Calibration of Large Liquid Argon Detectors Utilizing External Neutron Source

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Abstract

The purpose of my research was to use Geant4 simulations to design a neutron source capable of calibrating large liquid argon detectors. A general design was used to optimize each part of the moderator using two key parameters: thickness and material. I found that an initial moderating volume of elemental iron followed by a filtering volume of elemental sulfur provided an adequate flux of neutrons within the required energy range necessary for calibration. Multi-layer, Multi-material configurations of the filter were also tested, but due to sulfur's effectiveness and simplicity, it was chosen to be used as a good first approximation for the study. After the general design was completed, the findings were applied to the specific engineering specifications of the DUNE Far Detector. While these simulations were conducted for the purpose of calibrating DUNE, the applications of this new technique are relevant to all experiments using liquid argon. This fact coupled with the positive results of my simulation warrant further real world testing of the moderator's design as well as the eventual usage of the technique on DUNE and other experiments like it.

1 Purpose and Theory

A time projection chamber (TPC) is the most common form of neutrino and dark matter detectors. They function by setting up a uniform electric field through out the volume. This is accomplished by splitting the detector up into multiple sections each with a cathode plane, made of a resistive material, and multiple anode wire planes which combine to form a wire grid. When a neutrino interacts with the detector, its deposited energy ultimately manifests in the form of electrons. These free electrons then drift through the constant electric field and are deposited on the anode wire plane. Using the time, the magnitude of current through the wire, and the location of the wire in the grid, scientists are then able to reconstruct a 3-dimensional representation of the electron tracks, the position of the original event vertex, and the net energy deposition.

However, the net charge collected is dependent on the electric field strength. So, if the electric field is not perfectly uniform through out the detector, then some areas of the detector will record higher net charge than others given the same initial energy deposition. Furthermore, the purity of the argon can effect electron lifetimes and recorded noise my be different in different parts of the detector. Therefore, it is necessary to use a known energy deposition to tune specific areas of the TPC in order to get consistent data collection throughout the volume.

There are many strategies to producing such standard energy depositions. Chief among these schemes is the deployment of radioactive sources inside the detector's volume. The advantages to this technique are that the activity and location of the source are well known. However, there are clear draw backs to this scheme, especially when applied to large detectors such as DUNE. First, the source must be placed at varying locations inside the TPC which represents logistical and engineering challenges. Second, the presence of the source affects the surrounding electric field. And third, dropping equipment and radioactive material into the TPC represents a potential risk to the purity of the liquid argon.

Due to these challenges, a new strategy for calibrating large liquid argon detectors is required. One such method which solves all of these challenges is external neutron calibration. The neutron source can be placed on top of the detector without the need to open the cryostat. The neutrons can propagate through out the volume of the detector without altering the existing electric field. Conservatively, the source would need to run for 30 minutes and neutrino data collection can run in parallel during this time. This is a very quick time when compared to alternative techniques such as using cosmic muons which will take on the order of several months to calibrate the TPC.

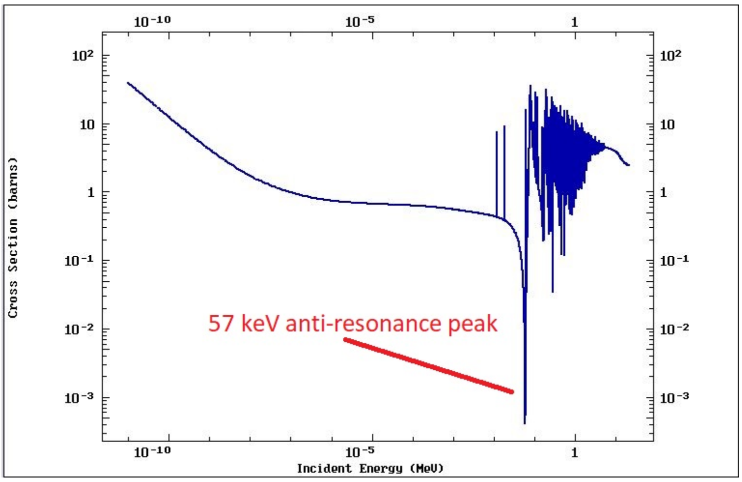


Figure 1: Plot of total neutron cross section as a function of incident energy [1]

The conceptual basis for external neutron calibration relies on a special property of argon-40's total neutron cross section. At a incident neutron energy equal to 57 keV, argon's total cross section is significantly decreased, as shown in Figure 1. At 57 keV, a neutron's mean free path inside argon is approximately 34 meters which is more than half the DUNE TPC length. This will allow neutrons to travel long distances inside the TPC before capturing. The goal of the neutron source is to send neutrons of energy just above 57 keV into the TPC volume so that they elastically scatter, losing energy, and fall into the anti-resonance saddle point upon which they are free to disperse throughout the detector ultimately capturing on an argon nucleus. Once the neutron is captured, the argon nucleus is left in an excited state and subsequently decays with an energy equal to the binding energy difference between Ar-40 and Ar-41, approximately 6.1 MeV. Finally, this measurable energy deposition signature can be used to calibrate the TPC.

2 Simulation Set Up

This section details the specific software, physics lists, and nuclear data files used to conduct the simulation. The section also includes a description of the detector volume, the general neutron source geometry configuration, and the parameters used to simulate the neutron gun.

2.1 Simulation Software Used

Version 10.04.p02 of Geant4 was used for this simulation. The following physics lists were also implemented: G4BosonConstructor, G4LeptonConstructor, G4MesonConstructor, G4BosonConstructor, G4BaryonConstructor, G4IonConstructor, and G4ShortLivedConstructor. Furthermore, the ENDF-VIII Neutron High Precision Library was used in order to more accurately simulate neutron interactions. The resulting data from the simulations were then fed into ROOT files to be processed and analyzed. The Qt4 visualization package was also used through out the project.All processes were run on a Linux Mint operating system.

2.2 Configuration of the Detector

The model of the liquid argon TPC in the simulation is based off DUNE's TPC specifications. The liquid argon pool is 58m x 14.5m x 12m. Then placed on top of the pool is a 0.8 m thick layer of argon gas to act as a buffer. These two volumes are contained in a 1 cm thick, stainless steel cryostat. The whole detector volume is wrapped in a 90 cm thick insulating layer of polypropylene. A cylindrical feed through port of radius 10 cm is added in the top center of the detector. A diagram of the detector's geometry is in Figure 2.

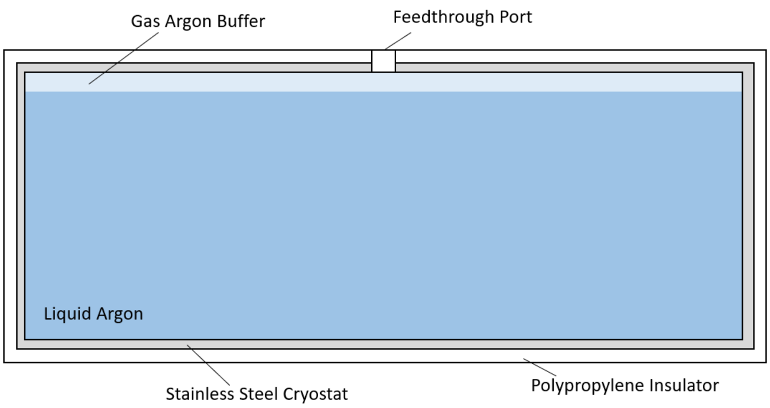


Figure 2: Simulated Detector Design

2.3 Configuration of the Neutron Source

The neutron source design is shown on Figure 3. An off axis configuration in which the neutron beam is reflected off an internal reflector before exiting the source was considered, however the final design was chosen for its simplicity and effectiveness. Furthermore, similar neutron source designs have been used successfully for Boron Neutron Capture Therapy [2] [3]. There are six components to the source's design. One, a deuterium-deuterium gun produces neutrons with energy roughly equal to 2.5 MeV. Two, the moderator volume efficiently cuts down the neutron energy from 2.5

MeV to 1 MeV. Three, the filter volume selects the specific energy needed for calibration, 57 keV to 87 keV. Four, a thermal absorbing volume of Lithium is placed at the entry to the argon pool in order to capture any neutrons that may have fallen below the 57 keV threshold. Five, the reflecting volume is added to increase efficiency by reflecting downward any back scattered neutrons. And six, the whole source is encased in a shielding volume for safety.

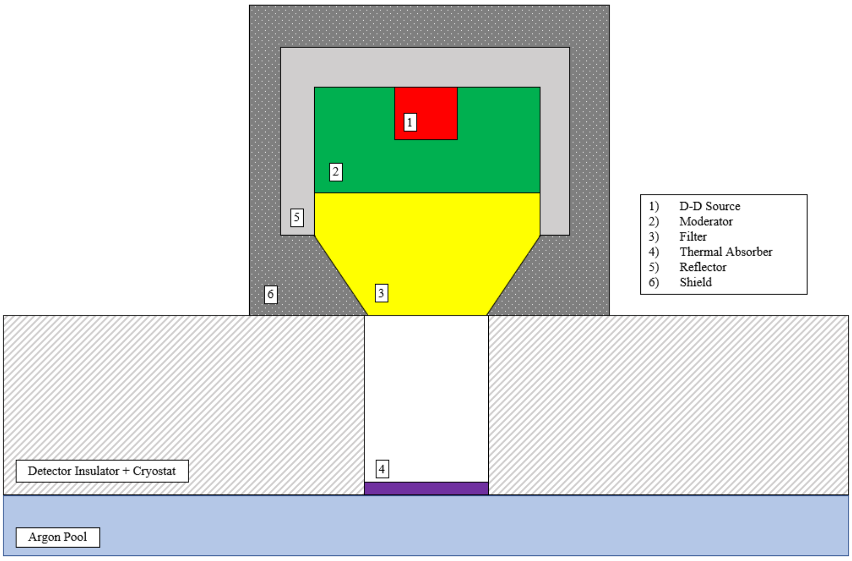


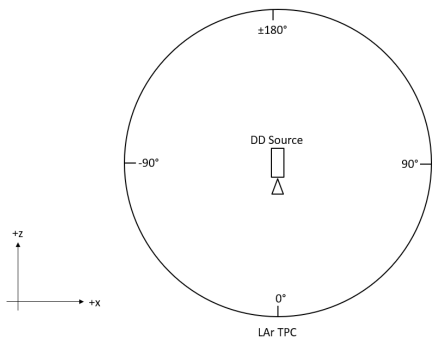
Figure 3: Design for a General Neutron Source

2.4 Simulating a Deuterium-Deuterium Neutron Gun

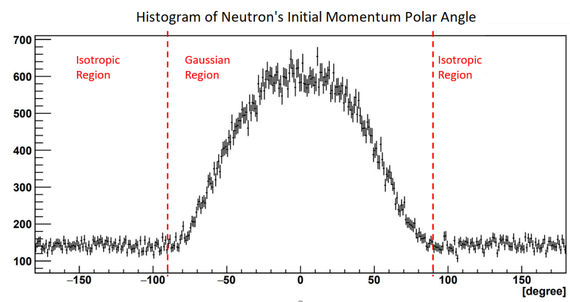
Unlike protons and electrons, neutrons can not be focused using electromagnetic fields. For this reason, the neutron source does not produce a tightly focused beam of neutrons. Instead, it shoots neutrons mostly straight but with some statistical uncertainties. This is not an insignificant factor, and therefore, must be accounted for in the simulation. Using initial momentum measurements of a D-D source made by R.F. Lang et al. [4], a probability distribution for the polar angle of initial momentum of the neutrons was constructed. The azimuth angle was taken to be isotropic. As Figure 4b shows, the probability distribution is split into two regions. The first region, titled 'Gaussian Region' on Figure 4b, covers angles in front of the neutron source and is characterized by the function:

$$f(cos(\theta)) = A + B\ cos^2(\theta) + C\ cos^4(\theta) \tag{1}$$

where A = 0.237, B = -0.051, and C = -0.130. The second region, behind the source, was not measured by R.F. Lang. It's probability was assumed to be isotropic and equal to the lowest value of the Gaussian region. The energy of the neutrons was set to 2.5 MeV.



(a) Defining the coordinate system



(b) Histogram of 100000 simulated neutron's initial direction

3 Neutron Source Optimization

The following are the optimization results for each component of the neutron source design. The components of the neutron source's design were optimized in the order that follows.

3.1 Moderator

The goal of the moderator is to efficiently cut down the neutrons energy from 2.5 MeV to 1 MeV. To accomplish this a material is needed with a high elastic cross section to degrade the energy quickly and low absorption cross section to ensure a high flux of neutrons are able to escape the volume. Using these two criterion, ten materials were selected to be tested. Each material was simulated for 100,000 neutron events and each trial was conducted with a constant thickness of 25 cm. As Figure 5 shows, Elemental iron was chosen to be the optimal moderating material because it out performs all other materials by nearly a factor of two. This result makes sense because iron, being a transition metal, has an atomic mass that is roughly in the middle of elements relevant to the study. This allows it to have a high elastic scattering cross section while also minimizing its absorption cross section. Future studies could investigate the moderating properties of other transition metals such as vanadium and titanium.

After the material of the moderator was determined, the thickness of the material was varied, and the number of neutrons leaving the moderator volume with an energy between 2.5 MeV and 57 keV were counted. Each thickness was simulated for 50,000 neutron events.If the moderator is too thin, the neutron will not elastically scatter enough times to fall into the desired energy range. Conversely, if the moderator is too thick, the neutron will scatter too many times and fall below the 57 keV threshold. As the results show, approximately 18 cm of iron maximizes the number of elastic scatters inside the moderator.

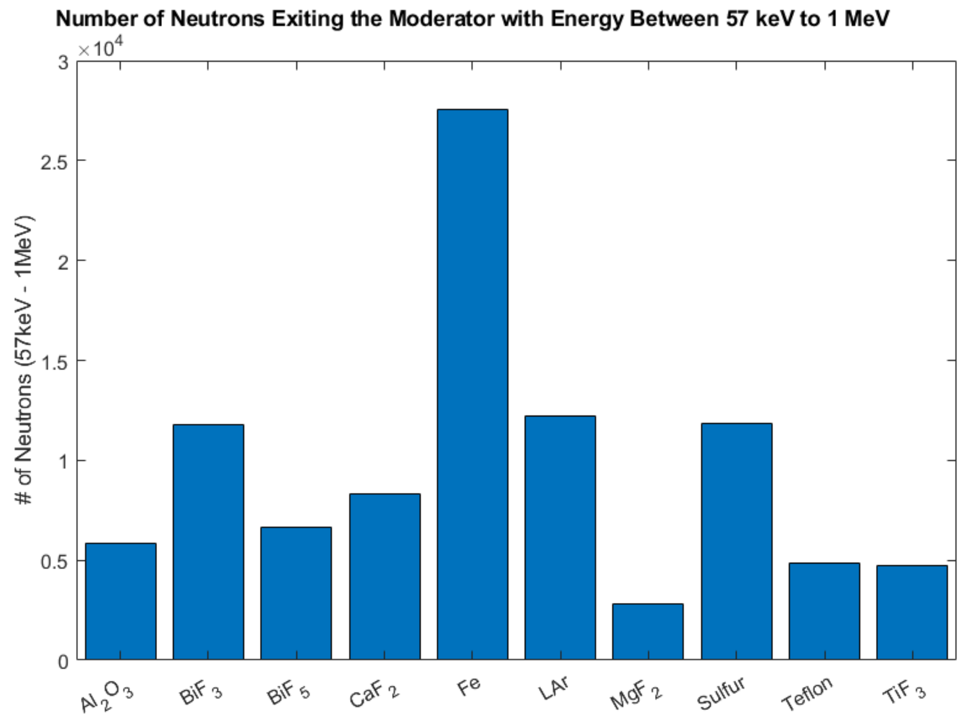


Figure 5: The moderating effectiveness of each material per 100,000 events

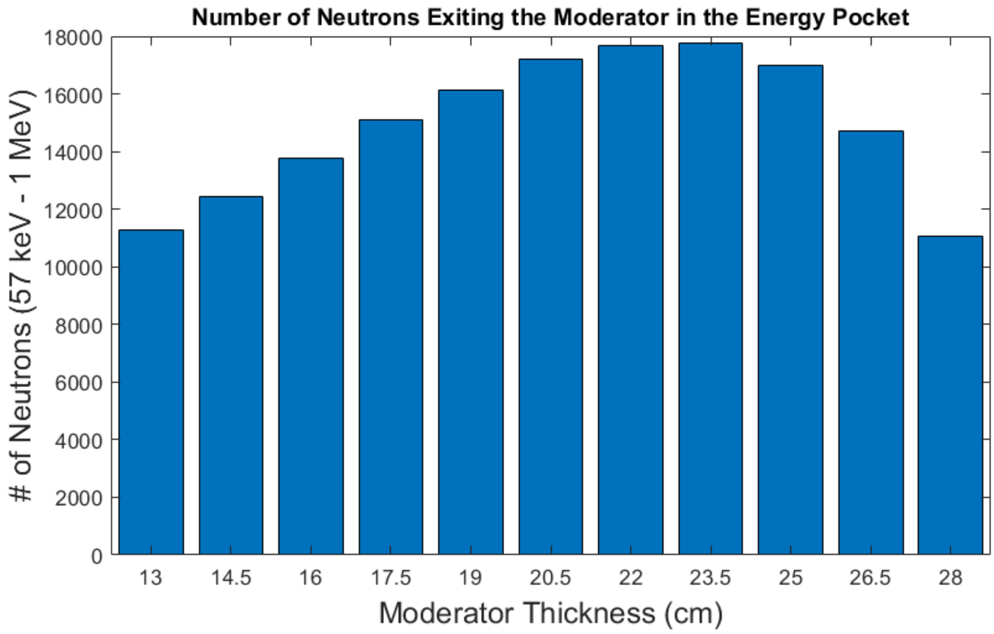


Figure 6: The effectiveness of varying moderator thicknesses in centimeters

3.2 Filter

The objective of the filter is to take the degraded energy spectrum from the moderator and select neutrons with energies within the necessary window from 57 keV to 87 keV. The easiest way to accomplish this is to select a material with an anti-resonance peak within this window. Liquid argon would clearly be the best material for this purpose however it also requires a cryostat which presents unreasonable engineering challenges. The best filter material was chosen to be Sulfur because it has an anti-resonance peak at 73 keV and can be used in powdered form. The number of neutrons exiting the filter with energies between 57 keV and 1 MeV were counted for varying thicknesses of the filter (see Figure 7). About 20 cm of sulfur is the optimal filter configuration.

Multi-layer, multi-material configurations were also investigated. Two main schemes were tested with varying material combinations. The first of these schemes was a two layer configuration in which the total filter thickness was divided into two layers of different material. The top layer was tested for varying materials while the material of second layer was chosen to be sulfur. The results of this are shown in blue in Figure 8. The second scheme tested was the sandwich configuration. The total filter volume was divided into thirds. The material for the top and bottom layers were sulfur while the material of the middle layer was varied. The results of this are shown in orange in Figure 8. When only counting the net number of neutrons that escape the filter inside the desired energy range, the pure sulfur configure out performs either of the multi-layer configurations. And when the two schemes are compared directly, the sandwich configuration out performs the two-layer configuration across all three materials. When the ratio of neutrons between 57 keV and 87 keV to the total number of escaped neutrons was taken, the sandwich configuration slightly out performs pure sulfur when Iron and BiF_3 are used as the second material (see Figure 9).So, while pure sulfur allows for the most neutrons of viable energy to escape the filter, the sandwich design produces a cleaner energy spectrum with fewer neutrons of too high or too low of energies.

Ultimately, a pure sulfur filter configuration with a thickness of 20 cm was chosen to be the most optimal because of its simplicity and ability to efficiently produce neutrons in the desired energy range. Further research is needed into multilayer configurations in order to determine their optimal effectiveness.

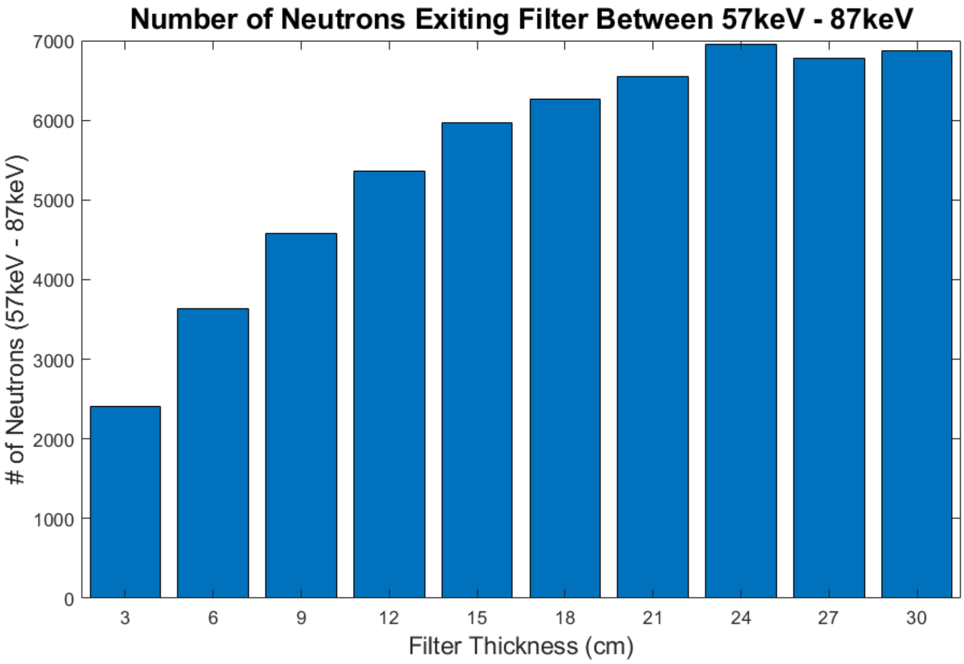


Figure 7: The effectiveness of varying sulfur filter thicknesses

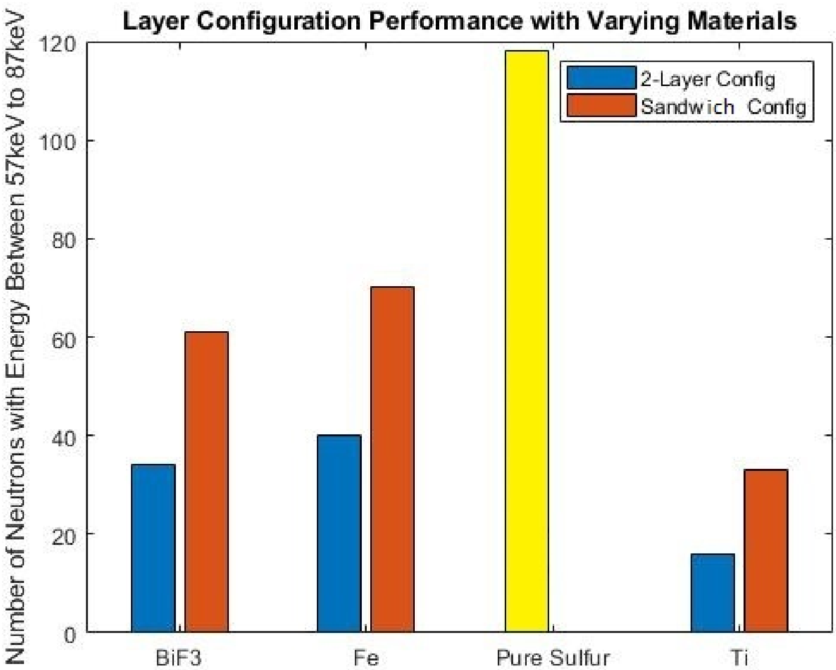


Figure 8: A direct comparison of two filter configurations with varying materials and pure sulfur as a bench mark

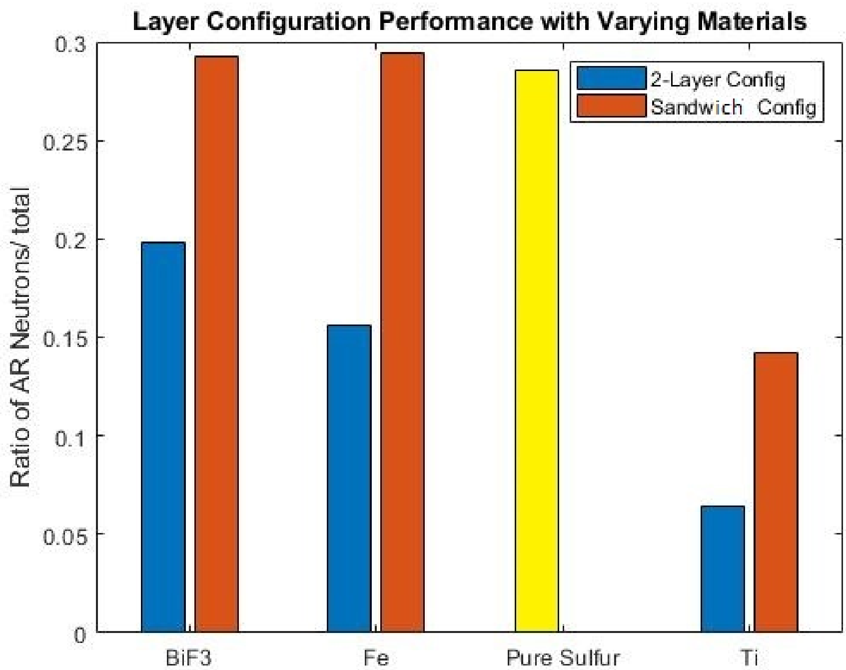


Figure 9: Comparing the ratio of neutrons within the energy range to the total number of neutrons escaping the filter volume

3.3 Reflector

The goal of the reflector is to increase the efficiency of the neutron source by reflecting any backscattered neutrons back toward the TPC's port. Two materials were studied as viable materials for the reflector: nickel and lead. These two were chosen for their high densities and high neutron elastic scattering cross sections. For both materials, ten reflecting thicknesses were simulated and the neutron flux exiting Filter 1 was measured. For reflector thicknesses above 12 cm, lead performs better. However, do to its high density, using more than 12 cm of lead as a reflecting volume would be impractical. Therefore, using less than 12 cm of nickel is the best option for the reflector. About 10 cm of nickel is enough to reflect most backscattered neutrons downward.

3.4 Shield

The objective of the shield is to block both scattered neutrons and gammas which are produced in the source as a result of neutron captures. Lithium-Polyethylene was chosen to be the material for the neutron shield because its rich in hydrogen and lithium atoms which yields a high neutron absorption cross section. Lithium-Polyethylene is also light weight, commercially available, and relatively inexpensive. The energy spectrum entering the shield has multiple peaks between 0.5 MeV and 1.5 MeV, and one major spike at 2.2 MeV. The shield is able to effectively block the lower energy peaks but is only able to degrade the intensity of the 2.2 MeV peak. This is because 2.2 MeV gammas are a characteristic signature for neutron captures on hydrogen; therefore, it is impossible to fully suppress gammas in this energy range solely using lithium-polyethylene, a hydrogen rich material. If one wanted to completely dampen the gamma output of the neutron source, then one could encase the source in lead. However, as was discussed in the Reflector section, surrounding any major portions of the source in lead would cause logistical problems.

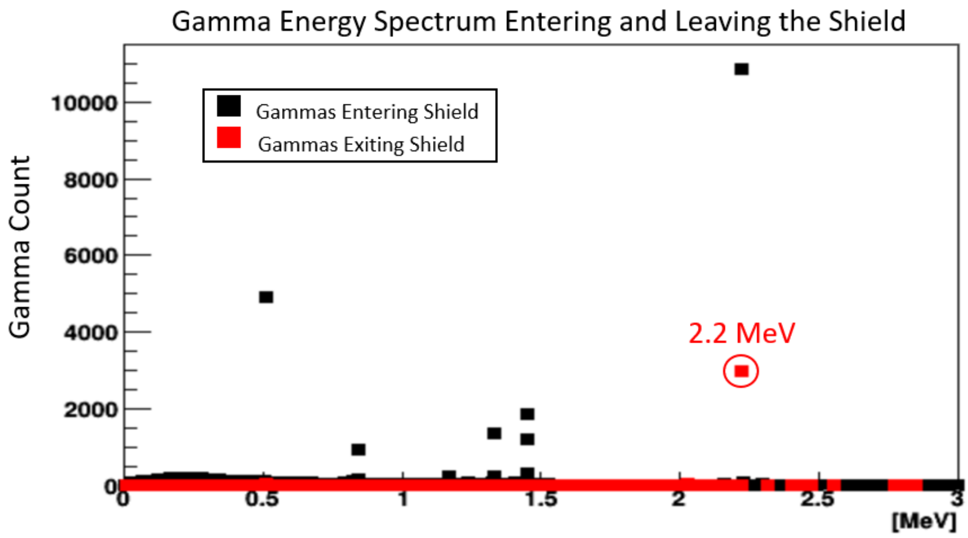


Figure 10: Lithium-Polyethylene shield is capable of totally capturing lower energy gammas and dampening 2.2 MeV gammas

So, a safe thickness of the lithium-polyethylene shield must be found such that it is capable of degrading the 2.2 MeV spike to safe levels. To accomplish this, ten shield thicknesses were simulated for 100,000 events. The dose of radiation from the 2.2 MeV was then calculated assuming a person standing 1 meter away absorbs all of the radiation. A plot of dosage as a function of thickness is shown in Figure 11 and the equations used to calculate dose is shown below.

$$flux = \frac{100\gamma}{4\pi(100cm)^2} \tag{2}$$

$$dose = Q[flux * \frac{\mu}{\rho} * E_{abs}] * (\frac{1.6x10^{-13}}{1MeV}) * (\frac{1000g}{1kg}) * (\frac{100rad}{1Gy}) * (\frac{1000mrad}{1rad}) \tag{3}$$

γ represents the number of escaped gammas with energy of 2.2 MeV. Q is equal to 1.00 for gamma radiation. μ represents the Mass Absorption Coeffecient and is equal to 0.0242 cm^{-1}. The density of human flesh, ρ, was assumed to be 1 g/cm^3. And, the energy absoption factor, E_{abs}, is equal to 1.40 MeV for 2.2 MeV gammas.

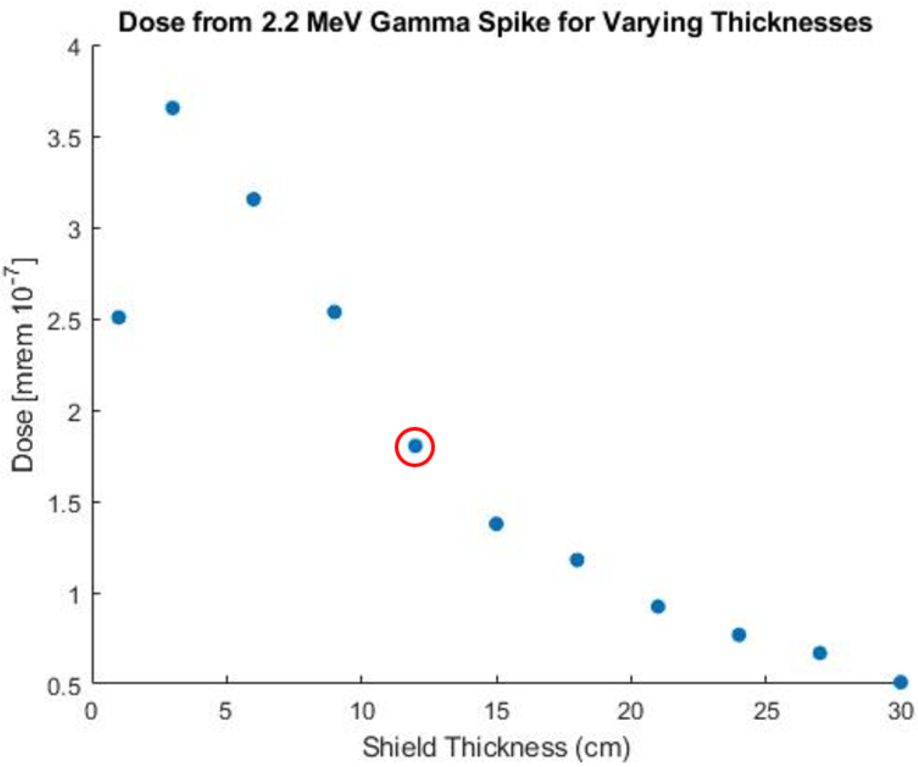


Figure 11: The first dose is low because the neutrons were able to scatter out of the source before being captured, lowering the gamma count

At approximately 12 cm, no neutrons escape the shield. Furthermore, the dose at this thickness is 1.803 $x10^{-7}$ mrem. The Nuclear Regulation Commission (NRC) sets the annual radiation dose for a nuclear worker to be 5 rem. This means that if the neutron source was to be ran everyday for a year, and the worker absorbed all the radiation from one meter away, the source could run 7.7 $x10^7$ shots per day and still be compliant with the NRC.Therefore, 12 cm of lithium-polyethylene shielding is the optimal shield thickness.

4 Overall Performance of the Neutron Source

In order for the calibration technique to be successful, it needs to be able to generate neutron captures throughout the volume of the detector. To do this it needs to be able to send neutrons into the TPC with energies between 57 keV and 87 keV. First, a compact volume of iron was used to degrade the energy of the neutrons from the 2.5 MeV D-D gun. Figure 12 shows the degraded energy spectrum centered mostly in the 57 keV to 87 keV range. Next, utilizing its 73 keV anti-resonance peak, the sulfur volume selects neutron energies within the desired range. This is shown in blue in Figure 12, the 73 keV peak is clearly visible. Finally the neutrons travel through the feed through port. The 73 keV peak has been decreased in magnitude due to neutron scatters inside the port however the peak still dominates the spectrum. This result is also confirmed by the neutron capture positions shown in Figure 13. By placing the neutron source centered on top of the detector, the source was able to produce neutron captures through out the volume. This result proves the viability of the calibration technique.

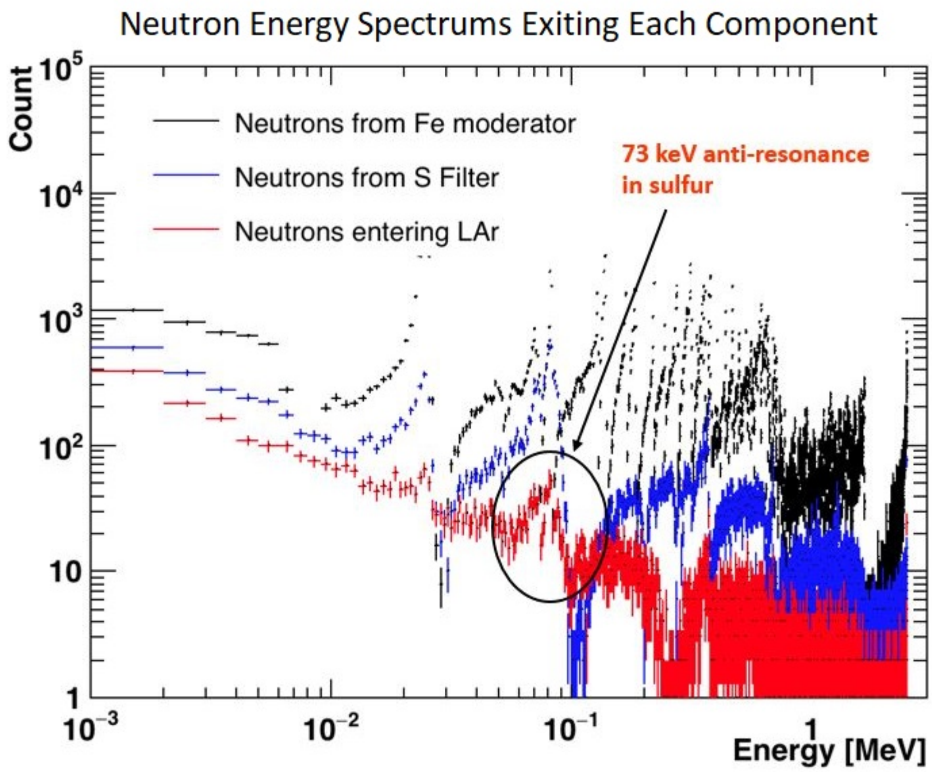
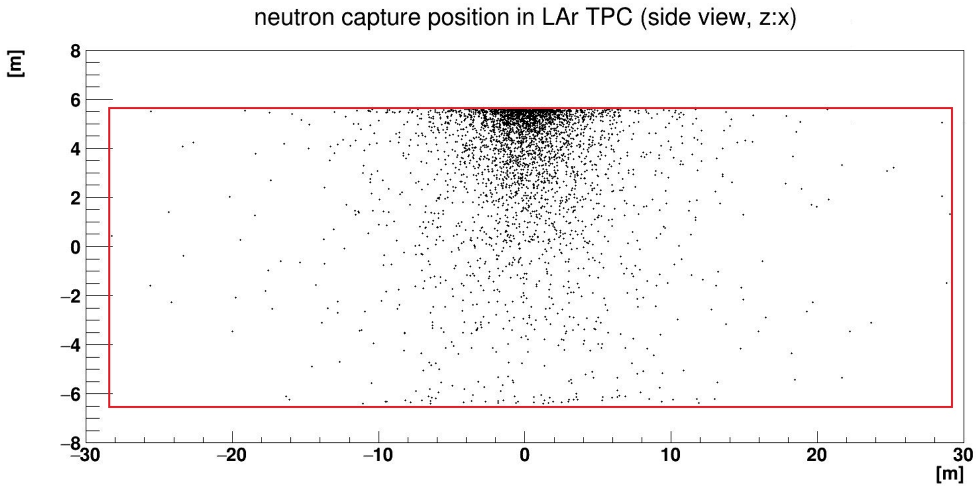
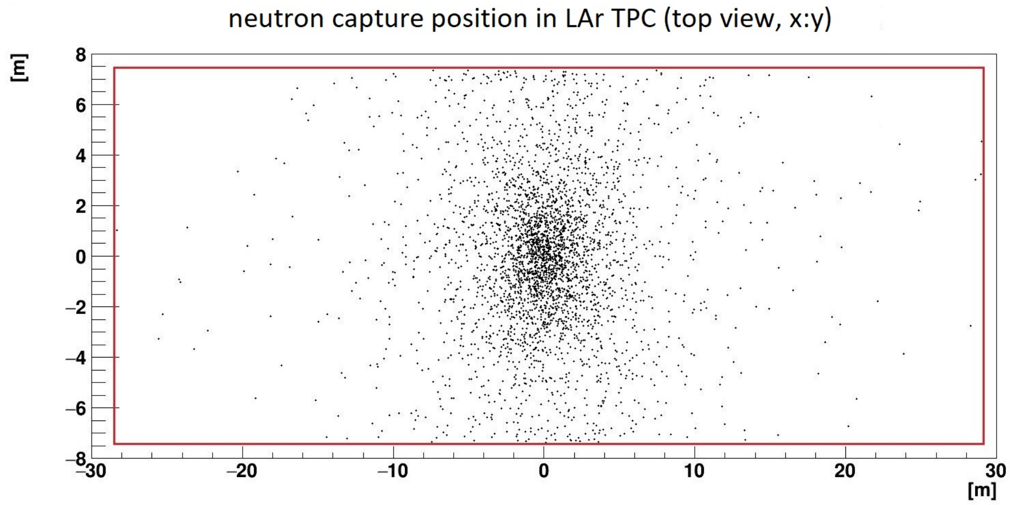


Figure 12: This figure show the energy spectrum of neutrons exiting each component of the neutron source design. Labeled on the graph is the desired peak of neutrons with energy roughly equal to 73 keV, just above liquid argon's anti-resonance peak at 57 keV.



(a) Side view of neutron capture positions inside liquid argon pool. Shown in red is the detector's perimeter.



(b) Top view of neutron capture positions inside liquid argon pool.

5 Conclusion

The objective of the study was to determine the feasibility of a external neutron calibration source as a means to calibrate large liquid argon detectors. To accomplish this, a general design of the source was simulated using Geant4. The source was optimized on the basis of two parameters: material and thickness. Neutron flux and number of neutrons within a selected energy region were the two methods used to quantify the performance of varying source configurations. As a result of these systematic simulations, it was found that the optimal configuration for the source used a 18 cm thick iron moderator and a 20 cm thick sulfur filter. This neutron source design is capable of generating a high flux of neutrons with in the appropriate energy range and produces neutron captures through out the detector's volume. This finding overwhelmingly proves the efficacy of the external neutron calibration technique. The result of this research is relevant to all neutrino and dark matter experiments using liquid argon detectors. In the future, real-world experiments of the neutron source design must be conducted to test the results of the simulations. And eventually, the source must be used to calibrate DUNE and other liquid argon experiments.

6 References

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[4] R.F. Lang *et al* Characterization of a Deuterium-Deuterium Plasma Fusion Neutron Generator (2017). *Nuclear Inst. and Methods in Physics Research*, A, Volume 879, p. 31-38.