCN outperformed the tail fraction method of PSD classification for SE segments. This resulted in a larger overall signal to background, which allowed us to relax veto window lengths so as to maximize the effective statistics of the dataset using ML. A 3.5% improvement in effective statistics was achieved over the traditional tail fraction method of particle identification.

Further applications of ML for event selection were detailed as well. This includes full waveform CNNs for positron identification based on PROSPECT simulations. Further work on accurate pulse simulations are required to utilize this in the PROSPECT data. This type of network could be applied to future neutrino experiments. Especially promising are solid state detectors which can provide greater spatial resolution for particle tracks to help distinguish positron event topology from electrons and gammas. Training CNNs (or GCNs which provide similar performance) based on accurate well-tuned simulations can simplify the otherwise complex analysis process for such a detector.

Table 6.7: Results from the ionization identification case study. The case study shows that a classifier is best for distinguishing ionization events from other event types.

Method	N Sigma	Threshold	Precision	Recall	F1 Score
E PSD Cut	1.82	n/a	0.9262	0.9905	0.9573
ML E PSD Cut	2.06	n/a	0.9263	0.9882	0.9562
ML Classifier	n/a	0.21	0.9529	0.9830	0.9667

Table 6.8: Table of cuts for nominal values as described in sections 5.4.1 and 5.5.2 and the reoptimized values when using ML-based SEER cuts. "Delay PSD" is the ^6Li neutron capture sigma width for the delay signal (which must be a single segment cluster), while "Delay E" is the sigma width of its energy. "Prompt PSD" is the sigma width of the electron-like band, "Muon E" is the energy above which a cluster is vetoed with a window shown by "Muon Veto". "Distance" is the maximum allowable distance in Z between the prompt and delay for delayed occurring in the (same, adjacent) segment as the prompt. "SE PSD" is the sigma width of the ionization-like SE PSD, "ML Score" is the ML ionization classification score for SE segments, "SE E" is the SE energy upper limit for SE segment hits, and "ML SE E" is the ML energy prediction for those hits.

Name	Nominal Value	ML Value
Delay PSD	2.2σ	2.2σ
Delay E	2.0σ	2.0σ
Prompt PSD	2.0σ	2.1σ
Muon E	$15.0 \text{ MeV}_{\text{ee}}$	$18.0 \text{ MeV}_{\text{ee}}$
distance	$(140, 60) \text{ mm}$	$(140, 70) \text{ mm}$
Fiducial Z	968 mm	984 mm
Pileup Veto	800 ns	650 ns
Recoil Veto	$[0, 200] \text{ us}$	$[0, 190] \text{ us}$
nCap Veto	$[-300, 300] \text{ us}$	$[-270, 270] \text{ us}$
Muon Veto	$[0, 200] \text{ us}$	$[0, 180] \text{ us}$
SE PSD	3.5σ	—
ML Score	—	0.035
SE E	$0.8 \text{ MeV}_{\text{ee}}$	—
ML SE E	—	$0.6 \text{ MeV}_{\text{ee}}$

Table 6.9: Results for IBD selection using nominal values, nominal values with ML SEER subbed in, and reoptimized values with ML SEER. A 3.5% increase in effective statistics is observed with the introduction of ML SEER.

	Nominal	Nominal + ML	ML Optimal
IBD Stats / Day	497.0	487.4	519.7
Signal : Correlated Background	3.33	3.50	3.27
Signal : Accidental Background	3.98	4.29	3.82
Effective Stats / Day	244.9	248.0	253.6

Chapter 7

Conclusion

There are a number of properties of the neutrinos that researchers are actively working to uncover. As more experiments are run, it seems that anomalies of various types keep arising in defiance of the 3 flavor neutrino model. With recent experiments such as BEST [112] confirming the "Gallium anomaly" and the still unexplained LSND anomaly, it is clear that high precision neutrino measurements are needed to tease out the underlying physical processes contributing to these discrepancies. Meanwhile, we have entered into the period of high precision neutrino measurements at short baseline for reactor measurements with PROSPECT and STEREO. PROSPECT was the first high precision measurement of the ^{235}U spectrum and found that the null hypothesis of no sterile neutrinos is preferred to the best-fit RAA parameter space by 2.5σ . In addition, the RAA has since decreased in significance to about 1σ due to reanalysis of the reactor spectra predictions coming from improved measurements of the beta decaying daughters via TAS measurements.

While the PROSPECT results do not confirm the sterile neutrino hypothesis, they do not totally exclude parts of the parameter space that could give rise to solutions to the Gallium anomaly. Additionally, the PROSPECT experiment found variations in the shape of the measured spectrum consistent with variations seen in Daya Bay and other reactor experiments. The shape anomaly points to the need for more high

precision measurements of reactor $\bar{\nu}_e$ with even great statistics in order to resolve this with the improving spectra predictions coming from TAS-based measurements of the fission daughter beta decay spectra.

So while much progress has been made in resolving the various issues that have arisen with short baseline neutrino detection from man-made sources, there is still a great deal of interesting physics to be uncovered with the next generation of $\bar{\nu}_e$ measurements at reactors. Measurements of CE ν NS at a reactor has still yet to be accomplished which in the future might provide access to the low energy portion of the reactor spectrum that is currently inaccessible with IBD based measurements. Central to any of these future measurements will be a detailed characterization of the reactor and cosmogenic backgrounds and analysis techniques to mitigate them. This thesis provided an in depth look at said backgrounds at the High Flux Isotope Reactor in Oak Ridge, TN. The work done characterizing the backgrounds will be useful for future experiments due to the detailed information regarding the backgrounds present along with a precise spatial identification of the primary source related to one of the neutron beamlines. This information provides guidance for targeted gamma shielding that has the potential to greatly reduce gamma related backgrounds in future experiments. It is also useful for understanding backgrounds relevant to fission product gamma ray spectroscopy.

Finally, the thesis also showed a novel application of machine learning techniques to reactor neutrino data. It was shown that these techniques can improve on traditional techniques, finding a 3.5% increase in effective statistics across the PROSPECT IBD dataset. With a well tuned simulation, one could leverage these techniques for data analysis in future experiments involving segmented readouts.

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Appendix

Appendix A

HFIR Experiment Hall Gamma Sources

A list of gammas and their corresponding parent isotopes found in the gamma spectra taken in the experiment hall at HFIR. is shown in table A.1. All isotopes are present coming from the direction of the reactor pool with the exception of ^{48}Ti , which is present in spectrum coming from the floor above the HB4 hot spot. Energies listed are from the most frequent gammas resulting from neutron capture except for Eu, Ar, Co, and K are decays from radioactive isotopes. Energies and yields are obtained from the nudat database [260] for radioactive decays and capgam [261] for neutron capture reactions. What follows is the gamma spectrum depicted in figure 3.6 broken up into various energy ranges with the peaks identified.

Table A.1:

Isotope	Energy [keV]	Yield [%]	reaction
^{59}Ni	11386.5	48.206	neutron capture
^{59}Ni	10054.14	18.43	neutron capture
^{59}Ni	9102.1	19.798	neutron capture

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Table A.1: (Continued)

^{53}Cr	9718.79	20	neutron capture
^{53}Cr	8884.81	56.203	neutron capture
^{53}Cr	7100.11	9.633	neutron capture
^{53}Cr	6645.64	12.291	neutron capture
^{63}Ni	9656.89	80.702	neutron capture
^{63}Ni	8311.45	9.825	neutron capture
^{54}Fe	9297.8	100	neutron capture
^{54}Fe	8886.4	18.636	neutron capture
^{58}Ni	8998.63	100	neutron capture
^{58}Ni	8533.71	47.839	neutron capture
^{58}Ni	8120.75	8.501	neutron capture
^{50}Cr	8512.2	37.5	neutron capture
^{50}Cr	8484.2	32.5	neutron capture
^{50}Cr	7362.6	15.525	neutron capture
^{50}Cr	6135.9	11.263	neutron capture
^{52}Cr	7938.58	100	neutron capture
^{52}Cr	7374.58	18.942	neutron capture
^{52}Cr	5618.23	32.287	neutron capture
^{52}Cr	5269	11.331	neutron capture
^{60}Ni	7819.56	100	neutron capture
^{60}Ni	7536.62	57.0388	neutron capture
^{27}Al	7724.034	96.0573	neutron capture

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Table A.1: (Continued)

^{27}Al	7693.398	12.366	neutron capture
^{56}Fe	7645.58	86.207	neutron capture
^{56}Fe	7631.18	100	neutron capture
^{56}Fe	7278.82	20.69	neutron capture
^{56}Fe	6018.42	34.138	neutron capture
^{56}Fe	5920.35	33.103	neutron capture
^{63}Cu	7916.26	100	neutron capture
^{63}Cu	7638	48.943	neutron capture
^{63}Cu	7307.31	27.0695	neutron capture
^{63}Cu	7253.05	12.538	neutron capture
^9Be	6809.61	100	neutron capture
^9Be	3367.45	49.165	neutron capture
^9Be	3443.406	16.84	neutron capture
^9Be	2590.014	32.929	neutron capture
^9Be	853.63	35.812	neutron capture
^{48}Ti	6760.12	54.15	neutron capture
^{48}Ti	6418.53	35.67	neutron capture
^{154}Eu	1274.43	34.83	radioactive decay
^{154}Eu	723.30	20.06	radioactive decay
^{152}Eu	778.9	12.93	radioactive decay
^{152}Eu	841.63	14.2	radioactive decay
^{152}Eu	963.38	11.6	radioactive decay

Continued on next page

Table A.1: (Continued)

^{152}Eu	964.01	14.51	radioactive decay
^{152}Eu	1085.84	10.11	radioactive decay
^{152}Eu	1112.08	13.67	radioactive decay
^{152}Eu	1408.01	20.87	radioactive decay
^{41}Ar	1293.64	99.16	radioactive decay
^{40}K	1460.82	10.66	radioactive decay
^{60}Co	1332.5	99.98	radioactive decay
^{60}Co	1173.2	99.85	radioactive decay

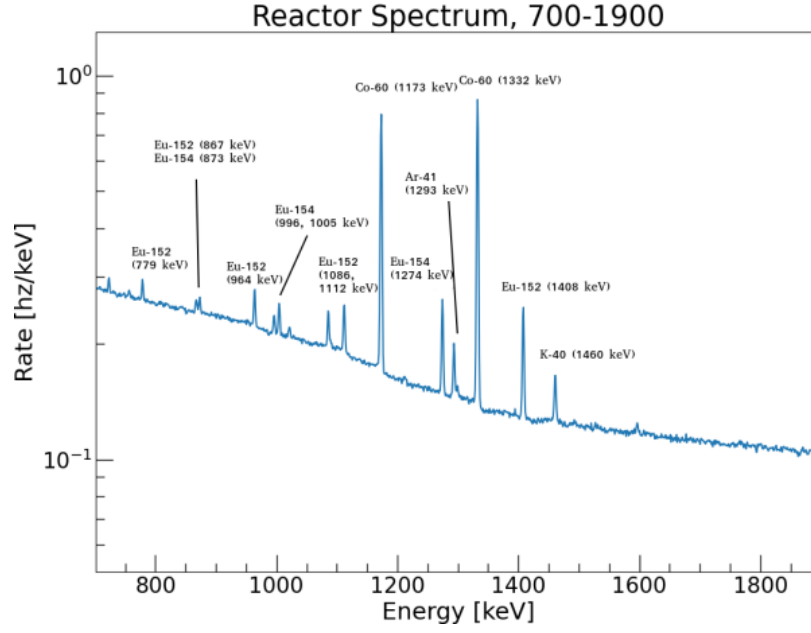


Figure A.1: Peaks labelled for spectrum taken under the MIF with collimator pointed at the reactor core, 700 - 1900 keV.

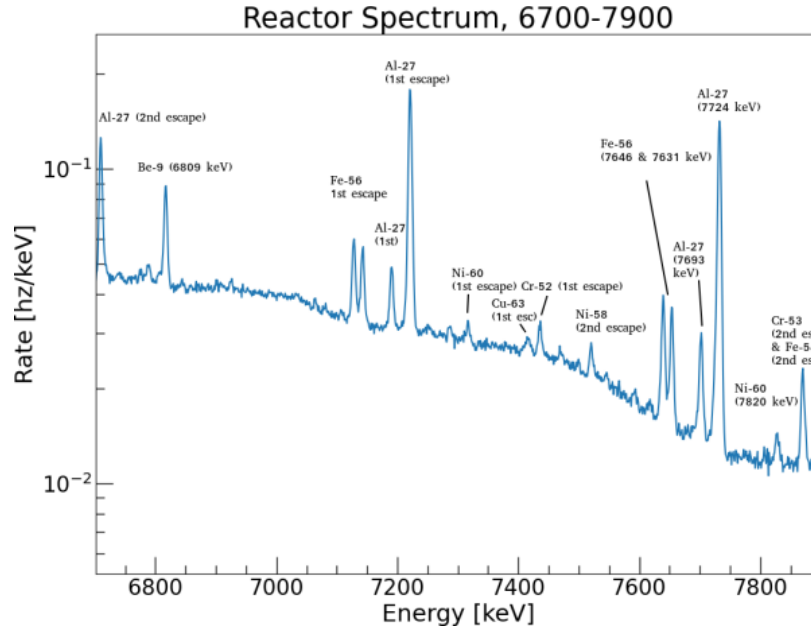


Figure A.2: Peaks labelled for spectrum taken under the MIF with collimator pointed at the reactor core, 6700 - 7900 keV.

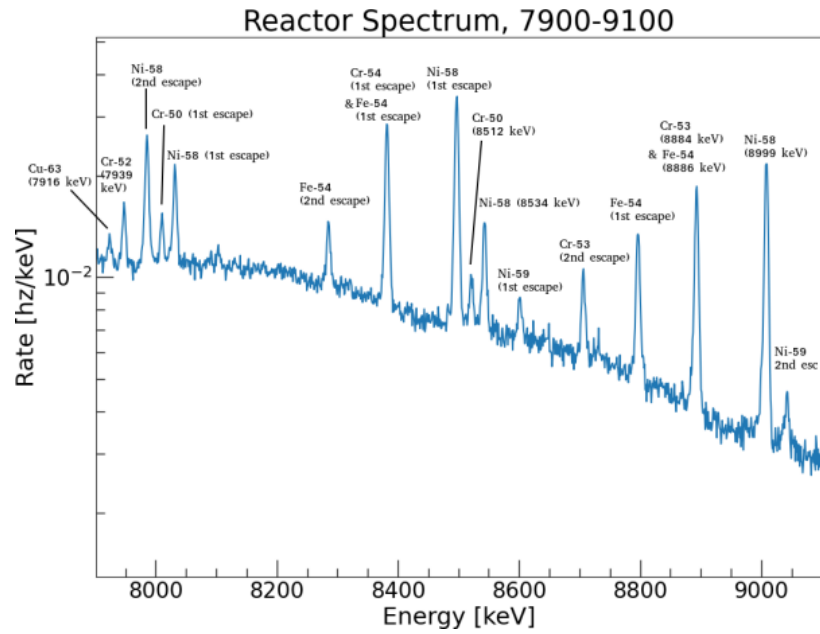


Figure A.3: Peaks labelled for spectrum taken under the MIF with collimator pointed at the reactor core, 7900 - 9100 keV.

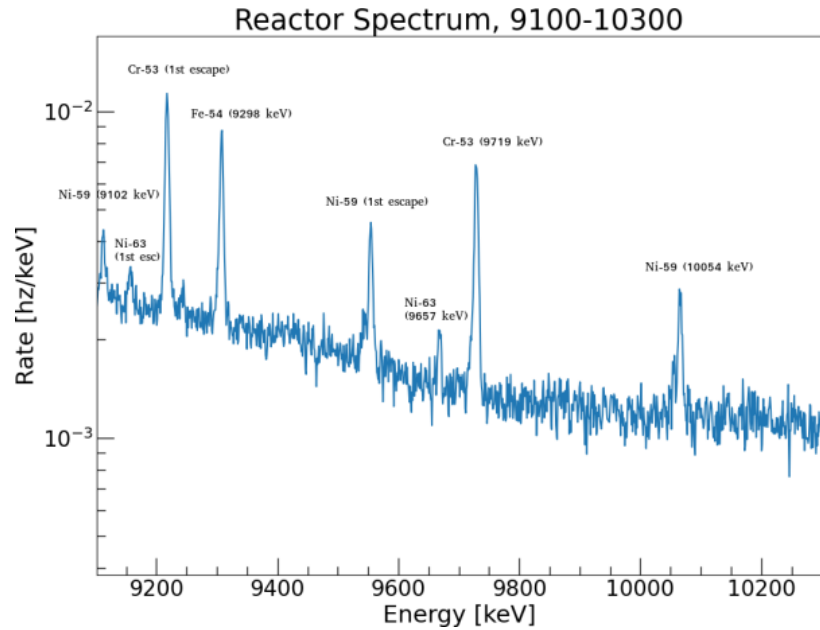


Figure A.4: Peaks labelled for spectrum taken under the MIF with collimator pointed at the reactor core, 9100 - 10300 keV.

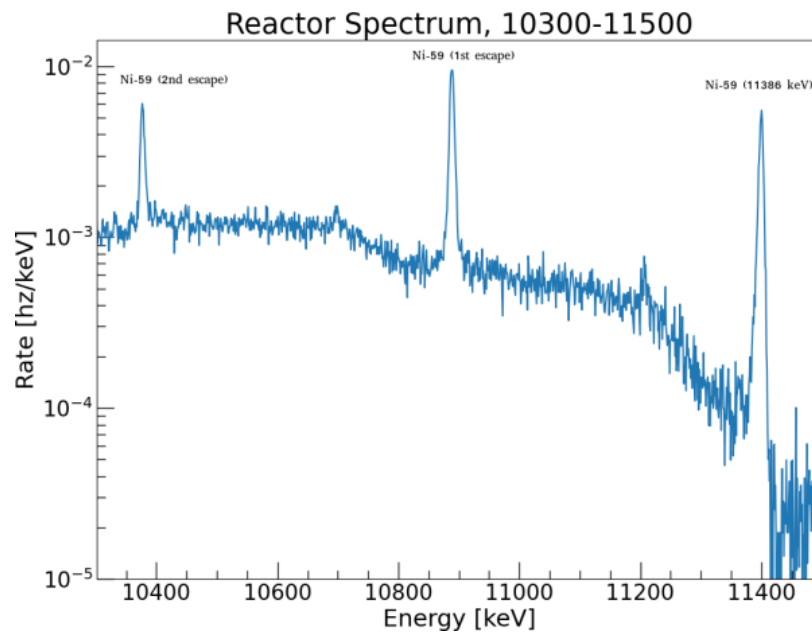


Figure A.5: Peaks labelled for spectrum taken under the MIF with collimator pointed at the reactor core, 10300 - 11500 keV.

Vita

Blaine A. Heffron was born in Birmingham, AL and moved to Mt. Pleasant, SC at the age of two. He was second of four children born to Susan and Greg Heffron. After graduating Wando High School, he attended The University of North Carolina at Chapel Hill, NC, graduating in 2012 with a Bachelors of Science in Physics. He then worked with an environmental engineering group at UNC before attending University of Tennessee at Knoxville in 2014. In addition to his primary work with the PROSPECT collaboration, he participated in experimental efforts at HRIBF, RIKEN, and visited Los Alamos to work on antineutrino calculations. He graduated with a Masters in Physics in 2017 then proceeded to work in web development and database software roles, including helping found a company, performing web development as an independent contractor, and working in tech support for CData. In 2019 he decided to return to Knoxville for his PhD in Physics, where he has continued working with the PROSPECT collaboration.