COATED MICRO-PARTICLES FOR IMPROVED NEUTRON DETECTION
WITH $^6$LiF:ZnS(Ag)

A Thesis in
Nuclear Engineering
by
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ABSTRACT

The supply of $^3$He has diminished due to the increased use in homeland security, medicine and science applications over the years, which has raised the price of the isotope $[1]$ This fact led to research on alternative ways of neutron detection. One of those ways is to use $^6$LiF:ZnS(Ag) scintillation detectors with $^6$Li acting as a neutron converter and the ZnS as inorganic scintillator that converts the energy of ionizing radiation into light to be detected by photon detectors. The Li is highly enriched in $^6$Li to a minimum of 95% to increase the neutron capture probability and therefore the tritium and alpha particle production. $[2]$ The Li comes with the chemical compound of LiF since the Li metal has highly reactive chemical properties.

The existing neutron detection technology employs mixing of $^6$LiF and ZnS(Ag) grains in an optically transparent binder which holds the mixture together. Although this detection approach works, it has some shortcomings such as opaqueness of ZnS to its own light, which limits the thickness of the detectors and clustering of grains of the same type. This effect results in deteriorated light production and light transport properties of the scintillator.

The proposed way to overcome these problems is to design a coated micro-particle detector that utilizes $^6$LiF coated with ZnS and the distribution of these particles throughout the active volume of the detector. MCNP6, GEANT4 and custom Monte Carlo code have been used to optimize the $^6$LiF micro-particle radius. GEANT4 has been used to optimize the ZnS coating thickness and the pitch, which is the distance between the two micro-particles. Moreover, the commercially available EJ-426 detectors were modeled in GEANT4 using LiF and ZnS grains distributed throughout the detection medium which is between two clear polyester sheets and the simulation results were compared to the experimental results for model validation.

The optimal dimension for the LiF radius was found to be 19μm and the optimal ZnS thickness was found to be 1μm. The best detectors were found to have the dimensions of 60μm pitch, 0.6mm thickness
and 80μm pitch, 1mm thickness, on the average performing 1.7 times better than the best performing existing technology. A code was written in GEANT4 to simulate the randomly distributed particles with varying radii and thicknesses as well as position and shape to test the proposed technology.
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Chapter 1 Introduction

Since neutrons are neutral particles with no charge, they do not cause primary ionization. The detection of neutrons relies on converting them into charged particles that can cause ionization in the detector medium for signal generation. There are several isotopes that have a high cross section for neutron capture and can be used as what is called a “neutron converter”. The main ones are \(^3\)He, \(^6\)Li and \(^{10}\)B, which have the reaction characteristics shown in Table 1.1.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Q-Value</th>
<th>Thermal neutron capture cross section</th>
</tr>
</thead>
<tbody>
<tr>
<td>(^{10})B + (^1)n → (^7)Li + (\frac{4}{2})α (ground state)</td>
<td>2.792 MeV</td>
<td>3840 barns</td>
</tr>
<tr>
<td>(^{10})B + (^1)n → (^7)Li * + (\frac{4}{2})α (excited state)</td>
<td>2.310 MeV</td>
<td></td>
</tr>
<tr>
<td>(^{6})Li + (^1)n → (\frac{4}{2})α + (\frac{3}{1})T</td>
<td>4.78 MeV</td>
<td>941 barns</td>
</tr>
<tr>
<td>(^3)He + (^1)n → (\frac{1}{1})p + (\frac{3}{1})T</td>
<td>0.764 MeV</td>
<td>5330 barns</td>
</tr>
</tbody>
</table>

Table 1.1 Neutron capture reactions in different isotopes and corresponding Q-values

Relatively low cross section of \(^6\)Li is offset by its high Q-value. Also, just like \(^3\)He, there is only one reaction channel, which does not release any gamma rays.

\(^6\)LiF:ZnS(Ag) detectors are produced by mixing LiF and ZnS powders together, which results in a highly inhomogeneous and nonuniform medium. As a result, several shortcomings of this type of detectors arise. First off, the performance between two “identical” detectors may differ due to the grain size variation and distribution of the grains during the mixing process. Clustering of grains may result in some portions of the detector medium not being sensitive to the neutrons. On top of all these, ZnS is a relatively opaque material even if it is activated with Ag to shift the light emission spectrum. Main advantages of ZnS are its brightness and high gamma rejection properties.
Coated micro-particle detectors are a promising technology, which would eliminate the clustering and nonuniformity of the detector medium. In collaboration with the Pennsylvania State University Material Science Department, a project has been started to coat the $^6$LiF with ZnS(Ag) to increase the light collection efficiency. These coated particles would then be distributed throughout the detector medium. The idea is to produce spherical micro-particles with fixed radius and coating thickness. In this work, optimizations of LiF radius, ZnS thickness, pitch size (center-to-center distance) and detector thickness were performed and different parameters were tested. After determining the promising geometries, randomization of LiF radius, ZnS thickness and position of particles was carried out to take into account the deviation from ideal geometries in the manufacturing process.

1.1 Theory

In this chapter, background theory for particle transport and scintillation mechanism is explained briefly. Necessary background knowledge is also provided about the parameters used in the simulations.

1.1.1 Neutron Transport

Neutrons don’t interact through the Coulomb force, therefore their transport in the media is a series of collisions with the nuclei. Neutrons may be scattered, captured or engaged in various other reactions. Neutron capture reaction by $^6$Li, which results in alpha and triton particles, is

$$^6\text{Li} + n(\text{thermal}) \rightarrow ^4\text{He}(2.05\text{MeV}) + ^3\text{H}(2.73\text{MeV})$$

The cross section of thermal neutron capture by $^6$Li is 941 barns.$^{[4]}$ Knowing the cross sections of various reactions in different media, the neutrons can be simulated.

1.1.2 Charged Particle Transport

Charged particles, $\alpha$ and T after the neutron capture by $^6$Li, lose their energy through excitation and ionization of the electrons in the media since they interact with the matter through the Coulomb force. Therefore, they can be assumed to lose their energy continuously through the interactions with multiple electrons.
They can be simulated using the continuous slowing down approximation (CSDA). Since the energy loss is a statistical phenomenon by its nature, energy straggling functions may be incorporated to take into account the stochastic effects in slowing down of charged particles. Energy loss can be given by the Bethe-Bloch formula\textsuperscript{[5]}

\[
- \frac{dE}{dx} = 0.1535 \frac{\rho z^2 Z}{A \beta^2} \left\{ \ln \left[ \frac{2m_e v^2 W_m}{I^2 (1 - \beta^2)} \right] - 2\beta^2 - \delta - U \right\} \left[ \frac{MeV}{cm} \right]
\]

[Eq. 1.1]

where \( W_m \) is the maximum energy transfer and it is given by

\[
W_m = 2m_e c^2 \beta^2 \gamma^2 \left[ 1 + \left( \frac{m_e}{m} \right)^2 + 2\gamma \left( \frac{m_e}{m} \right)^{-1} \right]
\]

[Eq. 1.2]

\( \delta \) and \( U \) are the density correction and shell correction factors, respectively.

Other parameters in the equation are given in Table-1.2.

| \( \rho \) | Mass density |
| \( z \) | Charge of the particle |
| \( Z \) | Atom number of the isotope |
| \( A \) | Mass number of the isotope |
| \( m_e \) | Electron mass |
| \( v \) | Charged particle velocity |
| \( I \) | Mean excitation energy |
| \( \beta \) | Ratio of the charged particle velocity to speed of light |
| \( \gamma \) | Lorentz factor |

\textit{Table-1.2 – Relevant Parameters in the Bethe-Bloch Formula}

No delta radiation (\( \delta \)-rays) are assumed to be produced in the simulations in this work due to relatively low energy of charged particles, which means the energy is deposited locally. After the charged particles lose all of their kinetic energy, they capture electrons and become neutralized.
1.1.3 Electron Transport in Scintillators

When the electrons are created in the scintillator by radiation, they are highly energetic, therefore they are sometimes called hot electrons. Through series of interactions, they lose their energy and become thermalized. These thermal electrons may travel to the luminescent centers to reach their ground level and produce light, which is called scintillation. There are other phenomena that may take place during the electron transport process, which result in non-radiative energy transfer. A simple illustration of such scintillation process is shown in Figure-1.1 [6].

![Figure-1-1 Basic schematic of electron transport in the inorganic scintillators](image)

Hot electrons produced through ionization undergo multiple electron-electron interaction and they can cause secondary excitations. Electrons are then thermalized and they occupy the bottom of the conduction band. Electrons finally migrate to luminescence centers or non-radiative centers.

The electron transport in a scintillator is not handled by the simulation packages used in this work. In GEANT4, the light is produced whenever the charged particle deposits its energy in the medium defined as a scintillator according to the scintillator yield $R_s$. \[ R_s = \frac{N_{ph}}{E_i} \] [Eq. 1.3]
where $N_{ph}$ and $E_i$ are number of photons emitted and the energy deposited in the scintillator, respectively. Simulation tools used in this work are described in Section 1.3.

### 1.1.4 Light Transport

When the scintillation photons are produced, they are typically in visible portion of the electromagnetic spectrum and they are called “light”; the actual range of energies depends on the context. The light may be absorbed, transmitted, reflected, refracted, or scattered. Each of these events has a certain probability of occurrence depending on the bulk material, surface properties and angle of incidence, which can be used to compute the light related properties such as radiant flux.

GEANT4 is a useful toolkit to simulate light or optical photons in scintillators and other media. There is a distinction between photons and optical photons in GEANT4, although they are the same in nature. “Regular” photon in GEANT4 is called “gamma” and the light is called “optical photon” when its wavelength is larger than the atomic spacing. Although they are essentially the same electromagnetic radiation whose only difference is the energy, GEANT4 introduces a distinction between the two. One reason is that for high energies, such as typical gamma or X-ray energies, the refractive indices of the materials are the same and there is no reflection or refraction. As for low energy photons, the wave nature of the electromagnetic radiation becomes important.

There are many parameters relevant for light transport that need to be entered into GEANT4; two of them are the wavelength dependent refractive index and absorption length for each material. In the present work, these properties for ZnS are especially crucial since ZnS is relatively opaque to its own light, which means its absorption length is small.

### 1.1.5 Electron Transport in a Photomultiplier Tube

Finally, when the light hits a PMT surface (photocathode), electrons are emitted via the photoelectric effect. Those electrons pass through the electrode and go through multiplication in dynodes until they are
collected in the anode. The electric charge is then converted into a signal that can be digitized in a
digitizer for post-processing.

The simulation of electrons can be handled in GEANT4; however, it wasn’t done in this work.
Quantum efficiency correction was applied on the collected light on the PMT surface.

1.2 Literature Review

Several papers were studied to obtain the required parameters and possible geometry configurations
for the simulations. GEANT4 doesn’t have a database for scintillators so the user needs to input necessary
parameters to carry out the simulations such as absorption length, refraction index, scintillator yield, and
so on. Also, since the scintillator material needs to be defined separately, several papers were used as a
guideline to get a general understanding of how to handle the geometry.

1.2.1 Optical Properties of ZnS

The wavelength dependent refractive index and the absorption length were obtained from the dielectric
function calculated in the reference[7].

The wave intensity attenuation can be described as[8]

\[ I(x) = I_0 \ast \exp \left(-2 \frac{\omega}{c} \kappa x\right) = I_0 \ast \exp(-\alpha x) \]  \[ \text{[Eq. 1.4]} \]

where \( \alpha, \omega, \kappa \) and \( c \) are the absorption coefficient, angular frequency, extinction coefficient and the speed
of light, respectively. Absorption coefficient can also be expressed as

\[ \alpha(E) = 2 \frac{\omega}{c} \kappa = \frac{\omega \ast \epsilon_2}{c \ast n} = \frac{4\pi \sigma_1}{n \ast c} = \frac{4\pi}{\lambda} \ast \kappa(E) \]  \[ \text{[Eq. 1.5]} \]

where \( \lambda \) is the wavelength and \( \epsilon_2 \) is the complex part of the dielectric function, which is equal to

\[ \epsilon_2 = \frac{4\pi}{\omega} \sigma_1 = 2n\kappa \]  \[ \text{[Eq. 1.6]} \]

where \( \sigma \) is the complex optical conductivity.
Knowing the energy dependent complex dielectric function, one can calculate the wavelength dependent refractive index, extinction coefficient and absorption coefficient using

\[ n(E) = \sqrt{\frac{\sqrt{\varepsilon_1(E)^2 + \varepsilon_2(E)^2 + \varepsilon_1(E)}}{2}} \quad [Eq. 1.7] \]

\[ \kappa(E) = \sqrt{\frac{\sqrt{\varepsilon_1(E)^2 + \varepsilon_2(E)^2 - \varepsilon_1(E)}}{2}} \quad [Eq. 1.8] \]

\[ \alpha(E) = \frac{4\pi}{\lambda} \cdot \kappa(E) \quad [Eq. 1.9] \]

These quantities can also be measured experimentally. Some work has been done to model the dielectric function for cubic ZnS using transition for various energy gaps, namely, \( E_0, E_0 + \Delta_0, E_1 \) and \( E_2 \) transitions. These transitions can be used to produce model dielectric function (MDF). Details can be found in the reference [7].

\( E_0 \) and \( E_0 + \Delta_0 \) transition:

\[ \varepsilon(E) = AE_0^{-1.5} \left\{ f(\chi_0) + 0.5 \ast \left( \frac{E_0}{E_0 + \Delta_0} \right)^{1.5} \ast f(\chi_{s.o.}) \right\} \quad [Eq. 1.10] \]

\( E_0 \) and \( E_0 + \Delta_0 \) gaps:

\[ \varepsilon(E) = \sum_{n=1}^{\infty} \frac{A_{0x}}{n^3} \left[ \frac{1}{E_0 - \frac{G_0}{n^2} - E - i\Gamma} - \frac{1}{2} \left( \frac{1}{E_0 + \Delta_0 - \frac{G_0}{n^2} - E - i\Gamma} \right) \right] \quad [Eq. 1.11] \]

\( E_1 \) transitions:

\[ \varepsilon(E) = \sum_{n=1}^{\infty} \frac{1}{(2n-1)^3} \frac{B_{1x}}{E_1 - \frac{G_1}{(2n-1)^2} - E - i\Gamma_1} \quad [Eq. 1.12] \]

\( E_2 \) transitions:

\[ \varepsilon(E) = \frac{C}{1 - \chi_2^2 - i\chi_2 Y} \quad [Eq. 1.13] \]
The dielectric function and the obtained energy dependent absorption coefficient are shown in Figure-1.2.

![Figure-1-2 a) Energy dependent dielectric function for different optical transitions [7] and b) energy dependent absorption coefficient in ZnS](image)

### 1.2.2 Geometry in the Simulations

Since the $^6$LiF:ZnS(Ag) is a powdery matrix and ZnS is the scintillator, they can’t be homogenized completely. Several papers were studied$^{[9,10,11]}$. Main purpose of those papers is to design a highly efficient cold neutron detector using LiF:ZnS:Binder matrix and GEANT4 was used in the simulations. The authors defined a spherical ZnS grain and placed it inside homogenous mixture of LiF and binder. After that, they replicated the geometry throughout the volume. A similar approach has been utilized in this work with the difference of LiF defined as an individual grain as well.

In reference $^{[11]}$, the authors report an optimization for ZnS grain size studying different concentration of LiF, ZnS and binder. They changed the detectors’ binder concentration in order to maximize the light output since their previous findings indicate poor light output from the detectors. They also made light transmission measurements and found out that the optimal grain size for ZnS is 8μm, which is the current standard. Using WLS fibers, they achieved high light output. WLS fibers can also be used with the coated micro-particles to improve the light collection efficiency even further.
1.3 Simulation Tools Used in This Work

The main simulation tool used in this work was GEANT4 because of its capability to simulate light as well as neutrons and charged particles. MCNP6 was used whenever there wasn’t any light transport simulation necessary. Custom made Monte Carlo code was also written to compare with the GEANT4 and MCNP6 for LiF radius optimization. SRIM was used for range calculations.

1.3.1 MCNP6

MCNP (Monte Carlo N-Particle) is a general purpose particle simulation software that uses Monte Carlo methods and it is developed by Los Alamos National Laboratory (LANL) [12]. Its application areas are radiation detection, nuclear reactor criticality calculations, shielding and many more. MCNP6 is the merger of two codes (MCNP5 and MCNPX). MCNPX (Monte Carlo N-Particle eXtended) is a code that can simulate different types of particles and nuclides.

1.3.2 GEANT4

GEANT4 (GEometry ANd Tracking) is a particle simulation toolkit that utilizes Monte Carlo methods [13]. It is developed by CERN and used in various applications such as high energy physics, medical physics, radiation detection and many others. It is written in C++ and it handles geometry, tracking, materials and complex particle physics ranging from high energy physics to optical physics. Therefore, it is a very useful toolkit to simulate the properties of scintillators. There is no built-in statistical checks in GEANT4; therefore they were implemented into the code to determine the statistical significance of the results. Implementation is explained in Section 3.3.

1.3.3 SRIM

SRIM (Stopping and Range of Ions in Matter) is a Monte Carlo software that can be used to calculate particle ranges in different materials and to compute displacement cross sections and radiation damage [14]. SRIM was used only to calculate the range of the charged particles in this work.
Chapter 2 Preliminary Work for Optimizing the Simulations and Experiments

Preliminary work was done to select the optimum and valid parameters for simulations and experiments. These were done primarily to reduce the uncertainty of the final simulations and experiments.

2.1 Optimum Thickness of Polyethylene for Experiments

Moderator thickness optimization was performed to determine the optimal thickness of a polyethylene moderator to get more thermalized neutrons from a $^{252}$Cf while minimizing the absorption and loss. MCNP6 and GEANT4 were used for this optimization. Watt spectrum was used in simulation codes to mimic $^{252}$Cf.

$^{252}$Cf energy spectrum is given by [15]

$$N(E) = \exp\left(-\frac{E}{a}\right) \times \sinh\left(\sqrt{bE}\right)$$  \hspace{1cm} [Eq. 2.1]

where $a$ and $b$ are fitting constants with numerical values of

$$a = 1.18 MeV, \quad b = 1.03419 MeV^{-1}$$

The Watt spectrum was obtained in GEANT4 using the direct sampling method [16].

$$w = a \times (-\log \xi_1 - \log \xi_2 \times \cos^2\left(\frac{\pi}{2} \times \xi_3\right))$$ \hspace{1cm} [Eq. 2.2]

$$x = w + \frac{a^2 \times b}{4} + (2 \times \xi_4 - 1) \times \sqrt{a^2 \times b \times w}$$ \hspace{1cm} [Eq. 2.3]

And the probability density distribution is

$$f(x) = \frac{2 \times \exp\left(-\frac{a \times b}{4}\right)}{\sqrt{\pi \times a^3 \times b}} \times \exp\left(-\frac{x}{a}\right) \times \sinh\sqrt{b \times x}$$ \hspace{1cm} [Eq. 2.4]
In the GEANT4 reference physics lists, the thermal scattering treatment \((S(\alpha,\beta)\) tables) is not included. The neutron physics list is modified by implementing the G4ParticleHPThermalScattering with the upper limit of 4eV. Thermal scattering treatment is important since chemical bonds of elements affect the neutron scattering cross section and using individual cross sections without considering the chemical bonds would be inaccurate. Especially for the polyethylene moderator, including the thermal scattering treatment with \(S(\alpha,\beta)\) tables is extremely important.

In MCNP6, \(S(\alpha,\beta)\) is activated by adding MT card that overrides the free-gas treatment.

The comparison between MCNP6 and GEANT4 is shown in Table-2.1.

<table>
<thead>
<tr>
<th>Thickness (cm)</th>
<th>MCNP6 (with (S(\alpha,\beta))) (Number of neutrons moderated per primary neutron)</th>
<th>GEANT4 (with (S(\alpha,\beta))) (Number of neutrons moderated per primary neutron)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>2.68E-4 ± 0.013 &lt;0.0253eV</td>
<td>4.40E-4 ± 0.021 &lt;0.0253eV</td>
</tr>
<tr>
<td>4</td>
<td>8.14E-4 ± 0.004 &gt;0.0253eV and &lt;0.045eV</td>
<td>13.5E-4 ± 0.012 &gt;0.0253eV and &lt;0.045eV</td>
</tr>
<tr>
<td>6</td>
<td>8.23E-4 ± 0.010 &gt;0.0253eV and &lt;0.045eV</td>
<td>14.7E-4 ± 0.011 &gt;0.0253eV and &lt;0.045eV</td>
</tr>
<tr>
<td>8</td>
<td>5.84E-4 ± 0.011 &gt;0.0253eV and &lt;0.045eV</td>
<td>10.9E-4 ± 0.014 &gt;0.0253eV and &lt;0.045eV</td>
</tr>
<tr>
<td>10</td>
<td>3.21E-4 ± 0.014 &gt;0.0253eV and &lt;0.045eV</td>
<td>6.98E-4 ± 0.017 &gt;0.0253eV and &lt;0.045eV</td>
</tr>
</tbody>
</table>

Table-2.1 MCNP6 and GEANT4 simulation results for different moderator (polyethylene) thickness

According to the results, a polyethylene block with 6-cm thickness is optimal for the neutron slowing down process. Therefore, 6-cm thick polyethylene blocks were used for the simulations and experiments. Although both simulation codes agree upon the optimal thickness of polyethylene, there is a significant discrepancy between the absolute values, which is a known issue in the thermal energy regime \cite{17}.
2.2 Optimal Distance of Source for Simulations

Since the $^{252}\text{Cf}$ source used in experiments is not exactly a point source, the experiments were performed to investigate the behavior of gamma rays and neutrons as a function of distance between the source and a EJ-309 liquid scintillator, which was chosen because of its diameter (4”) and PSD capabilities. In order to suppress the high gamma ray field, a lead block was placed between the source and the detector. The $^{252}\text{Cf}$ is shown in Figure-2.1 and its activity is 0.26mCi.

$^{252}\text{Cf}$ is contained in a stainless steel casing and the volume of it is very small\textsuperscript{[18]} so it is expected that it would behave as a point source. In Figure-2.2, schematic representation of the source is shown.
The solid angle subtended by the circular area to a point source can be represented by

\[
\omega = 2 \pi \left[ 1 - \frac{d}{\sqrt{d^2 + R^2}} \right]
\]

[Eq. 2.5]

where \( \omega \), \( d \) and \( R \) are the solid angle subtended by the detector, distance between the source and the detector and radius of the detector, respectively. A pulse shape discrimination (PSD) algorithm was written to separate the neutron and gamma pulses. Experimental setup is shown in Figure-2.3.
The behavior of the gamma ray counts and neutron counts are shown as a function of distance in Figure-2.4. Theoretical point source fitting is also shown in the same figure.

![Normalized Counts vs. Distance](image)

**Figure-2.4 – Theoretical point source behavior and the experimental values as a function of distance**

Since there was a lead block between the source and the detector, counts couldn’t be taken for distances below 8 cm. However, it is seen in Figure-2.4 that the gamma ray and neutron counts follow the same trend as a point source after 10 cm distance. Clearly, the point source behavior is dependent on the area of the detector. Still the results can be used to a first degree of approximation as if a point source was used.

A PSD code was written to discriminate between neutron and gamma events and Charge Integration Method (CIM) was used. Some ringing was present in the signals due to impedance mismatch therefore pulses were smoothed out to improve the PSD performance. CIM can be expressed as

\[
PSD = \frac{\int_{tail\ cutoff}^{full\ signal} Qdt}{\int_{0}^{full\ signal} Qdt} \approx \frac{\sum_{n=tail\ cutoff}^{full\ signal} Q_n}{\sum_{n=0}^{full\ signal} Q_n} \tag{Eq. 2.6}
\]

PSD between gammas and neutrons are shown in Figure-2.5 and the PSD code is shared in the Appendix A.
PSD figure of merit (FOM) is defined as:\[^{[20]}\]

\[
FOM = \frac{d}{FWHM_n + FWHM_g}
\]

[Eq. 2.7]

where d, FWHM_n and FWHM_g are the distance between the peaks of gamma and neutron peaks, full width at half maximum of neutrons and full width at half maximum of gammas, respectively. FOM is found to be 0.95. Although EJ-309 has very good PSD capabilities, ringing was present in the signals due to the impedance mismatching which affects the PSD. Although the ringing was eliminated with the post-processing code, the post-processing itself may have caused some information to be lost.

Full-scale simulations were performed with a $^{252}$Cf point source 8.5-cm away from the detector.
2.3 Lateral Light Transmission Measurements in $^{6}\text{LiF:ZnS(Ag)}$

Since combining the neutron transport, charged particle transport and light transport is extremely time consuming and memory demanding, measures were taken to optimize the best simulation geometry without losing the essential information. $^{6}\text{LiF:ZnS(Ag)}$ scintillators (EJ-426) used were 10cm*5cm with varying thicknesses and concentration.

The PMT employed in the experiments is Hamamatsu model H10580 with the diameter of 1” coupled to the scintillator with an optical grease (EJ-550). Therefore, the light produced at the edges of the scintillator not directly seen by the PMT has a low chance to reach the PMT because of two reasons. The first reason is that light production is isotropic, and the second reason is that ZnS is relatively opaque to its own luminescence so light cannot travel distance on the order of cm in the scintillator. The equipment used in the experiments is shown in Figure-2.6.
Three experiments were performed for 30 minutes acquisition time each. The first experiment was done without placing any borated polyethylene between the moderator and the scintillator. In the second experiment, borated polyethylene was directly placed in front of the portion of the scintillator seen by the PMT. In the third experiment, borated polyethylene blocks were placed at the edges of the scintillator. Pulses due to the thermal electron excitations were removed to count the neutrons more accurately in the post-processing. Experimental setup is shown in Figure-2.7.
Figure 2.7 a) Experimental setup without borated polyethylene b) Experimental setup with the borated polyethylene at the center c) Experimental setup with the borated polyethylene at the edges

Results are shown in Table 2.2.

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Count Rate (cpm) (30 minutes)</th>
<th>Removed neutron signals/Total registered neutron signals</th>
</tr>
</thead>
<tbody>
<tr>
<td>No Borated Polyethylene</td>
<td>1396.3 ± 6.82</td>
<td>0.0049</td>
</tr>
<tr>
<td>Borated Polyethylene at the center</td>
<td>158.2 ± 2.29</td>
<td>0.0514</td>
</tr>
<tr>
<td>Borated Polyethylene at the edges</td>
<td>1367.4 ± 6.75</td>
<td>0.0054</td>
</tr>
</tbody>
</table>

Table 2.2 Successfully registered neutron count rates and percentage of signals removed for each case.
Standard deviation for the count rate can be calculated using the best estimate value as

\[ \sigma_s = \sqrt{x} \]  
[Eq. 2.8]

\[ \sigma_{CR} = \frac{\sigma_s}{t} \]  
[Eq. 2.9]

where \( t \) is the measurement time.

The count rates are not same when the borated polyethylene is placed at the edges and when there is no borated polyethylene possibly due to the small fraction of light reaching the PMT. The other reason is the statistical uncertainty. A signal amplitude cutoff was determined with the “no-boron” case and the signals below this cutoff was removed. The percentage of removed signals to the total registered neutron signals is shown in Table-2.2 for the three cases. The high percentage (5\%) in the setup where borated polyethylene was at the center suggests that there are some contribution to the signal due to the \( \alpha \) particles and \( ^7 \)Li nuclei created through the neutron capture by \( ^{10} \)B. There are two reasons why these particles result in lower signal amplitudes; one is that the Q-value of the reaction is lower, other is that the reaction products are captured at the back of the scintillator. Still, there are some successfully registered neutron signals even when the boron was at the center. The reason is that boron doesn’t shield all the neutrons and some of the escaped neutrons interact with \( ^6 \)Li.

In Figure-2.8, the full integral value spectrum of no-boron case and boron-at-the-center case are shown. The number of rejected signals is almost the same for two cases even if there are much more neutron counts in the no-boron case.
Simulations were done to see the effect of $^{10}$B shielding on thermal neutrons. When the borated polyethylene was placed at the center, the reduction on the number of neutrons detected in experiments is

$$ reduction = \frac{1396.3 - 158.2}{1396.3} = 0.887 $$  \[Eq. 2.10\]

This result is compared to the simulation values in Table-2.3. The reduction rate in the neutron moderation events are similar to the experimental values.
<table>
<thead>
<tr>
<th>Configuration</th>
<th>MCNP6</th>
<th>GEANT4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Without Borated polyethylene at the center</td>
<td>7.64E-4 ± 0.008</td>
<td>6.84E-4 ± 0.017</td>
</tr>
<tr>
<td>With Borated polyethylene at the center</td>
<td>1.21E-4 ± 0.023</td>
<td>1.32E-4 ± 0.039</td>
</tr>
<tr>
<td>Reduction of the number of neutrons (experimentally)</td>
<td>0.887</td>
<td>0.887</td>
</tr>
<tr>
<td>Reduction of the number of neutrons (simulation)</td>
<td>0.842</td>
<td>0.807</td>
</tr>
</tbody>
</table>

*Table-2-3* Comparison of the moderation with and without borated polyethylene using MCNP6 and GEANT4

The simulations performed with full length and width of the detectors produced similar results with no detection of photons created at the regions not directly seen by the PMT. In Figure-2.9, the 1” diameter PMT is situated next to the scintillator medium.

![Figure 2-9](image)

*Figure 2-9* a) Simulation of EJ-426-0-0032 in GEANT4 with full length and width b) Simulation of 0.032cm coated particle detector in GEANT4 with full length and width
From these results, it was determined that simulating the portion of the scintillator directly seen by the PMT is sufficiently accurate as well as time and memory saving. Therefore, 1.5cm*1.5cm detectors were simulated with varying thicknesses.
Chapter 3 Experiments and Model Validation

Four different EJ-426 neutron detector sheets with different thicknesses and different $^6$LiF:ZnS(Ag) ratios were used in the experiments. The experimental setup is shown in Figure-3.1.

![Figure-3-1](image1) ![Figure-3-1](image2)

*Figure-3-1 a) Experimental setup showing the scintillator between PMT and the moderator b) Same experimental setup showing the position of the source*

Measurements were taken with each scintillator for 30 minutes. In order to calculate the absolute neutron detection efficiency (neutron detected in the scintillator versus the number of neutrons emitted from $^{252}$Cf source), the neutron emission rate was calculated.

Compositions of some materials used in the simulations such as polyester were obtained from reference [21]. Since there is no built-in statistical checks in GEANT4, standard deviation and variance calculations were implemented into the simulation code.
3.1 Californium Neutron Emission Rate Calculation

$^{252}$Cf activity and the neutron emission rate can be calculated from the initial source activity, half-life and specific neutron emission rate of the source.

The source activity was 1mCi ± 0.15 on 11/20/2013 and the experiments were conducted on 01/09/2019, so the elapsed time between the two dates is 1876 days. The half-life of $^{252}$Cf is 965.4 days.

Therefore, the decay constant is

$$\lambda = \frac{\ln(2)}{T_{1/2}} = \frac{\ln(2)}{965.4 \text{d}} = 7.18 \times 10^{-4} \text{d}^{-1}$$  \[Eq.3.1\]

and

$$\alpha = \alpha_0 \times \exp(-\lambda \times t) = 1mCi \times \exp(-7.18 \times 10^{-4} \times \text{d}^{-1} \times 1876\text{d}) = 0.26mCi$$  \[Eq.3.2\]

Therefore, the total number of $^{252}$Cf nuclei is

$$N_{Cf} = \frac{\alpha}{\lambda} = \frac{0.26mCi \times \frac{3.7 \times 10^{10} \text{Bq}}{1\text{Ci}} \times \frac{1\text{Ci}}{1000\text{mCi}}}{7.18 \times 10^{-4} \times \text{d}^{-1} \times \frac{1\text{d}}{24 \times 60 \times 60 \text{s}}} = 1.158 \times 10^{15} \#$$  \[Eq.3.3\]

The $^{252}$Cf mass is

$$m_{Cf} = \frac{N_{Cf} \times M_{Cf}}{N_A} = \frac{1.158 \times 10^{15} \# \times 252 \text{g/mol}}{0.602 \times 10^{24} \times \frac{\#}{\text{mol}}} = 4.847 \times 10^{-7} \text{g} = 484.7 \text{ng}$$  \[Eq.3.4\]

where $N_A$ and $M_{Cf}$ are the Avogadro’s number and molar mass of $^{252}$Cf, respectively.

The specific activity of $^{252}$Cf [15] is

$$\gamma = 2.314 \times 10^{12} \frac{n}{g - s}$$

Finally, the neutron emission rate is

$$\dot{N} = \frac{\gamma \times m_{Cf}}{10^9 \frac{ng}{g}} = \frac{2.314 \times 10^{12} \frac{n}{g - s} \times 484.7 \text{ng}}{10^9 \frac{ng}{g}} = 1,121,596 \frac{n}{s}$$  \[Eq.3.5\]
3.2 Experimental Results with EJ-426

Experimental results for the four sheets are shown in Table-3.1. The naming convention for the detectors is that composition and detector thickness follow the detector type. As an example, EJ-426-0-0032 represents the EJ-426 detector with LiF:ZnS composition as 1:3 and thickness of 0.032cm. HD stands for 1:2 composition for LiF:ZnS.

<table>
<thead>
<tr>
<th>Detector</th>
<th>Measurement time (minutes)</th>
<th>Number of source neutrons</th>
<th>Number of neutron events detected</th>
<th>Number of neutrons detected per neutron</th>
<th>Mean value of full integral</th>
</tr>
</thead>
<tbody>
<tr>
<td>EJ-426-0032</td>
<td>30</td>
<td>2.02E+9</td>
<td>70283</td>
<td>3.48E-5</td>
<td>1.41E+5</td>
</tr>
<tr>
<td>EJ-426-HD-0032</td>
<td>30</td>
<td>2.00E+9*</td>
<td>68922</td>
<td>3.45E-5</td>
<td>1.62E+5</td>
</tr>
<tr>
<td>EJ-426-0-0060</td>
<td>30</td>
<td>2.02E+9</td>
<td>70006</td>
<td>3.47E-5</td>
<td>1.39E+5</td>
</tr>
<tr>
<td>EJ-426-HD-0060</td>
<td>30</td>
<td>2.02E+9</td>
<td>82036</td>
<td>4.06E-5</td>
<td>1.34E+5</td>
</tr>
</tbody>
</table>

Table-3.1 – Experimental results of four different scintillator with absolute efficiency and mean signal amplitude. * Experiment done some time after the other three.

In the experiments, record length was set to 300 with each sample being 2ns and high voltage was set to 1000V.

Neutron pulses have a long decay time while the random excitations are fast because they are solely associated with the PMT. Therefore, neutron pulses were separated from the raw pulses using their characteristic long tail. Example of a neutron pulse, a random excitation and an exponential fit with 110ns decay time are shown in Figure-3.2.
Figure 3-2 a) Neutron pulse in EJ-426 b) Random PMT excitation c) A neutron pulse with the fit of a single exponential having a decay time of 110ns

\[ I(t) = A \exp \left( -\frac{t}{\tau} \right) \]  

[Eq. 3.6]

where \( \tau \) is the decay time.
When the detection efficiencies of the four scintillators are compared, EJ-426-0-032, EJ-426-HD-0032 and EJ-426-0-060 have similar efficiencies within one standard deviation if the measurement is assumed to follow the normal distribution. EJ-426-HD-060 has a higher neutron detection efficiency as expected since there are more neutron capture events in the medium due to the both increased ratio of LiF:ZnS and increased mass of $^6\text{Li}$. Although its thickness is larger, it can be argued that more neutron capture eventually offsets the light transport deterioration.

Mean value of full integral represents the average magnitude of the signal amplitude coming from the neutron detection events. Since not all neutron events result in the exact same energy deposition in ZnS due to the mixed powder geometry and light transport is not same for every event, the thick detectors have lower signal amplitude due to the light attenuation in the detector medium.

### 3.3 Implementation of Statistical Checks in GEANT4

Statistical checks were implemented in the GEANT4 to measure the quality of the simulations.

\[
\sigma_s^2 = \frac{1}{N-1} \sum (x_i - \bar{x})^2 \quad [Eq.3.7]
\]

\[
\sigma_{s,x}^2 = \frac{\sigma_s^2}{N} \quad [Eq.3.8]
\]

\[
\sigma_{s,x} = \sqrt{\sigma_{s,x}^2} \quad [Eq.3.9]
\]

\[
f_{sd} = \frac{\sigma_{s,x}}{\bar{x}} \quad [Eq.3.10]
\]

where $x_i$ and $\bar{x}$ are the measurement of the quantity of interest for the $i^{th}$ event and mean value of the quantity of interest, respectively.\[23]

In order for the results to have a statistical significance, the fractional standard deviation needs to be lower than a certain value. It is generally accepted that if the relative error is lower than 0.1, the statistics are sound\[24]. If the relative error is between 0.1 and 0.2, the results are considered to be questionable. If it is above 0.5, the results are unreliable.
Also, the standard deviation must decrease with the number of histories and the decrease rate must follow \( \frac{1}{\sqrt{N}} \). The implementation was tested with an example and Table-3.2 and Figure-3.3 show the results.

<table>
<thead>
<tr>
<th>Number of histories (N)</th>
<th>Standard Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>5000</td>
<td>0.0306</td>
</tr>
<tr>
<td>10000</td>
<td>0.0213</td>
</tr>
<tr>
<td>50000</td>
<td>0.0094</td>
</tr>
<tr>
<td>100000</td>
<td>0.0067</td>
</tr>
</tbody>
</table>

*Table-3.2 – Statistical implementation check in GEANT4 with different number of histories*

The decrease rate is close to \( \frac{1}{\sqrt{N}} \). Since randomness is in the nature of Monte Carlo methods, it is not perfectly \( \frac{1}{\sqrt{N}} \).

Error propagation is carried out using
\[
\sigma_w = w \sqrt{\left(\frac{\partial w}{\partial u}\right)^2 \sigma_u^2 + \left(\frac{\partial w}{\partial v}\right)^2 \sigma_v^2}
\]  
[Eq. 3.11]

where \(u\) and \(v\) are the obtained quantities, and \(w\) is the quantity of interest.

### 3.4 Geometry of the Simulations of EJ-426

Since LiF and ZnS are powders mixed together to produce the detector medium, those two powders need to be simulated individually. Work has been done to simulate such geometry by defining ZnS and LiF:binder mixture separately. The authors created a ZnS grain as a spherical volume and put it in a unit cell and replicated the geometry to produce the detector active volume.

In this work, respecting the LiF:ZnS ratio, ZnS and LiF grains were modeled as spherical volumes and put in a cubical unit cell of binder. Then, this geometry was replicated. In all of the simulations, \(^6\)Li enrichment is set to 95\% (atom percent). The representation of a unit cell is shown in Figure-3.4.

![Figure-3-4 Unit cell used in EJ-426 scintillator simulations. Blue, red and green represent LiF, ZnS and binder, respectively.](image)

After the unit cell was replicated and placed in the detector medium, the full scale simulations were performed. The active volume of the detector was placed between two polyester sheets. In reference [11], optimization work was done for scintillator mixtures and ZnS phosphor size was reported to be 8\(\mu\)m, which is the current standard size. For the simulations, LiF and ZnS grain sizes are selected as 4\(\mu\)m and 8\(\mu\)m in diameter, respectively. In Figure-3.5, a GEANT4 simulation is shown with the moderator, detection sheet and the PMT surface.
3.5 Simulations of EJ-426 Detectors

The specifications of the detectors were taken from the ELJEN website\textsuperscript{(2)}.

The calculation of $^6\text{Li}$ mass in the detectors is carried out as

$$M_{^6\text{Li}} = N_{^6\text{Li}} \times V \times 6 \times 1.66 \times 10^{-24}$$  \hspace{1cm} [Eq. 3.12]

$$M_{^6\text{Li}} = 8.81 \times 10^{21} cm^{-3} \times 0.032 cm \times 5 cm \times 10 cm \times 6 \frac{amu}{\#} \times 1.66 \times 10^{-24} \frac{g}{amu} = 140 mg$$  \hspace{1cm} [Eq. 3.13]

In Table-3.3 and Table-3.4, the simulation results are shown for four detector sheets with different compositions and different thicknesses.
The mean number of photons detected per neutron event decreases as the thickness of the detector and the concentration of $^6$Li increase, which is in agreement with the experiments with the exception of EJ-426-0060-HD. The highest efficiency was obtained with the EJ-426-0032-HD contrary to experiments where the highest detection efficiency was obtained with EJ-426-0060-HD. Also, in simulations, the thinner detectors were favored in general which might mean that absorption coefficient of ZnS was overestimated.
0.044eV was chosen as a cutoff energy to approximate the thermal neutron detection efficiency and it was obtained from the MCNP6 simulations which involved the LiF:ZnS:binder geometry.

Figure-3.6 shows the neutron energy at the time of capture by $^6$Li. There is a peak at thermal energy (0.0253eV) but higher and lower energy neutrons may also cause alpha and triton production.

PTRAC card was used to get detailed information from the simulations and a MATLAB script was written to obtain the energy distribution. The code is given in Appendix B with a sample MCNP6 input.

The reason why the cutoff is implemented is that not the same number of neutrons is moderated when the detector geometry is changed although the moderator geometry is not changed. It is the random nature of Monte Carlo methods. Still, both absolute detection efficiency and the thermal neutron detection efficiency are tabulated.
3.6 Comparison of Simulations and Experiments

Comparison between the simulations and experiments is shown in Table-3.5. Quantum efficiency (QE) correction was done based on the number of photons crossing the PMT surface in a single event. The peak quantum efficiency of the PMT (H10580) is 0.2724 so the events resulting below 4 photons crossing the PMT were discarded. Since the simulations were done with the source emitting neutrons only in the positive-z direction, the simulation results are divided by 2 before comparing them to the experiments.

Percentage error between the experimental results and the simulation results is calculated as

\[
\text{Percentage error} = \frac{|N_{\text{experimental}} - N_{\text{simulation}}|}{N_{\text{experimental}}} \quad [Eq.3.14]
\]

where N is the quantity of interest.

<table>
<thead>
<tr>
<th>Detector</th>
<th>Number of neutrons detected per neutron (experimental)</th>
<th>Number of neutrons detected per neutron (no additional material)</th>
<th>Percentage Error</th>
<th>Number of neutrons detected per neutron (with additional materials)</th>
<th>Percentage Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>EJ-426-0032</td>
<td>3.48E-5 ± 0.15*</td>
<td>3.20E-4 ± 0.026</td>
<td>0.08</td>
<td>5.60E-5 ± 0.039</td>
<td>0.61</td>
</tr>
<tr>
<td>EJ-426-HD-0032</td>
<td>3.45E-5 ± 0.15*</td>
<td>4.55E-5 ± 0.028</td>
<td>0.32</td>
<td>5.85E-5 ± 0.092</td>
<td>0.70</td>
</tr>
<tr>
<td>EJ-426-0060</td>
<td>3.47E-5 ± 0.15*</td>
<td>2.65E-5 ± 0.040</td>
<td>0.24</td>
<td>4.20E-5 ± 0.109</td>
<td>0.21</td>
</tr>
<tr>
<td>EJ-426-HD-0060</td>
<td>4.06E-5 ± 0.15*</td>
<td>3.15E-5 ± 0.063</td>
<td>0.22</td>
<td>4.73E-5 ± 0.119</td>
<td>0.17</td>
</tr>
</tbody>
</table>

Table-3.5 – Comparison between experiments and simulations of four different EJ-426 detectors. *252Cf activity uncertainty, which is explained below.

Since the simulations shown in Figure-3.5 don’t take into account the scattering of neutrons from the floor and the box surfaces, more detailed simulations were performed with additional materials including the stainless steel casing of 252Cf. Moreover, clustering of grains were mimicked using a different kind of unit cell approach.
H10580 is a type of PMT that is useful for scintillation counting and the peak quantum efficiency of the photocathode is 0.27, which is used for the QE correction. The spectral response range of the PMT, however, is 300-600nm, which means some photons are less likely to cause the photoelectric effect. The exact function of the spectral response characteristic was unknown so typical PMT response was mimicked to see the PMT effect and the results are shown in Table-3.6.

<table>
<thead>
<tr>
<th>Detector</th>
<th>Number of neutrons detected per neutron (experimental)</th>
<th>Number of neutrons detected per neutron (constant Q.E.)</th>
<th>Percentage Error</th>
<th>Number of neutrons detected per neutron (Wavelength dependent Q.E.)</th>
<th>Percentage Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>EJ-426-0032</td>
<td>3.48E-5 ± 0.15*</td>
<td>5.60E-5 ± 0.077</td>
<td>0.61</td>
<td>5.56E-5 ± 0.077</td>
<td>0.60</td>
</tr>
<tr>
<td>EJ-426-HD-0032</td>
<td>3.45E-5 ± 0.15*</td>
<td>5.85E-5 ± 0.092</td>
<td>0.70</td>
<td>5.85E-5 ± 0.092</td>
<td>0.70</td>
</tr>
<tr>
<td>EJ-426-0-0060</td>
<td>3.47E-5 ± 0.15*</td>
<td>4.20E-5 ± 0.109</td>
<td>0.21</td>
<td>3.90E-5 ± 0.113</td>
<td>0.12</td>
</tr>
<tr>
<td>EJ-426-HD-0060</td>
<td>4.06E-5 ± 0.15*</td>
<td>4.73E-5 ± 0.119</td>
<td>0.17</td>
<td>3.80E-5 ± 0.132</td>
<td>0.06</td>
</tr>
</tbody>
</table>

Table-3.6 Comparison between experiments and simulations of four different EJ-426 detectors with constant PMT QE and varying PMT QE

Figure-3-7 a) Simulation with additional materials included b) Eight unit cells together with clustering of ZnS and LiF grains
According to Table-3.5, the simulations mostly underestimate the number of neutrons detected when only the portion of the geometry was taken into consideration since the neutrons scattered from surfaces may find their way into the moderator again and consequently the detector. When the whole geometry is simulated, there is a clear overestimation of the detection. Since the powders are mixed in a random manner with different grain size, the simulation geometry doesn’t exactly reflect the actual scintillator medium, where there could be clustering of the same type of the material at certain places. For example, if there are lots of $^6$LiF clustered at some location, captured neutrons wouldn’t result in light production and if there are lots of ZnS clustered at some location, neutrons wouldn’t be captured in the first place. Other possibility is that some portions of the detector may be solely filled with binder. Simulations assume a highly regular geometry without any clustering, which is one of the reasons of the overestimation. Another reason might be the uncertainties in light properties for production and transport. In simulations, ZnS was assumed to produce 50000 photons/MeV [9]. Also, as seen from Table-3.6, when the wavelength dependency for quantum efficiency is applied, the neutron detection goes down as expected since the constant QE assumes all of the photons have the same probability of photoelectric effect and that probability is 0.27 when there are other photons which would less likely to produce photoelectrons.

Effort has been made to address the clustering issue creating a unit cell seen in Figure-3.7(b); however, it didn’t produce much effect as expected since arranging the geometry as in Figure-3.7(b) actually creates more free space for light to travel although light production decreases due to the clustering.

There are several sources of error as well including the uncertainty in the $^{252}$Cf activity, uncertainty in the moderation of neutrons (between GEANT4 and MCNP6) and uncertainty in the optical properties of ZnS. Uncertainty in the activity of $^{252}$Cf is ±15% [18], which is a considerable amount. The uncertainty in $^{252}$Cf makes the accurate validation of the simulations impossible.
ROOT was used to analyze the data obtained from GEANT4. ROOT is a data analysis program developed by CERN.\cite{25}

The photon energy spectrum crossing the PMT surface is shown in Figure 3.8 with the Gaussian fit.

![Figure 3.8 Energy spectrum of photons that hit the PMT surface in GEANT4](image)
Scintillation light is produced throughout the detector medium almost uniformly because of the homogeneity of the medium. However, due to the attenuation of the neutrons, less light is expected to be generated in the distant regions from the moderator. But since the detector sheet is very thin, neutron attenuation doesn’t have much effect. In Figure-3.9, the moderator is at the back of the detector (thickness coordinate = -0.2mm) and the PMT is at the face of the detector sheet (thickness coordinate = 0.2mm).

*Figure-3.9 Locations of photons produced per primary neutron in 0.032cm EJ-426-0 detector*
In Figure-3.10, location of the production of the detected photons are shown. As expected, although light is produced deeper in the scintillator volume, those photons cannot travel much without being absorbed by the opaque medium. Consequently, the photons that are detected are the ones produced at the front side of the detector. As we move towards the deeper regions of the detector, the count of photons vanishes. Also, when the thickness of the detector increases, there is even more dramatic decrease of photons reaching the PMT due to more ZnS in the way.
In Figure-3.11, the PMT response is shown for EJ-426-0032-0 and EJ-426-060-0. When the thickness is increased from 0.032cm to 0.060cm, the PMT response is shifted towards the left side of the spectrum. Consequently, there is less neutron detection and fewer number of photons per detection.

Although the simulation results don’t match well with the experiment values due to lots of uncertainties with both neutron part and light part of the simulations, they have given a reference to compare the coated micro-particle geometries.
Chapter 4 Coated Micro-Particles

In order to convert the higher portion of the charged particle energy to the light production and increase the light collection, it is proposed for the $^6$LiF to be coated by ZnS so that the charged particles have a higher chance to produce light in ZnS. The design of this geometry requires optimizations at various levels. One important parameter to consider is the range of $\alpha$ and $T$ in LiF and ZnS. Optimization took place at the following different levels:

1) It is desired to have a neutron converter volume (LiF) as large as possible to capture the neutrons. At the same time, it shouldn’t be too large, otherwise the charged particles wouldn’t travel to the scintillating crystal (ZnS).

2) It is desired that the scintillating volume is as large as possible for the charged particles to deposit much of their energy before leaving it. However, it shouldn’t be too large since ZnS is not transparent to its own luminescence and the light produced may not get out.

3) It is desired to have a transparent volume as large as possible to allow the light to travel to the photodetector without being absorbed. At the same time, it shouldn’t be too large since it would occupy the space that could be filled with LiF and ZnS; thereby reducing both the neutron capture probability and the light production.

4) It is desired to have a detector as thick as possible to capture most neutrons. However, that would reduce the light collection efficiency because of the opaqueness of ZnS to its own light.
In Figure-4.1(a), the representation of grains of LiF and ZnS distributed inside a binder geometry is shown. Coated particle geometry is shown in Figure-4.2(b).

Since there are four different parameters that need to be considered simultaneously, a convention was devised so that the comparison can be made easier.

A quantity is expressed as a letter with four subscripts, i.e. $D_{\text{RLiF}\cdot t\text{ZnS}\cdot \text{pitch}\cdot \text{thickness}}$. For examples, $D_{19\cdot 4\cdot 80\cdot 320}$ means “detector with $r_{\text{LiF}} = 19\mu m$, $t_{\text{ZnS}} = 4\mu m$, pitch = 80$\mu m$ and thickness 320$\mu m$”.

4.1 Optimization with Single Unit Cell

LiF radius and ZnS thickness can be optimized using a single unit cell approximation. The relevant tally for LiF radius optimization process is the energy deposited in ZnS per primary neutron and the relevant tally for ZnS thickness optimization is the number of light photons escaping the unit cell per primary neutron.
4.1.1 Range Calculations

Alpha and triton ranges in LiF and ZnS were calculated using three different Monte Carlo codes; MCNP6, GEANT4 and SRIM. Analytical calculation was also performed with the range calculated as

\[
R(T) = \int_0^T \left( -\frac{dE}{dx} \right)^{-1} dE
\]

where R is the range and T is the kinetic energy of the particle. Stopping power is calculated using Bethe-Bloch formula with density effect and shell correction neglected. The code is in Appendix C with the SRIM results.

In Table 4.1, the range values are shown for alpha and triton particles in LiF and ZnS. Although there are discrepancies between the calculation approaches, the numbers are close to each other.

<table>
<thead>
<tr>
<th>Medium/Computational Tool</th>
<th>Range of Alpha (μm)</th>
<th>Range of Triton (μm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>LiF (Analytical)</td>
<td>4.0</td>
<td>29</td>
</tr>
<tr>
<td>LiF (Simulation-MCNP6)</td>
<td>6.5</td>
<td>31.5</td>
</tr>
<tr>
<td>LiF (Simulation-SRIM)</td>
<td>6.1</td>
<td>34.1</td>
</tr>
<tr>
<td>LiF (Simulation-GEANT4)</td>
<td>5.2</td>
<td>33.8</td>
</tr>
<tr>
<td>ZnS (Analytical)</td>
<td>7.3</td>
<td>37</td>
</tr>
<tr>
<td>ZnS (Simulation-MCNP6)</td>
<td>7.5</td>
<td>34.5</td>
</tr>
<tr>
<td>ZnS (Simulation-SRIM)</td>
<td>6.0</td>
<td>32.3</td>
</tr>
<tr>
<td>ZnS (Simulation-GEANT4)</td>
<td>6.0</td>
<td>32.0</td>
</tr>
</tbody>
</table>

Table 4.1 – Calculated range values for alpha and triton particles with four different tools

FMESH tally was used to calculate the range of particles in MCNP6. The tally allows to split the geometry into bins which gives a better resolution in terms of range. The MCNP6 results are shown in Figure 4.2.
4.1.2 LiF Radius Optimization

Optimization was performed using three different Monte Carlo codes; MCNP6, GEANT4, and custom made Monte Carlo code. Different models (Vavilov energy straggling and CSDM) in MCNP6 were also tested but because of the energies of interest, they didn’t produce different results. In GEANT4, QGSP_BERT_HP (Quark-Gluon String Model_Bertini Cascade Model_High Precision Neutron Model) was used in the simulations.

Concentric spheres were created and placed in a cubical volume. A thermal neutron pencil source (mono-directional point source) was pointed to the center of the geometry and the energy deposition in ZnS was tallied. A sphere is symmetrical along its azimuthal and polar angle; therefore, there is no difference between point source at the center or pencil source at some distance in terms of optimization.

The LiF radius was varied keeping the ZnS thickness constant and at a relatively large value since the only thing that is important is how LiF radius affects the energy deposition.
The schematic representation of a unit cell is shown in Figure-4.3.

![Figure-4-3 Unit cell representation of the coated particle geometry (MCNP6-VISED)](image)

The optimization results are shown in Table-4.2 and Figure-4.4.

<table>
<thead>
<tr>
<th>( R_{LiF} ) (µm)</th>
<th>( t_{ZnS} ) (µm)</th>
<th>Energy Deposition in ZnS per primary neutron in MCNP6 (MeV) (with Continuous Slowing Down Model)</th>
<th>Energy Deposition in ZnS per primary neutron in MCNP6 (MeV) (with Vavilov Model)</th>
<th>Energy Deposition in ZnS per primary neutron in GEANT4 (MeV) (with QGSP_BERT_HP)</th>
<th>Energy Deposition in ZnS per primary neutron in Custom Monte Carlo code</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>90</td>
<td>0.252 ± 0.0066</td>
<td>0.252 ± 0.0066</td>
<td>0.257 ± 0.0092</td>
<td>0.249 ± 0.0094</td>
</tr>
<tr>
<td>11</td>
<td>90</td>
<td>0.265 ± 0.0063</td>
<td>0.265 ± 0.0063</td>
<td>0.273 ± 0.0088</td>
<td>0.264 ± 0.0089</td>
</tr>
<tr>
<td>12</td>
<td>90</td>
<td>0.277 ± 0.0060</td>
<td>0.277 ± 0.0060</td>
<td>0.281 ± 0.0085</td>
<td>0.274 ± 0.0086</td>
</tr>
<tr>
<td>13</td>
<td>90</td>
<td>0.287 ± 0.0057</td>
<td>0.287 ± 0.0057</td>
<td>0.301 ± 0.0080</td>
<td>0.281 ± 0.0082</td>
</tr>
<tr>
<td>14</td>
<td>90</td>
<td>0.294 ± 0.0055</td>
<td>0.294 ± 0.0055</td>
<td>0.307 ± 0.0078</td>
<td>0.288 ± 0.0080</td>
</tr>
<tr>
<td>15</td>
<td>90</td>
<td>0.300 ± 0.0054</td>
<td>0.300 ± 0.0054</td>
<td>0.310 ± 0.0074</td>
<td>0.295 ± 0.0077</td>
</tr>
<tr>
<td>16</td>
<td>90</td>
<td>0.304 ± 0.0052</td>
<td>0.304 ± 0.0052</td>
<td>0.318 ± 0.0073</td>
<td>0.295 ± 0.0076</td>
</tr>
<tr>
<td>17</td>
<td>90</td>
<td>0.306 ± 0.0051</td>
<td>0.306 ± 0.0051</td>
<td>0.321 ± 0.0072</td>
<td>\textbf{0.302 ± 0.0074}</td>
</tr>
<tr>
<td>18</td>
<td>90</td>
<td>\textbf{0.307 ± 0.0050}</td>
<td>\textbf{0.307 ± 0.0050}</td>
<td>0.326 ± 0.0071</td>
<td>0.301 ± 0.0052</td>
</tr>
<tr>
<td>19</td>
<td>90</td>
<td>0.307 ± 0.0050</td>
<td>0.307 ± 0.0050</td>
<td>\textbf{0.327 ± 0.0070}</td>
<td>0.297 ± 0.0052</td>
</tr>
<tr>
<td>20</td>
<td>90</td>
<td>0.304 ± 0.0049</td>
<td>0.304 ± 0.0049</td>
<td>0.327 ± 0.0067</td>
<td>0.294 ± 0.0051</td>
</tr>
<tr>
<td>21</td>
<td>90</td>
<td>0.300 ± 0.0049</td>
<td>0.300 ± 0.0049</td>
<td>0.322 ± 0.0068</td>
<td>0.292 ± 0.0051</td>
</tr>
<tr>
<td>22</td>
<td>90</td>
<td>0.294 ± 0.0049</td>
<td>0.294 ± 0.0049</td>
<td>0.319 ± 0.0066</td>
<td>0.288 ± 0.0051</td>
</tr>
</tbody>
</table>

\[\text{Table-4.2 – Optimization of LiF radius with MCNP6 and GEANT4}\]
There are discrepancies between the codes possibly due to the slightly different thermal neutron data in GEANT4 and MCNP6 as mentioned in Section 2.1. Still, they give almost the same optimal radius for LiF. MCNP6 gives 18μm, GEANT4 gives 19μm and custom made Monte Carlo code with ENDF-VI libraries gives 17μm as the optimal radius. In MCNP6, there is a very slight difference between the 18μm and 19μm to the point they are identical up to the third digit. Since the rest of the simulations were done mainly with GEANT4, 19μm radius was considered to be the optimal. From the range values, it is clear that most of the alpha energy is lost without reaching ZnS. In order for the alpha particles to reach ZnS, they need to be produced within a distance of 4μm from the scintillator. Although making the unit cell smaller would highly increase the light production for a given neutron, neutron capture efficiency would decrease significantly, reducing the effective energy deposition.

Detectors with different LiF radii were also tested and compared to the 19μm case. The results are in Section 4.2.2.
Energy deposition map in a unit cell is shown in Figure-4.5.

![Energy Deposition in a unit cell (MeV) yz projection](image)

**Figure-4.5 Energy deposition map in a unit cell**

As can be seen from Figure-4.5, most of the energy of the charged particles is deposited within approximately 8μm radius, which is well within the optimal radius of LiF. Therefore, most of the energy is lost without any light production.

### 4.1.3 ZnS Thickness Optimization

After determining the optimum radius of LiF, the focus was switched to GEANT4 for its capability to simulate scintillation light. While ZnS produces light, at the same time it absorbs its own luminescence. Similar approach was utilized to find out the optimum ZnS thickness as was done determining the LiF radius; concentric unit spheres were constructed and the amount of light getting out of the ZnS per primary neutron event was tallied. LiF thickness was kept constant at its optimal value and the results are shown in Table-4.3 and Figure-4.6.
Optimal thickness is determined to be 1 µm for ZnS. Still, the results are too close to each other. Therefore, simulations were also performed with 2 µm ZnS and it was shown that for high pitch
geometries, 2μm ZnS performed better than 1μm case due to less light absorption by blocking layers. However, the results are well within the error range. The sharp decrease is replaced by a smoother drop after 8μm up to 12μm due to the number of light photons competing with the high absorption coefficient of ZnS.

The emission spectrum and the absorption coefficient used in GEANT4 simulations are shown in Figure-4.7.

![Emission and absorption spectrum of ZnS(Ag)](image)

*Figure-4.7 Emission and absorption spectra used in GEANT4 for ZnS*
In Figure-4.8, the energy deposition distribution is shown for three different ZnS thicknesses.

There is a sharp drop at approximately 2.7 MeV when the ZnS coating thickness is 34μm, which corresponds to the events where a triton deposits its full energy into the ZnS. Since alpha particles and tritons are created with opposite momenta, it is highly likely when the triton deposits its full energy in ZnS that all of the alpha particle energy will be deposited in LiF.
In Figure 4.9, the number of light photons leaving the unit cell is shown for two ZnS thicknesses since when ZnS is 34μm, almost no light can be collected.

34μm ZnS thickness is enough to have all the energy of alpha and triton particles since it is the range of T in ZnS. Although only 8% of the maximum possible energy deposition is achieved in 1μm ZnS, this ZnS coating thickness performs better due to the improved light transport properties. 130keV corresponds to 6500 light photons produced. On the average, 975 of them can leave the ZnS volume without being absorbed, which corresponds to 15% of the average number of light produced. However, when the ZnS is 34μm, almost no light can escape the unit cell. Therefore, the ratio of the amount of light that can be collected to the theoretical maximum of light production is just 1.2%. Most frequent light output for 1μm and 4μm ZnS thickness are both roughly 660 photons but 1μm ZnS has a tail in the upper portion of the spectrum which makes it brighter. The reason the figures are plotted in a way that shows the upper portion is to show the light output corresponding to the mean energy deposition in the scintillator, which are 6500 and 22500 light photons for 1μm and 4μm, respectively. However, in 4μm, the maximum number of photons leaving the unit cell is roughly 5000, which is less than that of 1μm ZnS.
Since the pitch and thickness optimizations require the use of multiple unit cells, they were performed using the entire detector volume.

4.2 Optimization with Multiple Unit Cells with Full-Scale Simulations of Coated Micro-Particle Detectors

Pitch and the detector thickness optimization require the use of multiple unit cells since the presence of other unit cells affects the overall performance of the detector.

The unit cell was replicated and placed in the detector volume. LiF radius was kept constant in all of the simulations however cases were simulated with 2μm, 4μm and 8μm coating thickness to see how well the coated particles perform with even larger ZnS thicknesses. When the optimal geometry was found, randomization of position of micro-particles, randomization of LiF radius and randomization of the ZnS thickness were implemented to reveal the overall performance.

4.2.1 Calculation of Mass of $^6\text{Li}$ for Coated Micro-Particle Detectors

$^6\text{Li}$ is assumed to be 95% enriched in weight,

$$\frac{1}{M_{\text{Li}}} = \left(\frac{1 - \epsilon}{7} + \frac{\epsilon}{6}\right)^{-1} \Rightarrow M_{\text{Li}} = 6.04 g \quad [Eq.4.2]$$

The mass of $^6\text{Li}$ is calculated for coated particles as follows

$$\text{Volume of LiF in a unit cell} = \frac{4}{3} \pi * (19 * 10^{-4} \text{cm})^3 = 2.87 * 10^{-8} \text{cm}^3 \quad [Eq.4.3]$$

$$\text{Number of } ^6\text{Li atoms in a unit cell} = 2.87 * 10^{-8} \text{ cm}^3 * \frac{2.635 * 0.602 * 10^{24}}{25.04} * 0.95 \frac{\#}{\text{cm}^3} = 1.73 * 10^{15} \# \quad [Eq.4.4]$$

$$\text{Mass of } ^6\text{Li in a unit cell} = 1.73 * 10^{15} \# * 6 \frac{\text{amu}}{\#} * 1.66 * 10^{-24} \frac{g}{\text{amu}} = 17.2 * 10^{-9} g \quad [Eq.4.5]$$

For 0.032cm*5cm*10cm detector with 80μm pitch
Total mass of $^6Li = 4 \times 625 \times 1250 \times 17.2 \times 10^{-9} = 53.8 \text{mg}$  \[ Eq. 4.6 \]

4.2.2 Comparison of Different Thicknesses in Micro-Particle Detectors

Full scale simulations were performed to compare the pitch, detector thickness and ZnS thickness altogether. The results are tabulated and plotted for comparison.

4.2.2.1 0.032cm Thick Detector

The results for a 0.032cm detector are shown in Table-4.4 and Table-4.5. The highest absolute detection efficiency is found with $D_{1.5-50-320}$ whereas highest signal amplitude (the mean number of photons detected) is found with $D_{1.80-320-320}$ where n.a. stands for non-aligned. Non-aligned geometry is where the micro-particles are placed in alternating layers instead of being directly placed behind the particles in front.
<table>
<thead>
<tr>
<th>ZnS thickness (μm)</th>
<th>Pitch (μm)</th>
<th>Number of neutrons detected per primary neutron</th>
<th>Number of neutrons detected per primary neutron (corrected with Q.E.)</th>
<th>Number of photons detected per primary neutron</th>
<th>Mean number of photons detected</th>
<th>Mass of $^6\text{Li}$ (mg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>40</td>
<td>1.45E-4 ± 0.048</td>
<td>8.23E-5 ± 0.064</td>
<td>8.37E-3</td>
<td>13.20</td>
<td>430</td>
</tr>
<tr>
<td>1</td>
<td>50</td>
<td>2.07E-4 ± 0.035</td>
<td>1.50E-4 ± 0.041</td>
<td>9.73E-3</td>
<td>16.89</td>
<td>206</td>
</tr>
<tr>
<td>1</td>
<td>60 (n.a.)</td>
<td>1.58E-4 ± 0.032</td>
<td>1.39E-4 ± 0.035</td>
<td>1.31E-2</td>
<td>25.82</td>
<td>120</td>
</tr>
<tr>
<td>1</td>
<td>60</td>
<td>1.57E-4 ± 0.046</td>
<td>1.38E-4 ± 0.049</td>
<td>1.13E-2</td>
<td>26.30</td>
<td>120</td>
</tr>
<tr>
<td>2</td>
<td>60</td>
<td>1.41E-4 ± 0.053</td>
<td>1.16E-4 ± 0.053</td>
<td>9.85E-3</td>
<td>22.06</td>
<td>120</td>
</tr>
<tr>
<td>4</td>
<td>60</td>
<td>1.27E-4 ± 0.051</td>
<td>1.01E-4 ± 0.057</td>
<td>6.25E-3</td>
<td>17.13</td>
<td>120</td>
</tr>
<tr>
<td>8</td>
<td>60</td>
<td>9.40E-5 ± 0.073</td>
<td>5.70E-5 ± 0.094</td>
<td>2.34E-3</td>
<td>10.45</td>
<td>120</td>
</tr>
<tr>
<td>1</td>
<td>70</td>
<td>1.03E-4 ± 0.057</td>
<td>9.37E-5 ± 0.060</td>
<td>1.04E-2</td>
<td>31.65</td>
<td>70</td>
</tr>
<tr>
<td>4</td>
<td>70</td>
<td>1.00E-4 ± 0.058</td>
<td>8.13E-5 ± 0.064</td>
<td>5.00E-3</td>
<td>24.92</td>
<td>70</td>
</tr>
<tr>
<td>8</td>
<td>70</td>
<td>7.57E-5 ± 0.066</td>
<td>5.70E-5 ± 0.076</td>
<td>3.80E-3</td>
<td>20.57</td>
<td>70</td>
</tr>
<tr>
<td>1</td>
<td>80</td>
<td>8.33E-5 ± 0.045</td>
<td>7.63E-5 ± 0.047</td>
<td>9.19E-3</td>
<td>34.02</td>
<td>54</td>
</tr>
<tr>
<td>2</td>
<td>80</td>
<td>7.33E-5 ± 0.058</td>
<td>6.35E-5 ± 0.063</td>
<td>6.62E-3</td>
<td>31.47</td>
<td>54</td>
</tr>
<tr>
<td>4</td>
<td>80</td>
<td>7.52E-5 ± 0.047</td>
<td>6.28E-5 ± 0.051</td>
<td>4.73E-3</td>
<td>29.07</td>
<td>54</td>
</tr>
<tr>
<td>8</td>
<td>80</td>
<td>6.20E-5 ± 0.057</td>
<td>4.88E-5 ± 0.064</td>
<td>2.20E-3</td>
<td>23.04</td>
<td>54</td>
</tr>
<tr>
<td>1</td>
<td>100</td>
<td>4.33E-5 ± 0.048</td>
<td>3.81E-5 ± 0.051</td>
<td>5.59E-3</td>
<td>36.99</td>
<td>26</td>
</tr>
<tr>
<td>2</td>
<td>100</td>
<td>4.38E-5 ± 0.062</td>
<td>4.00E-5 ± 0.065</td>
<td>4.94E-3</td>
<td>31.07</td>
<td>26</td>
</tr>
<tr>
<td>4</td>
<td>100</td>
<td>4.36E-5 ± 0.046</td>
<td>3.79E-5 ± 0.049</td>
<td>3.52E-3</td>
<td>32.65</td>
<td>26</td>
</tr>
<tr>
<td>8</td>
<td>100</td>
<td>3.33E-5 ± 0.071</td>
<td>3.00E-5 ± 0.074</td>
<td>2.22E-3</td>
<td>35.11</td>
<td>26</td>
</tr>
<tr>
<td>1</td>
<td>80 (n.a.)</td>
<td>8.88E-5 ± 0.043</td>
<td>8.25E-5 ± 0.045</td>
<td>1.10E-2</td>
<td>37.21</td>
<td>54</td>
</tr>
<tr>
<td>4</td>
<td>80 (n.a.)</td>
<td>8.14E-5 ± 0.050</td>
<td>6.84E-5 ± 0.054</td>
<td>4.27E-3</td>
<td>28.75</td>
<td>54</td>
</tr>
<tr>
<td>8</td>
<td>80 (n.a.)</td>
<td>6.53E-5 ± 0.062</td>
<td>5.43E-5 ± 0.068</td>
<td>3.06E-3</td>
<td>22.62</td>
<td>54</td>
</tr>
</tbody>
</table>

Table 4-4 – Simulation results for different coated particle detectors with mean signal amplitude and absolute detection efficiency. Number of photons detected per primary neutron and the mass of $^6\text{Li}$ in each detector are also shown. The detector thickness is 0.032cm.
Detector | Neutron capture efficiency (captured/neutrons below 0.044eV) | Neutron detection efficiency (detected/captured) | Overall neutron detection efficiency (detected/neutron below 0.044eV) | Overall neutron detection efficiency (corrected with quantum efficiency) | LiF:ZnS mass ratio
---|---|---|---|---|---
D19-1-40-320 | 1.43* ± 0.034 | 0.211 ± 0.053 | 0.301 ± 0.055 | 0.171 ± 0.069 | 1:0.26
D19-1-50-320 | 0.921 ± 0.034 | 0.492 ± 0.043 | 0.453 ± 0.042 | 0.327 ± 0.047 | 1:0.26
D19-1-60-320 (non aligned) | 0.585 ± 0.031 | 0.580 ± 0.041 | 0.339 ± 0.038 | 0.298 ± 0.039 | 1:0.26
D19-1-60-320 | 0.594 ± 0.044 | 0.564 ± 0.058 | 0.335 ± 0.053 | 0.294 ± 0.056 | 1:0.26
D19-2-60-320 | 0.578 ± 0.049 | 0.528 ± 0.066 | 0.305 ± 0.061 | 0.251 ± 0.066 | 1:0.54
D19-4-60-320 | 0.619 ± 0.044 | 0.447 ± 0.062 | 0.277 ± 0.058 | 0.221 ± 0.063 | 1:1.20
D19-8-60-320 | 0.639 ± 0.052 | 0.312 ± 0.084 | 0.200 ± 0.080 | 0.121 ± 0.099 | 1:2.90
D19-1-70-320 | 0.377 ± 0.052 | 0.604 ± 0.072 | 0.227 ± 0.063 | 0.208 ± 0.066 | 1:0.26
D19-4-70-320 | 0.382 ± 0.051 | 0.561 ± 0.072 | 0.214 ± 0.064 | 0.174 ± 0.069 | 1:1.20
D19-8-70-320 | 0.387 ± 0.052 | 0.448 ± 0.080 | 0.173 ± 0.072 | 0.125 ± 0.081 | 1:2.90
D19-1-80-320 | 0.301 ± 0.040 | 0.605 ± 0.057 | 0.182 ± 0.049 | 0.167 ± 0.050 | 1:0.26
D19-2-80-320 | 0.291 ± 0.050 | 0.560 ± 0.073 | 0.163 ± 0.063 | 0.141 ± 0.067 | 1:0.54
D19-4-80-320 | 0.306 ± 0.039 | 0.526 ± 0.058 | 0.161 ± 0.051 | 0.134 ± 0.055 | 1:1.20
D19-8-80-320 | 0.288 ± 0.044 | 0.460 ± 0.069 | 0.132 ± 0.060 | 0.104 ± 0.067 | 1:2.90
D19-1-100-320 | 0.157 ± 0.041 | 0.618 ± 0.061 | 0.097 ± 0.050 | 0.085 ± 0.053 | 1:0.26
D19-2-100-320 | 0.156 ± 0.053 | 0.631 ± 0.079 | 0.099 ± 0.065 | 0.090 ± 0.067 | 1:0.54
D19-4-100-320 | 0.163 ± 0.038 | 0.584 ± 0.057 | 0.095 ± 0.048 | 0.083 ± 0.051 | 1:1.20
D19-8-100-320 | 0.148 ± 0.053 | 0.485 ± 0.086 | 0.072 ± 0.073 | 0.064 ± 0.077 | 1:2.90
D19-1-80-320 (non aligned) | 0.308 ± 0.039 | 0.620 ± 0.055 | 0.191 ± 0.047 | 0.177 ± 0.049 | 1:0.26
D19-4-80-320 (non aligned) | 0.314 ± 0.043 | 0.576 ± 0.062 | 0.181 ± 0.054 | 0.152 ± 0.058 | 1:1.20
D19-8-80-320 (non aligned) | 0.292 ± 0.050 | 0.497 ± 0.076 | 0.145 ± 0.066 | 0.120 ± 0.072 | 1:2.90

*Efficiencies more than 1 simply means that more neutrons above 0.044 eV are captured.

Table 4-5: Detailed information of the simulations of different coated particle detectors with thickness of 0.032cm showing the thermal neutron detection efficiency.
In Figure 4.10, the locations of the production of photons in coated particle detector D_{19-4:80-320} are shown. The production pattern is rather smooth as a function of detector thickness since the thickness is very low. Clearly, the photons are only produced in the four layers occupied by the micro-particles.

Comparison of the locations of “photons produced that are detected” is made in Figure 4.11 for six different cases. When the pitch decreases, more layer can be put into the detector with the same thickness. More layers increase the neutron capture efficiency but they also block the light coming from the back layers. When the pitch was increased to 80 μm, the light can be collected from the back layers more efficiently as can be seen in the figure. As expected, the ZnS thickness has an adverse effect on light collection.
Figure 4.11: Location of photons produced which are successfully registered as detection in 0.032 cm coated particle detector for:

a) $t=1$ micron, $p=60$ microns  
b) $t=1$ micron, $p=80$ microns  
c) $t=4$ microns, $p=60$ microns  
d) $t=4$ microns, $p=80$ microns  
e) $t=8$ microns, $p=60$ microns  
f) $t=8$ microns, $p=80$ microns
The numbers shown in Figure-4.11 are the number of photons per primary neutron. The mean number of photons per detected neutron is different and they are shown in Figure-4.12. In the figure, the PMT response of various detectors is shown. When the pitch increases, the signal amplitude increases due to the better light collection properties. Again, ZnS thickness has the adverse effect on the signal amplitude since it absorbs the light before it reaches the PMT. For 80μm pitch, the signal amplitude is much better than what the commercially available detectors provide.

Since the number of photons detected is different in all the cases, comparison is hard looking at Figure-4.11. Figures relative to the worst case (D_{19.8-80-320}) were made and they are shared in Appendix E.
Figure 4.12 PMT response in 0.032 cm coated particle detector for:

- a) t=1 micron, p=60 microns
- b) t=1 micron, p=80 microns
- c) t=4 microns, p=60 microns
- d) t=4 microns, p=80 microns
- e) t=8 microns, p=60 microns
- f) t=8 microns, p=80 microns
The geometry was arranged such that the layers are aligned with each other. Another configuration was tested with alternating layers not blocking the immediate layer as shown in Figure-4.13. The non-aligned versions give slightly better results than their counterparts in terms of neutron detection efficiency. In Figure-4.14, difference between the $D_{19-1:80-320}$ and $D_{19-1:80-320-n.a}$ is shown. There are much more light spikes at the back layers when the layers are alternating.

![Non-aligned geometry for coated particles](image)

Figure-4.13 Non-aligned geometry for coated particles

![Location of photons that are detected](image)

Figure-4.14 Location of photons that are detected for a) $D_{19-1:80-320}$ and b) $D_{19-1:80-320}$ non-aligned geometry.

The absolute detection efficiency with QE correction as a function of pitch for 0.032cm coated micro-particle detector is shown in Figure-4.15.
The absolute detection efficiency is highest when the pitch is 60μm however the decrease in the efficiency for 1μm ZnS and 4μm ZnS is sharper. The reason is that decreasing the pitch doesn’t improve the detection efficiency for 8μm ZnS as much as for 1μm or 4μm ZnS due to worsened light propagation properties.

Non-aligned cases show a consistent improvement over aligned cases. Still, the results are very close and well within the error range. The error bars weren’t put into the figures since they render the graph unreadable when there are lots of data points on top of each other.
4.2.2.2 0.060cm Thick Detector

The results for 0.060cm detector are shown in Table-4.6 and Table-4.7. The highest absolute detection efficiency is found with D_{19-1-60-600} whereas the highest signal amplitude is found with D_{19-1-100-600} as expected since more light can be collected when the medium is transparent.

<table>
<thead>
<tr>
<th>ZnS thickness (µm)</th>
<th>Pitch (µm)</th>
<th>Number of neutrons detected per primary neutron</th>
<th>Number of neutrons detected per neutron primary (corrected with Q.E.)</th>
<th>Number of photons detected per primary neutron</th>
<th>Mean number of photons detected</th>
<th>Mass of $^6$Li (mg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>40</td>
<td>8.13E-5 ± 0.091</td>
<td>4.67E-5 ± 0.119</td>
<td>3.22E-3</td>
<td>14.08</td>
<td>806</td>
</tr>
<tr>
<td>1</td>
<td>50</td>
<td>2.88E-4 ± 0.048</td>
<td>1.13E-4 ± 0.067</td>
<td>7.81E-3</td>
<td>10.91</td>
<td>413</td>
</tr>
<tr>
<td>1</td>
<td>60</td>
<td>2.36E-4 ± 0.046</td>
<td>1.54E-4 ± 0.057</td>
<td>1.10E-2</td>
<td>15.48</td>
<td>240</td>
</tr>
<tr>
<td>2</td>
<td>60</td>
<td>2.14E-4 ± 0.056</td>
<td>1.35E-4 ± 0.070</td>
<td>8.24E-3</td>
<td>13.09</td>
<td>240</td>
</tr>
<tr>
<td>4</td>
<td>60</td>
<td>1.70E-4 ± 0.054</td>
<td>8.70E-5 ± 0.076</td>
<td>3.49E-3</td>
<td>10.38</td>
<td>240</td>
</tr>
<tr>
<td>8</td>
<td>60</td>
<td>9.00E-5 ± 0.105</td>
<td>4.60E-5 ± 0.147</td>
<td>5.37E-3</td>
<td>10.12</td>
<td>240</td>
</tr>
<tr>
<td>1</td>
<td>80</td>
<td>1.38E-4 ± 0.038</td>
<td>1.24E-4 ± 0.040</td>
<td>9.54E-3</td>
<td>27.50</td>
<td>120</td>
</tr>
<tr>
<td>2</td>
<td>80</td>
<td>1.36E-4 ± 0.043</td>
<td>1.12E-4 ± 0.047</td>
<td>7.84E-3</td>
<td>22.54</td>
<td>120</td>
</tr>
<tr>
<td>4</td>
<td>80</td>
<td>1.16E-4 ± 0.044</td>
<td>9.22E-5 ± 0.049</td>
<td>4.85E-3</td>
<td>20.10</td>
<td>120</td>
</tr>
<tr>
<td>8</td>
<td>80</td>
<td>9.97E-5 ± 0.058</td>
<td>7.17E-5 ± 0.068</td>
<td>3.43E-3</td>
<td>14.71</td>
<td>120</td>
</tr>
<tr>
<td>1</td>
<td>100</td>
<td>9.32E-5 ± 0.038</td>
<td>8.30E-5 ± 0.049</td>
<td>1.05E-2</td>
<td>31.49</td>
<td>52</td>
</tr>
<tr>
<td>2</td>
<td>100</td>
<td>8.04E-5 ± 0.050</td>
<td>7.06E-5 ± 0.053</td>
<td>7.37E-3</td>
<td>31.47</td>
<td>52</td>
</tr>
</tbody>
</table>

Table-4-6 -- Simulation results for different coated particle detectors with mean signal amplitude and absolute detection efficiency. Number of photons detected per primary neutron and the mass of $^6$Li in each detector are also shown. The detector thickness is 0.060cm.
<table>
<thead>
<tr>
<th>Detector</th>
<th>Neutron capture efficiency (captured/neutrons below 0.044eV)</th>
<th>Neutron detection efficiency (detected/captured)</th>
<th>Overall neutron detection efficiency (detected/neutron below 0.044eV)</th>
<th>Overall neutron detection efficiency (corrected with quantum efficiency)</th>
<th>LiF:ZnS mass ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_{19-1-40-600}$</td>
<td>2.05* ± 0.047</td>
<td>0.088 ± 0.094</td>
<td>0.180 ± 0.098</td>
<td>0.103 ± 0.126</td>
<td>1:0.26</td>
</tr>
<tr>
<td>$D_{19-1-50-600}$</td>
<td>1.49* ± 0.043</td>
<td>0.322 ± 0.055</td>
<td>0.480 ± 0.059</td>
<td>0.251 ± 0.074</td>
<td>1:0.26</td>
</tr>
<tr>
<td>$D_{19-1-60-600}$</td>
<td>0.985 ± 0.046</td>
<td>0.498 ± 0.056</td>
<td>0.491 ± 0.056</td>
<td>0.319 ± 0.066</td>
<td>1:0.26</td>
</tr>
<tr>
<td>$D_{19-2-60-600}$</td>
<td>0.985 ± 0.053</td>
<td>0.450 ± 0.067</td>
<td>0.443 ± 0.067</td>
<td>0.279 ± 0.080</td>
<td>1:0.54</td>
</tr>
<tr>
<td>$D_{19-4-60-600}$</td>
<td>1.02* ± 0.047</td>
<td>0.364 ± 0.063</td>
<td>0.371 ± 0.064</td>
<td>0.191 ± 0.083</td>
<td>1:1.20</td>
</tr>
<tr>
<td>$D_{19-8-60-600}$</td>
<td>1.01* ± 0.065</td>
<td>0.190 ± 0.115</td>
<td>0.192 ± 0.115</td>
<td>0.098 ± 0.154</td>
<td>1:2.90</td>
</tr>
<tr>
<td>$D_{19-1-80-600}$</td>
<td>0.469 ± 0.036</td>
<td>0.611 ± 0.048</td>
<td>0.287 ± 0.043</td>
<td>0.257 ± 0.045</td>
<td>1:0.26</td>
</tr>
<tr>
<td>$D_{19-2-80-600}$</td>
<td>0.487 ± 0.041</td>
<td>0.610 ± 0.054</td>
<td>0.297 ± 0.049</td>
<td>0.245 ± 0.053</td>
<td>1:0.54</td>
</tr>
<tr>
<td>$D_{19-4-80-600}$</td>
<td>0.494 ± 0.039</td>
<td>0.526 ± 0.054</td>
<td>0.260 ± 0.049</td>
<td>0.207 ± 0.054</td>
<td>1:1.20</td>
</tr>
<tr>
<td>$D_{19-8-80-600}$</td>
<td>0.506 ± 0.046</td>
<td>0.425 ± 0.069</td>
<td>0.215 ± 0.064</td>
<td>0.155 ± 0.073</td>
<td>1:2.90</td>
</tr>
<tr>
<td>$D_{19-1-100-600}$</td>
<td>0.295 ± 0.036</td>
<td>0.683 ± 0.049</td>
<td>0.202 ± 0.041</td>
<td>0.180 ± 0.053</td>
<td>1:0.26</td>
</tr>
<tr>
<td>$D_{19-2-100-600}$</td>
<td>0.285 ± 0.044</td>
<td>0.613 ± 0.063</td>
<td>0.175 ± 0.054</td>
<td>0.153 ± 0.057</td>
<td>1:0.54</td>
</tr>
</tbody>
</table>

Table 4-7 -- Detailed information of the simulations of different coated particle detectors with thickness of 0.060cm showing the thermal neutron detection efficiency. *Efficiencies more than 1 simply means that more neutrons above 0.044 eV are captured.
4.2.2.3 0.1cm Thick Detector

The results for 0.1cm detector are shown in Table-4.8 and Table-4.9. The highest absolute detection efficiency is found with D_{19.1-80-1000} whereas the highest signal amplitude is found with D_{19.1-100-1000} as expected again since more light can be collected when the medium is transparent.

<table>
<thead>
<tr>
<th>ZnS thickness (μm)</th>
<th>Pitch (μm)</th>
<th>Number of neutrons detected per primary neutron</th>
<th>Number of neutrons detected per primary neutron (corrected with Q.E.)</th>
<th>Number of photons detected per primary neutron</th>
<th>Mean number of photons detected</th>
<th>Mass of 6Li (mg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>40</td>
<td>4.00E-5 ± 0.158</td>
<td>2.80E-5 ± 0.189</td>
<td>1.09E-3</td>
<td>12.56</td>
<td>1344</td>
</tr>
<tr>
<td>1</td>
<td>50</td>
<td>1.63E-4 ± 0.064</td>
<td>7.13E-5 ± 0.097</td>
<td>5.68E-3</td>
<td>8.84</td>
<td>688</td>
</tr>
<tr>
<td>1</td>
<td>60</td>
<td>2.21E-4 ± 0.055</td>
<td>1.07E-4 ± 0.079</td>
<td>6.15E-3</td>
<td>10.65</td>
<td>384</td>
</tr>
<tr>
<td>2</td>
<td>60</td>
<td>2.00E-4 ± 0.071</td>
<td>1.01E-4 ± 0.099</td>
<td>6.64E-3</td>
<td>8.89</td>
<td>384</td>
</tr>
<tr>
<td>4</td>
<td>60</td>
<td>1.42E-4 ± 0.069</td>
<td>6.13E-5 ± 0.104</td>
<td>2.82E-3</td>
<td>8.45</td>
<td>384</td>
</tr>
<tr>
<td>8</td>
<td>60</td>
<td>7.60E-5 ± 0.115</td>
<td>3.40E-5 ± 0.171</td>
<td>1.64E-3</td>
<td>7.61</td>
<td>384</td>
</tr>
<tr>
<td>1</td>
<td>80</td>
<td>2.05E-4 ± 0.040</td>
<td>1.58E-4 ± 0.046</td>
<td>1.09E-2</td>
<td>18.15</td>
<td>206</td>
</tr>
<tr>
<td>2</td>
<td>80</td>
<td>1.64E-4 ± 0.055</td>
<td>1.17E-4 ± 0.065</td>
<td>5.31E-3</td>
<td>17.37</td>
<td>206</td>
</tr>
<tr>
<td>4</td>
<td>80</td>
<td>1.62E-4 ± 0.045</td>
<td>1.08E-4 ± 0.056</td>
<td>4.27E-3</td>
<td>14.68</td>
<td>206</td>
</tr>
<tr>
<td>8</td>
<td>80</td>
<td>1.01E-4 ± 0.070</td>
<td>5.15E-5 ± 0.099</td>
<td>2.06E-3</td>
<td>12.57</td>
<td>206</td>
</tr>
<tr>
<td>1</td>
<td>100</td>
<td>1.34E-4 ± 0.050</td>
<td>1.20E-4 ± 0.053</td>
<td>1.14E-2</td>
<td>26.68</td>
<td>86</td>
</tr>
<tr>
<td>2</td>
<td>100</td>
<td>1.35E-4 ± 0.054</td>
<td>1.11E-4 ± 0.060</td>
<td>8.60E-3</td>
<td>24.51</td>
<td>86</td>
</tr>
</tbody>
</table>

Table 4.8 -- Simulation results for different coated particle detectors with mean signal amplitude and absolute detection efficiency. Number of photons detected per primary neutron and the mass of 6Li in each detector are also shown. The detector thickness is 0.1cm.
## Table 4.9

<table>
<thead>
<tr>
<th>Detector</th>
<th>Neutron capture efficiency (captured/neutrons below 0.044eV)</th>
<th>Neutron detection efficiency (detected/captured)</th>
<th>Overall neutron detection efficiency (detected/neutron below 0.044eV)</th>
<th>Overall neutron detection efficiency (corrected with quantum efficiency)</th>
<th>LiF:ZnS mass ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>D19-1-40-1000</td>
<td>2.52 ± 0.056</td>
<td>0.036 ± 0.161</td>
<td>0.090 ± 0.165</td>
<td>0.063 ± 0.195</td>
<td>1:0.26</td>
</tr>
<tr>
<td>D19-1-50-1000</td>
<td>1.99 ± 0.047</td>
<td>0.182 ± 0.069</td>
<td>0.363 ± 0.075</td>
<td>0.159 ± 0.104</td>
<td>1:0.26</td>
</tr>
<tr>
<td>D19-1-60-1000</td>
<td>1.41 ± 0.050</td>
<td>0.344 ± 0.064</td>
<td>0.485 ± 0.067</td>
<td>0.235 ± 0.088</td>
<td>1:0.26</td>
</tr>
<tr>
<td>D19-2-60-1000</td>
<td>1.39 ± 0.061</td>
<td>0.313 ± 0.081</td>
<td>0.436 ± 0.085</td>
<td>0.220 ± 0.110</td>
<td>1:0.54</td>
</tr>
<tr>
<td>D19-4-60-1000</td>
<td>1.34 ± 0.051</td>
<td>0.232 ± 0.076</td>
<td>0.312 ± 0.079</td>
<td>0.135 ± 0.111</td>
<td>1:1.20</td>
</tr>
<tr>
<td>D19-8-60-1000</td>
<td>1.46 ± 0.060</td>
<td>0.110 ± 0.121</td>
<td>0.161 ± 0.124</td>
<td>0.072 ± 0.178</td>
<td>1:2.90</td>
</tr>
<tr>
<td>D19-1-80-1000</td>
<td>1.31 ± 0.035</td>
<td>0.330 ± 0.047</td>
<td>0.434 ± 0.048</td>
<td>0.333 ± 0.053</td>
<td>1:0.26</td>
</tr>
<tr>
<td>D19-2-80-1000</td>
<td>0.703 ± 0.051</td>
<td>0.501 ± 0.068</td>
<td>0.352 ± 0.064</td>
<td>0.252 ± 0.073</td>
<td>1:0.54</td>
</tr>
<tr>
<td>D19-4-80-1000</td>
<td>0.779 ± 0.041</td>
<td>0.462 ± 0.055</td>
<td>0.360 ± 0.053</td>
<td>0.240 ± 0.062</td>
<td>1:1.20</td>
</tr>
<tr>
<td>D19-8-80-1000</td>
<td>0.739 ± 0.052</td>
<td>0.308 ± 0.081</td>
<td>0.228 ± 0.078</td>
<td>0.116 ± 0.104</td>
<td>1:2.90</td>
</tr>
<tr>
<td>D19-1-100-1000</td>
<td>0.437 ± 0.048</td>
<td>0.652 ± 0.064</td>
<td>0.285 ± 0.057</td>
<td>0.256 ± 0.059</td>
<td>1:0.26</td>
</tr>
<tr>
<td>D19-2-100-1000</td>
<td>0.464 ± 0.052</td>
<td>0.621 ± 0.069</td>
<td>0.288 ± 0.062</td>
<td>0.237 ± 0.067</td>
<td>1:0.54</td>
</tr>
</tbody>
</table>

*Efficiencies more than 1 simply means that more neutrons above 0.044 eV are captured.*
In Figure-4.14, the three detector thicknesses are compared keeping the ZnS thickness and the pitch constant.

According to Figure-4.16, the back layers contribute more to the photon detection relative to the front layers when the detector thickness decreases as expected. However, number of photons detected per primary neutron peaks at the intermediate thickness of 0.6mm. Figures relative to D_{19-4-80-1000} are shared in Appendix E.
In Figure-4.17, the PMT response is shown for three different thicknesses with same ZnS thickness and pitch.

![Graphs showing PMT response for different thicknesses](image)

*Figure-4.17 PMT response for a) D_{19.4-80-320}, b) D_{19.4-80-600} and c) D_{19.4-80-1000}*

It is clearly seen that when the thickness is increased, number of photons detected per neutron detection (signal amplitude) decreases drastically.
In Figure 4.18, thicknesses and pitches are compared keeping the ZnS thickness constant as 1μm.

There are three distinct regions identified. When the pitch is 40μm, the highest neutron detection efficiency is obtained with 0.032cm detector. As the pitch is increased, the thicker detectors become more feasible with 0.1cm detector eventually having the highest efficiency and the overall highest efficiency was obtained with 80μm pitch, 0.1cm detector. The reason for the different behavior is that the pitch can’t be so large for the thin detectors since the neutron capture probability decreases sharply; however when the thickness is increased, larger pitch can be utilized since there are more layers to put the micro-particles into.
In Figure-4.19, different detector thicknesses are compared with varying ZnS thicknesses keeping the pitch constant as 80µm.

As seen in Figure-4.19, the detection efficiency is highest when the detector thickness is 0.6mm for 8µm ZnS thickness and 80 microns pitch. For 1µm and 4µm cases, 0.1cm detector gives the highest efficiency. The reason for different behavior between the ZnS thicknesses is that thicker detectors combined with thicker ZnS deteriorate the light transport properties to the point that after some thickness, neutron capture efficiency is overwhelmed by the light absorption in the medium.
The apparent non-stop increase for the 1μm ZnS prompt to test even thicker detectors. In Table-4.10 and Figure-4.20, it is seen that the detection efficiency reaches a peak at 1.25mm detector.

<table>
<thead>
<tr>
<th>Detector</th>
<th>Number of neutrons detected per primary neutron</th>
<th>Number of neutrons detected per primary neutron (corrected with Q.E.)</th>
<th>Number of photons detected per primary neutron</th>
<th>Mean number of photons detected</th>
<th>Mass of $^6$Li (mg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_{19-1-80-1250}$</td>
<td>$2.37E-4 \pm 0.041$</td>
<td>$1.60E-4 \pm 0.050$</td>
<td>$9.93E-3$</td>
<td>16.33</td>
<td>275</td>
</tr>
<tr>
<td>$D_{19-1-80-1500}$</td>
<td>$2.46E-4 \pm 0.045$</td>
<td>$1.52E-4 \pm 0.057$</td>
<td>$7.54E-3$</td>
<td>13.57</td>
<td>326</td>
</tr>
<tr>
<td>$D_{19-1-80-2000}$</td>
<td>$2.61E-4 \pm 0.044$</td>
<td>$1.48E-4 \pm 0.058$</td>
<td>$8.78E-3$</td>
<td>12.16</td>
<td>429</td>
</tr>
</tbody>
</table>

Table-4.10 Simulation results for increased thickness for $D_{19-1-80-x}$

![Absolute Detection Efficiency vs Detector Thickness for 1μm ZnS and 80μm pitch](image)

Figure-4.20 Absolute neutron detection efficiency as a function of detector thickness for t=1 micron and p=80 microns
In Figure-4.21, different detector thicknesses are compared with varying ZnS thicknesses keeping the pitch constant as 60μm.

For 60μm pitch, the trend is different which tells that there is no single “best” optimization pattern that all of the parameters and configurations would follow. 0.06 cm thick detector gives the best absolute detection efficiency when the ZnS thickness is 1μm. This is expected because when the ZnS thickness is 4μm or 8μm and the pitch is 60μm, the light transport properties suffer significantly.

Since radius of LiF is 19μm, most of the charged particle energy is lost before leaving the neutron converter volume. Keeping the same LiF mass in the detector sheet, different radii were tested and the results are presented in Table-4.11.
<table>
<thead>
<tr>
<th>LiF diameter (µm)</th>
<th>Pitch (µm)</th>
<th>Number of neutrons detected per primary neutron</th>
<th>Mean number of photons detected</th>
<th>Light production (relative to D$_{19.1-60-600}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.5</td>
<td>15</td>
<td>5.90E-5 ± 0.130</td>
<td>9.3</td>
<td>4.00</td>
</tr>
<tr>
<td>19</td>
<td>30</td>
<td>9.25E-5 ± 0.074</td>
<td>10.3</td>
<td>2.00</td>
</tr>
<tr>
<td>38</td>
<td>60</td>
<td>1.54E-4 ± 0.057</td>
<td>15.5</td>
<td>1.00</td>
</tr>
<tr>
<td>76</td>
<td>120</td>
<td>1.43E-4 ± 0.059</td>
<td>21.1</td>
<td>0.50</td>
</tr>
<tr>
<td>380</td>
<td>600</td>
<td>3.40E-5 ± 0.121</td>
<td>31.6</td>
<td>0.10</td>
</tr>
</tbody>
</table>

*Table 4-11 Comparison of different LiF radii keeping the mass constant*

By reducing the diameter, much more micro-particles can be placed in the same geometry. Although the neutron capture probability doesn’t change due to the same concentration of LiF in the geometries, the light production increases up to 4-fold since the charged particles can deposit more of their energy in the scintillator. However, placing more of them also reduces the transparency of the detector sheet, which is evident from the mean number of photons detected.

By increasing the diameter, light production highly suffers however, when a successful detection takes place, the signal amplitude is much higher due to the increased transparency of the sheet. Overall, deviating from the optimal size, which was found with one unit cell approximation, doesn’t increase the total neutron detection efficiency.

### 4.2.3 Final Comparison of the Detectors

Final comparison of the detectors was made to determine the best detector geometry using various parameters, including the mass of $^6$Li in the detectors.

#### 4.2.3.1 Detection Efficiency

The detection efficiencies of different detectors are compared including the commercially available EJ-426 detectors. Two approaches are utilized to compare the efficiencies with one being the absolute detection efficiency (number of neutrons detected per primary neutron) and thermal neutron detection efficiency (number of neutrons detected per neutron moderated below 0.044eV). The reason for this distinction is to take into account the uncertainties in the moderation within the same geometry.
Taking a look at both approaches, $D_{19-1.50-320}$ and $D_{19-1.80-1000}$ have the highest absolute and thermal detection efficiency compared to the other detectors with the same thickness. For the 0.06 cm detector case, the detector with the highest absolute efficiency is different than that of highest thermal neutron detection efficiency possibly due to poor statistics.

EJ-426 detectors perform better compared to only few cases where there are deviations from optimal ZnS thickness and pitch such as $D_{19-4.80-320}$ and $D_{19-1.40-600}$. However, when the optimal parameters are used, the detection efficiency is much better than that of EJ-426 detectors. In Figure 4.22 and Figure 4.23, the absolute detection efficiency and thermal neutron detection efficiency are shown.

*Figure 4.22 Comparison of the absolute neutron detection efficiency of the detectors*
4.2.3.2 Performance Parameter

Other important parameters besides the neutron detection efficiency are the signal amplitude and the mass of $^6$Li in the detectors. Performance parameters are defined in order to evaluate the detector performance in a healthier manner. They take into account the neutron detection efficiency, signal amplitude and mass of $^6$Li to determine the optimal detector with the best cost-effective option.

First performance parameter can be defined as the product of absolute neutron detection efficiency and the mean number of photons hitting the PMT surface per neutron detection event.

$$\text{Performance parameter} = P.P.1 = \text{abs}(\eta) * \mu * 10^3$$  \[\text{Eq.\:4.7}\]

where $\eta$ and $\mu$ are detection efficiency and mean number of photons per detection.
Figure 4.24 shows that the non-aligned geometries perform better when the other parameters are fixed. Apart from that, $D_{19-1-60-320}$, $D_{19-1-80-600}$ and $D_{19-1-100-1000}$ have very high performance compared to the other detectors with the same thickness. What is noted is that the detector thickness and pitch are related and there is no single pitch value that is optimal for every thickness since light transport efficiency is getting higher when pitch increases however it decreases when the thickness increases. Therefore, as the thickness increases, pitch also needs to increase for a better performance.

Second performance parameter can be defined as the product of thermal neutron detection efficiency and the mean number of photons hitting the PMT surface per neutron detection event.

$$Performance\ parameter = P.P.\ 2 = \eta \times \mu$$  \[Eq. 4.8\]
Almost the same behavior is observed as the first performance parameter beside the fact that D\textsubscript{19:1-100-600} performs better compared to P.P.1.

Third performance parameter can be defined as the product of thermal neutron detection efficiency and the mean number of photons hitting the PMT surface per neutron detection event divided by the mass of \textsuperscript{6}Li in the detector.

\[
\text{Performance parameter} = P.P.\ 3 = \frac{\eta \cdot \mu}{M_{\text{Li}}} \cdot 10^2 \quad [\text{Eq. 4.9}]
\]
Detectors with larger pitches are favored in terms of P.P.3 since the detection efficiency doesn’t increase at the same rate of increase of mass of $^6\text{Li}$ in the detectors. P.P.3 can be used to evaluate to cost-effectiveness of the detectors.

In Table-4.12, the detection efficiencies and performance parameters are presented. In Table-4.13, detection efficiencies and performance parameters relative to EJ-426-HD-0032 are presented.
<table>
<thead>
<tr>
<th>Geometry</th>
<th>Absolute neutron detection efficiency</th>
<th>Thermal neutron detection efficiency</th>
<th>Performance Parameter 1</th>
<th>Performance Parameter 2</th>
<th>Performance Parameter 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>EJ-426-0-0032</td>
<td>6.40E-5</td>
<td>0.142</td>
<td>1.09</td>
<td>2.42</td>
<td>1.73</td>
</tr>
<tr>
<td>EJ-426-HD-0032</td>
<td>9.10E-5</td>
<td>0.204</td>
<td>1.40</td>
<td>3.15</td>
<td>1.42</td>
</tr>
<tr>
<td>D19-1-40-320</td>
<td>8.23E-5</td>
<td>0.171</td>
<td>1.09</td>
<td>2.26</td>
<td>0.52</td>
</tr>
<tr>
<td>D19-1-50-320</td>
<td>1.50E-4</td>
<td>0.327</td>
<td>2.53</td>
<td>5.52</td>
<td>2.68</td>
</tr>
<tr>
<td>D19-1-60-320</td>
<td>1.38E-4</td>
<td>0.294</td>
<td>3.63</td>
<td>7.73</td>
<td>6.47</td>
</tr>
<tr>
<td>D19-4-80-320</td>
<td>1.01E-4</td>
<td>0.221</td>
<td>1.73</td>
<td>3.79</td>
<td>3.17</td>
</tr>
<tr>
<td>D19-8-60-320</td>
<td>5.70E-5</td>
<td>0.121</td>
<td>0.60</td>
<td>1.26</td>
<td>1.06</td>
</tr>
<tr>
<td>D19-1-80-320</td>
<td>7.63E-5</td>
<td>0.167</td>
<td>2.60</td>
<td>5.68</td>
<td>10.6</td>
</tr>
<tr>
<td>D19-4-80-320</td>
<td>6.28E-5</td>
<td>0.134</td>
<td>1.83</td>
<td>3.90</td>
<td>7.24</td>
</tr>
<tr>
<td>D19-8-80-320</td>
<td>4.88E-5</td>
<td>0.104</td>
<td>1.12</td>
<td>2.40</td>
<td>4.45</td>
</tr>
<tr>
<td>D19-1-100-320</td>
<td>3.81E-5</td>
<td>0.085</td>
<td>1.41</td>
<td>3.14</td>
<td>12.1</td>
</tr>
<tr>
<td>EJ-426-0-0060</td>
<td>5.30E-5</td>
<td>0.118</td>
<td>0.84</td>
<td>1.88</td>
<td>0.71</td>
</tr>
<tr>
<td>EJ-426-HD-0060</td>
<td>6.30E-5</td>
<td>0.134</td>
<td>1.07</td>
<td>2.27</td>
<td>0.55</td>
</tr>
<tr>
<td>D19-1-40-600</td>
<td>4.67E-5</td>
<td>0.103</td>
<td>0.66</td>
<td>1.45</td>
<td>0.18</td>
</tr>
<tr>
<td>D19-1-50-600</td>
<td>1.13E-4</td>
<td>0.251</td>
<td>1.23</td>
<td>2.74</td>
<td>0.66</td>
</tr>
<tr>
<td>D19-1-60-600</td>
<td>1.54E-4</td>
<td>0.319</td>
<td>2.38</td>
<td>4.94</td>
<td>2.06</td>
</tr>
<tr>
<td>D19-4-60-600</td>
<td>8.70E-5</td>
<td>0.191</td>
<td>0.90</td>
<td>1.98</td>
<td>0.83</td>
</tr>
<tr>
<td>D19-8-60-600</td>
<td>4.60E-5</td>
<td>0.098</td>
<td>0.47</td>
<td>0.99</td>
<td>0.41</td>
</tr>
<tr>
<td>D19-1-80-600</td>
<td>1.24E-4</td>
<td>0.257</td>
<td>3.41</td>
<td>7.07</td>
<td>5.89</td>
</tr>
<tr>
<td>D19-4-80-600</td>
<td>9.22E-5</td>
<td>0.207</td>
<td>1.85</td>
<td>4.16</td>
<td>3.47</td>
</tr>
<tr>
<td>D19-8-80-600</td>
<td>7.17E-5</td>
<td>0.155</td>
<td>1.05</td>
<td>2.28</td>
<td>1.90</td>
</tr>
<tr>
<td>D19-1-100-600</td>
<td>8.30E-5</td>
<td>0.180</td>
<td>2.61</td>
<td>5.67</td>
<td>10.9</td>
</tr>
<tr>
<td>D19-1-40-1000</td>
<td>2.80E-5</td>
<td>0.063</td>
<td>0.35</td>
<td>0.79</td>
<td>0.06</td>
</tr>
<tr>
<td>D19-1-50-1000</td>
<td>7.13E-5</td>
<td>0.159</td>
<td>0.63</td>
<td>1.41</td>
<td>0.20</td>
</tr>
<tr>
<td>D19-1-60-1000</td>
<td>1.07E-4</td>
<td>0.235</td>
<td>1.14</td>
<td>2.50</td>
<td>0.65</td>
</tr>
<tr>
<td>D19-4-60-1000</td>
<td>6.13E-5</td>
<td>0.135</td>
<td>0.52</td>
<td>1.14</td>
<td>0.30</td>
</tr>
<tr>
<td>D19-8-60-1000</td>
<td>3.40E-5</td>
<td>0.072</td>
<td>0.26</td>
<td>0.55</td>
<td>0.14</td>
</tr>
<tr>
<td>D19-1-80-1000</td>
<td>1.58E-4</td>
<td>0.333</td>
<td>2.87</td>
<td>6.04</td>
<td>2.93</td>
</tr>
<tr>
<td>D19-4-80-1000</td>
<td>1.08E-4</td>
<td>0.240</td>
<td>1.59</td>
<td>3.52</td>
<td>1.71</td>
</tr>
<tr>
<td>D19-8-80-1000</td>
<td>5.15E-5</td>
<td>0.116</td>
<td>0.65</td>
<td>1.46</td>
<td>0.71</td>
</tr>
<tr>
<td>D19-1-100-1000</td>
<td>1.20E-4</td>
<td>0.256</td>
<td>3.20</td>
<td>6.83</td>
<td>7.94</td>
</tr>
</tbody>
</table>

Table 4-12 – Absolute neutron detection efficiency, Thermal neutron detection efficiency, First Performance Parameter, Second Performance Parameter and Third Performance Parameters of the detectors
Simulations have shown that coated micro-particles can significantly increase both the neutron detection and light collection efficiency. With these results, the detectors with the highest efficiencies were found to be $D_{19\cdot1\cdot60\cdot600}$ and $D_{19\cdot1\cdot80\cdot1000}$ performing 1.69 and 1.73 times better than the best performing...
existing technology, respectively. \( D_{19-1-60-320}, D_{19-1-80-600} \) and \( D_{19-1-100-1000} \) give the highest performance parameters. Their performance parameters are more than 2 times better than the performance parameter of EJ-426-HD-0032.

### 4.2.4 Randomization of the Geometry

In all of the cases, the coated particles are assumed to be the same without any deviation from prescribed radius, thickness or pitch. The positions of the coated particles are also assumed to be regular. In the actual manufacturing process, the perfect geometry is highly unlikely; therefore position, radius, and thickness randomization was done. Of course, since there are thousands of particles in a detector, complete randomization is nearly impossible. Instead, a randomization was performed with a finite group of particles and those cells were replicated. Randomized cells are shown in Figure-4.27 with the highly regular geometry.

#### 4.2.4.1 Randomization of the Position, LiF Radius and ZnS Thickness

**Figure 4-27**

a) Symmetrical geometry with fixed LiF and ZnS thicknesses  
b) 2x2x5 Randomized geometry with randomized LiF and ZnS size  
c) 4x2x5 Randomized geometry with randomized LiF and ZnS size  
d) 4x4x5 Randomized geometry with randomized LiF and ZnS size
Randomization range of LiF radius is from 18μm to 20μm and randomization range of ZnS thickness is from 0.2μm to 4μm. The results of symmetrical, 2x2x5, 4x2x5, 4x4x5, 5x10x10 and 10x10x10 randomized geometries are shown in Table-4.14

<table>
<thead>
<tr>
<th>Detector</th>
<th>Number of neutrons detected per neutron (corrected with Q.E.)</th>
<th>Number of photons detected per neutron</th>
<th>Mean number of photons detected</th>
<th>Absolute neutron detection efficiency (Relative to EJ-426-HD-0032)</th>
<th>Relative Performance Parameter 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Symmetrical</td>
<td>1.54E-4 ± 0.057</td>
<td>1.1E-2</td>
<td>15.48</td>
<td>1.69</td>
<td>1.70</td>
</tr>
<tr>
<td>2x2x5 Randomized with LiF and ZnS fixed</td>
<td>1.43E-4 ± 0.042</td>
<td>8.3E-3</td>
<td>14.85</td>
<td>1.57</td>
<td>1.51</td>
</tr>
<tr>
<td>2x2x5 Randomized</td>
<td>1.11E-4 ± 0.042</td>
<td>7.3E-3</td>
<td>13.19</td>
<td>1.21</td>
<td>1.04</td>
</tr>
<tr>
<td>4x2x5 Randomized with LiF and ZnS fixed</td>
<td>1.50E-4 ± 0.047</td>
<td>8.4E-3</td>
<td>14.65</td>
<td>1.64</td>
<td>1.56</td>
</tr>
<tr>
<td>4x2x5 Randomized</td>
<td>1.18E-4 ± 0.053</td>
<td>7.3E-3</td>
<td>12.12</td>
<td>1.29</td>
<td>1.02</td>
</tr>
<tr>
<td>4x4x5 Randomized with LiF and ZnS fixed</td>
<td>1.48E-5 ± 0.041</td>
<td>9.9E-3</td>
<td>14.14</td>
<td>1.62</td>
<td>1.49</td>
</tr>
<tr>
<td>4x4x5 Randomized</td>
<td>1.15E-4 ± 0.047</td>
<td>6.1E-3</td>
<td>12.23</td>
<td>1.26</td>
<td>1.00</td>
</tr>
<tr>
<td>5x10x10 Randomized with LiF and ZnS fixed</td>
<td>1.47E-4 ± 0.048</td>
<td>9.3E-3</td>
<td>14.33</td>
<td>1.62</td>
<td>1.50</td>
</tr>
<tr>
<td>10x10x10 Randomized with LiF and ZnS fixed</td>
<td>1.52E-4 ± 0.041</td>
<td>1.1E-2</td>
<td>15.93</td>
<td>1.67</td>
<td>1.73</td>
</tr>
<tr>
<td>10x10x10 Randomized</td>
<td>1.25E-4 ± 0.045</td>
<td>6.5E-3</td>
<td>13.14</td>
<td>1.37</td>
<td>1.17</td>
</tr>
</tbody>
</table>

Table-4.14 Results for randomized geometries with LiF and ZnS fixed and with LiF and ZnS size also randomized

When only the position of the particles is randomized, the absolute neutron detection efficiency doesn’t degrade much although there is a clear decrease in it. The reason is that there may be clustering of particles stopping light from propagating. When LiF radius and ZnS thickness are also randomized in addition to the position randomization, the detection efficiency and performance parameter are worsened significantly as expected since, now, in addition to the clustering issues, there are particles with highly
unfavorable dimensions. Still, when the number of particles that are randomized increases, there is no noticeable effect on detection efficiency and signal amplitude.

For 10x10x10 randomization, simulations were done with runs having different seed; therefore having different pseudorandom numbers to see the effect of the randomization on the simulations with varying positions of particles. The mean value of the simulation is found to be 1.52E-4.

4.2.4.2 Randomization of Shape and Orientation

In addition to the randomization of position, radius and thickness, shapes of the unit cells are also randomized as well as their orientation to approximate the manufacturing. The general ellipsoid equation can be given as

\[ 1 = \frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} \]  

[Eq. 4.10]

where a, b and c are the semiaxes.

The sphere is the general case of the ellipsoid when all the semiaxes are equal. The deviation from perfect sphericity can be randomized choosing a, b and c within a prescribed range. Three cases were tried with different ranges; therefore different degree of deviation from the sphericity. Since an ellipsoid is not symmetric along its three semiaxes, transformation matrix was applied in GEANT4 to randomly orient them. In Figure-4.28, the deviation from perfectly aligned symmetrical and spherical case to randomly oriented irregular and ellipsoid case is shown.

Figure-4-28 Randomization of the shape and orientation of the unit cells
In Table 4.15, three different deviation are shown with the range of semiaxis randomization. In all cases, 1000 particles are randomized.

<table>
<thead>
<tr>
<th>Semiaxis range</th>
<th>Number of neutrons detected per neutron (corrected with Q.E.)</th>
<th>Number of photons detected per neutron</th>
<th>Mean number of photons detected</th>
<th>Absolute neutron detection efficiency (Relative to EJ-426-HD-0032)</th>
<th>Relative Performance Parameter 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>LiF(17.8μm-21.8μm) ZnS(0.2μm-2.2μm)</td>
<td>1.42E-4 ± 0.059</td>
<td>9.04E-3</td>
<td>14.38</td>
<td>1.56</td>
<td>1.46</td>
</tr>
<tr>
<td>LiF(13.6μm-21.6μm) ZnS(0.4μm-4.4μm)</td>
<td>1.19E-4 ± 0.065</td>
<td>6.56E-3</td>
<td>15.23</td>
<td>1.31</td>
<td>1.29</td>
</tr>
<tr>
<td>LiF(5.2μm-21.2μm) ZnS(0.8μm-8.8μm)</td>
<td>0.73E-4 ± 0.117</td>
<td>3.21E-3</td>
<td>19.83</td>
<td>0.80</td>
<td>1.03</td>
</tr>
</tbody>
</table>

*Table 4-15 Results for shape and orientation randomization*

When the shape and the orientation of the unit cells are randomized, the detection efficiency goes down because of the deviation of the perfect geometry. However, except for extreme cases, the coated particle geometry performs significantly better than the existing technology.

### 4.2.4.2 Randomization of the Imperfections of the Coating

It is also possible to have partially coated micro-particles in the manufacturing process, which would result in escape of some of the charged particles from the medium without any energy deposition. Randomization of this sort of manufacturing fault has been performed and shown in Figure 4.29.

![Figure 4-29 Randomization of coating faults. a) Perfect coating, b) 90<theta<180, 180<phi<360, c) 0<theta<180, 0<phi<360](image-url)
In the case b, the randomization was performed with the zenith angle and azimuthal angle ranging between 90 to 180 and 180 to 360, respectively. In the case c, they are between 0 to 180 and 0 to 360, respectively. The results for the partial coating are presented in Table-4.16.

<table>
<thead>
<tr>
<th>Coating</th>
<th>Number of neutrons detected per neutron (corrected with Q.E.)</th>
<th>Number of photons detected per neutron</th>
<th>Mean number of photons detected</th>
<th>Absolute neutron detection efficiency (Relative to EJ-426-HD-0032)</th>
<th>Relative Performance Parameter 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Perfect Coating</td>
<td>1.54E-4 ± 0.057</td>
<td>1.1E-2</td>
<td>15.48</td>
<td>1.69</td>
<td>1.70</td>
</tr>
<tr>
<td>Coating shell randomized with 90&lt;θ&lt;180 and 180&lt;ϕ&lt;360</td>
<td>1.50E-4 ± 0.047</td>
<td>1.1E-2</td>
<td>21.04</td>
<td>1.64</td>
<td>2.25</td>
</tr>
<tr>
<td>Coating shell randomized with 0&lt;θ&lt;180 and 0&lt;ϕ&lt;360</td>
<td>9.90E-5 ± 0.058</td>
<td>9.9E-3</td>
<td>34.97</td>
<td>1.09</td>
<td>2.47</td>
</tr>
</tbody>
</table>

Table 4-16 Results for partial coating with randomized position

Even when the partial coating is applied, both neutron detection efficiency and the performance parameter are higher than the best performing commercially available detector. Partial coating decreases the light production however it allows the produced light to reach the PMT more easily since ZnS concentration is reduced on the way of the light.

### 4.2.5 Further Possible Improvements for Light Collection

There are several options to increase the light collection efficiency, which involves wavelength shifting (WLS) fibers and highly reflective mirrors. Several authors investigated the use of wavelength shifting fibers as a means of collecting light out of the scintillator.[27] WLS fibers absorb a photon at one wavelength and emit them at another; thereby shifting the spectrum. WLS fibers are used to collect light more efficiently and uniformly. Also, they are used to match the light spectrum with the photosensor’s spectral response characteristic to increase the quantum efficiency. WLS fibers take advantage of the total internal reflection of light which occurs when the refractive index of the first medium is greater than that of the second medium. Therefore, cladding material needs to be carefully selected.
However, using WLS fibers brings another step of optimization process, which needs to be done in order to find the number of WLS fibers and number of layers to put them into while keeping the neutron capture efficiency and light production as high as possible.

Mirrors can also be used to increase the probability of collecting light from the back layers. When the light is isotopically produced, some of them have no chance of hitting the photosensor if they are released in the opposite direction. Highly reflective aluminum layers can be used to reflect them. Preliminary GEANT4 simulation was done to see the effect of 95% reflective aluminum mirror with polished surface. In GEANT4, optical surfaces can be defined and accurately represented with many options of surface characteristics. For D_{19.1-60.600}, the reflective mirror increases the efficiency of neutron detection 13% compared to completely unreflected case.
Chapter 5 Monte Carlo Code Development for Coated Micro-Particles

Effort has been made to develop a Monte Carlo code involving only coated particles with LiF, ZnS and binder and repeated placement of this geometry. The incentive for having an additional code is to be able to compare the light related properties with GEANT4. In this chapter, a brief introduction to the theory of Monte Carlo methods is given and the steps as well as the algorithms are explained.

5.1 A Brief Introduction to Sampling Process

Monte Carlo methods take advantage of the random nature of the radiation interaction processes. Random numbers are generated to determine the various parameters of the particles during its life such as the distance it travels, what kind of interaction it undergoes and etc. So the essential part of a Monte Carlo code is to sample a random number. Since the softwares use algorithms to generate the random numbers, they are not truly random but pseudorandom numbers.

Position of source neutrons

Position of source neutrons can be sampled in case of a distributed source as

\[ x_0 = a_x \, \xi + b_x \quad [Eq. 5.1(a)] \]

\[ y_0 = a_y \, \xi + b_y \quad [Eq. 5.1(b)] \]

\[ z_0 = a_z \, \xi + b_z \quad [Eq. 5.1(c)] \]

where \( \xi \) is a random number between 0 and 1 and coefficients of \( a \) and \( b \) are the limits to restrict the position into a pre-defined space.
**Direction of source neutrons**

Next step is to determine the neutron direction with random numbers. Assuming isotropic emission and scattering, azimuthal angle can be sampled as

\[
\int_0^\phi \frac{d\phi'}{2\pi} = \xi, \quad \phi = 2\pi \xi
\]

[Eq. 5.2]

Zenith angle can be sampled as

\[
\int_{-1/2}^{1/2} d\mu' = \xi, \quad \mu = 2\xi - 1
\]

[Eq. 5.3]

**Energy of the source neutrons**

Energy can be assigned to source neutrons if the probability density function is known. Random number is generated and the corresponding energy is recovered from the cumulative probability distribution as

\[
\int_0^E PDF(E')dE' = \xi
\]

[Eq. 5.4]

It is not always required to directly solve the integral and sample afterwards. Sampling can also be done if the CDF is known at discrete energy steps. Random numbers can then be used to find the corresponding energy values.

**Checking the boundaries**

Depending on the geometry of the materials, the volume in which the particles propagate can be expressed in terms of surface equations. For example, when considering a spherical volume, the particles are inside of the sphere only if

\[
(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2 < R_s^2
\]

[Eq. 5.5]

where \(R_s\) is the radius of the sphere and \(x_0, y_0\) and \(z_0\) are the locations of the origin of the sphere. When, the particle escapes the inner sphere, it would then start propagating in the outer sphere. When it is in the
cubical geometry, the simple plane equations defining six different planes of the cube are sufficient to check if the particle is inside the volume. A somewhat tricky part arises when the particle is in the outer volumes. Since, after propagation, the particle may end up being in the same volume while having passed through the inner volumes. In this case, surface conditions must be checked along the particle trajectory and if it hits a surface, above procedure must be repeated.

5.2 Neutron Simulation

Neutrons interact at discrete steps and the distance between interactions can be sampled using the PDF

\[
PDF = \Sigma_t \ast \exp(-\Sigma_t \ast x) \rightarrow Collision \ probability \quad [Eq.5.6]
\]

\[
\int_0^x \Sigma_t \ast \exp(-\Sigma_t \ast x') = \xi \quad [Eq.5.7]
\]

\[
x = -\frac{1}{\Sigma_t} \ast \ln(\xi) \quad [Eq.5.8]
\]

Neutron is stopped at the distance \(x\) and whether it is in the same volume is checked. If it escapes the volume, the above process is repeated taking into account the distance traveled in the previous volume. In the repeated structure case, if the neutron escapes the unit cell, it is then propagated as if it is at the opposite side of the unit cell updating the real position values while keeping the position for unit cell within the boundary of that unit cell. If the neutron escapes the volume \((x_{real}, y_{real}, z_{real}>Boundary)\), then it is stopped and counted as leakage.

If it doesn’t escape the volume, the isotope that it interacts is determined according to the composition of the materials and one of the several interaction takes place depending on the relative cross sections.

Energy change in isotropic scattering in the center of mass (COM) frame \(s\)-wave scattering\(^{281}\) can be handled as

\[
E' = \left[\frac{(1 + \alpha) + (1 - \alpha) \ast cos\theta_c}{2}\right] \ast E \quad [Eq.5.9]
\]
where $\alpha$ and $\theta_c$ are collision parameter and scattering angle in COM frame, respectively. Collision parameter is defined as

$$\alpha = \left(\frac{A-1}{A+1}\right)^2$$  \hspace{1cm} [Eq. 5.10]

where $A$ is the mass number of the scattering nucleus.

Angle in the laboratory frame can be found by

$$\theta_L = \arctan \left( \frac{\sin \theta_c}{\frac{1}{A} + \cos \theta_c} \right)$$  \hspace{1cm} [Eq. 5.11]

In MATLAB, atan2 function should be used to find the correct quadrature into which the scattering occurs.

Shortest distance to a spherical boundary can be found using

$$x_{\text{new}} = x_0 + d \cdot \Omega_x$$  \hspace{1cm} [Eq. 5.12(a)]

$$y_{\text{new}} = y_0 + d \cdot \Omega_y$$  \hspace{1cm} [Eq. 5.12(b)]

$$z_{\text{new}} = z_0 + d \cdot \Omega_z$$  \hspace{1cm} [Eq. 5.12(c)]

$$R^2 = d^2 + 2d(x_0\Omega_x + y_0\Omega_y + z_0\Omega_z) + (x_0^2 + y_0^2 + z_0^2)$$  \hspace{1cm} [Eq. 5.13]

Positive root for $d$ can be found from Equation 5.13.

### 5.3 Charged Particle Simulation

When a neutron is captured by $^6\text{Li}$, $\alpha$ and T particles are created. Since energy of the neutrons is normally very low for this interaction compared to the energy gained by the charged particles, it can be assumed that two charged particles are created with opposite momenta. Charged particles can be assumed interacting with the electrons continuously in their passage since there are multiple collisions happening through Coulomb force. Eq.1.1 can be used to describe the energy loss of the charged particle using a
small step size $dx$. For thin absorbers, or when $\frac{\xi}{W_m} \ll 1$, Landau solution for energy fluctuation can also be implemented.

$\xi$ is defined as

$$\xi = 0.1535 \times x \times \frac{\rho \times Z^2 \times Z}{A \times \beta^2}, \text{where } x \text{ is the absorber thickness} \quad [Eq. 5.14]$$

For tritons, the condition is satisfied and the most probable energy loss can be given as \[5\]

$$\epsilon_{mp} = \epsilon + \left( \lambda_0 + \beta^2 + \ln \left( \frac{\xi}{W_m} \right) + 1 - C_E \right) \quad [Eq. 5.15]$$

where $\epsilon, \lambda_0 \text{ and } C_E$ are the mean energy loss, peak value of Landau distribution and Euler’s constant, respectively.

After each step of charged particle transportation, photons are produced and their locations and their numbers are put into arrays for photon propagation after the current charged particle event is done.

In Figure-5.1 Bragg’s curve is shown obtained from the custom Monte Carlo code. In Figure-5.2, number of photon distribution is shown for different ZnS thicknesses.
Figure-5-1 Bragg’s curve for triton in custom Monte Carlo code

Figure-5-2 Light production distribution with different ZnS thickness in custom Monte Carlo
5.4 Light Simulation

Light transport is still in the progress to be implemented to the code. It can be handled using the relevant governing equation, which are Beer-Lambert law, Fresnel equations and Snell’s law.

Beer-Lambert formula is used to describe the attenuation of the light in the medium as

\[ I(x) = I_0 \exp(-\mu_a x) \]  \hspace{1cm} \text{[Eq. 5.16]}

where \( \mu_a \) is the wavelength dependent absorption coefficient of the material. The boundary process for light is different than that of neutrons or gamma rays since the mismatch between boundaries may result in refraction, reflection or total internal reflection. When the photon reaches a boundary, the refractive indices between the two media are checked. If the refractive index of the first medium is greater than that of the second medium, then, depending on the angle of incidence with respect to the surface normal, total internal reflection may occur and the zenith angle is reversed.

Snell’s law states that

\[ n_1 \sin(\theta_1) = n_2 \sin(\theta_2) \]  \hspace{1cm} \text{[Eq. 5.17]}

And

\[ \theta_1 = \arcsin \left( \frac{n_2}{n_1} \right), \text{when } \theta_2 \text{ is } 90^\circ \]  \hspace{1cm} \text{[Eq. 5.18]}

So, the critical angle can be checked against the normal incidence angle and whether the light is totally reflected can be determined.

In order to evaluate the Fresnel refraction and Fresnel reflection, reflectance can be calculated using the angle of incidence and the final angle obtained from Snell’s law. Average of the s- and p-polarization can be used to calculate the reflectance as

\[ R_{ave} = \frac{1}{2} \left[ \frac{\sin^2(\alpha_i - \alpha_f)}{\sin^2(\alpha_i + \alpha_f)} + \tan^2(\alpha_i - \alpha_f) \right] \tan^2(\alpha_i + \alpha_f) \]  \hspace{1cm} \text{[Eq. 5.19]}
If the random number generated is less than the reflectance, then reflection occurs; otherwise, light is transmitted. Of course, this approach is rather crude since it doesn’t take into account the wave nature of the light; however it can be improved with weighting factors.

Since the medium in which the light propagation is simulated is extremely small in this case (microns), some additional measures can be taken to kill the light if it is trapped inside a volume with total internal reflection. There are still trapping issues in the code for light propagation.

In the current phase of the code, the wave nature of the light is not present and light is regarded merely a particle, which is not true.

The Monte Carlo algorithm is shown in Figure-5.3.
Initiate a neutron with energy $E$ and in volume $A$.

Move the neutron. Did the neutron cross a boundary?

Find the isotope that the neutron interacts and find the interaction. Was it scattered?

Calculate the final energy of the neutron after scattering. Change the angle.

Did the neutron escape the unit cell?

Continue propagating the neutron by putting it on the boundary.

Was the neutron escaped the entire medium?

Shift its position so that it starts in the next unit cell.

Did the neutron escape the entire medium?

Was it in ZnS?

Score the energy and continue propagating.

Is its energy below the critical value?

Set the momentum directions of alpha and triton. Propagate them.

Was it absorbed in $^6$Li?

Produce alpha and triton.

Produce photons.

Was it in ZnS?

Kill and score the remaining energy.

Is $N <$ Prescribed Number of Histories?

Stop.
Figure 5-3 Algorithm in custom Monte Carlo code

Set the position of the photon

Absorption

Leak

Move the photon. Did it cross the boundary?

Did the photon escape the entire medium?

Put it on the boundary. Check the incident angle. Is it greater than the critical angle?

Total internal reflection. Change the angle

Change the angle

Did the photon escape the unit cell?

Continue propagating the photon by putting it on the boundary

Is it reflected?

Y

N

N

Y

N

Shift its position so that it starts in the next unit cell

N
Chapter 6 Summary and Conclusion

GEANT4 was used extensively to evaluate the performance of the proposed coated micro-particle technology. Neutron transport, charged particle transport and light transport were simulated in both coated micro-particle detectors and in existing technology with different compositions and thicknesses. Model validations with commercially available detectors were made although there were lots of uncertainties with source, detector medium and optical constants, which were discussed in previous chapters.

Coated micro-particle optimization was performed on four different levels which are LiF radius, ZnS coating thickness, pitch and detector thickness. Detailed simulations were performed to find the best geometries with optimal parameters. Many metrics were used to evaluate the detector performances and the coated micro-particle detectors were compared to existing technology, which gave promising results.

Randomization of the coated micro-particles was performed to take into consideration the manufacturing imperfections. Even with the deviations from optimal parameters, it was shown that the coated micro-particle detectors performed better.

Coated micro-particle detectors have shown to improve both neutron detection efficiency and the light output. Ideal geometries increased the neutron detection efficiency by up to 1.7 compared to the best performing existing technology. Particle pitch and the detector thickness have been shown to be interrelated. 0.6mm thick detector gave the highest neutron detection efficiency with 60μm pitch while 1mm detector gave the highest neutron detection efficiency with 80μm.

There are issues that need to be addressed and improvements that need to be made. ZnS absorption coefficients need to be measured experimentally since there are disagreements between different sources. For future work, wavelength dependent LiF, ZnS and binder refraction indices, absorption coefficients and Rayleigh scattering lengths will be measured. More realistic quantum efficiency with spectral response characteristic can be modeled. Also, spatial dependency can be included since the quantum
efficiency is also space dependent. More realistic emission spectrum for ZnS(Ag) should be included. Well calibrated neutron source will be obtained for validation of the simulations. Knowing the microstructure and the grains size distribution of the specific detectors, simulations can be modeled more accurately.

Still, it is shown that, given the exact same parameters, coated micro-particle detectors perform much better than the existing technology. Although, ZnS thickness, pitch and detector thickness are subject to change with more accurate data, it would still perform better with the optimized parameters.
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Appendix A – Pulse Post-Processing Code

fileID = fopen('CF_252_neutron_15min.dat', 'r', 'a');
if fileID == -1, error('Cannot open file: %s', 'LYSO0.dat'); end
format = 'int16';
DET = fread(fileID, Inf, format);
fclose(fileID);
record_length = 300; % Record length each point represents 2 ns
[size_data_row, size_data_column] = size(DET); % size of the raw data
number_pulses = floor(size_data_row/record_length); % number of pulses

baseline_range = 50;
pulse_raw = zeros(number_pulses,record_length); %Raw Pulse initialization
baseline = zeros(number_pulses,1); % baseline initialization
pulse = zeros(number_pulses,record_length); % pulse initialization
for i = 1:number_pulses
    pulse_raw(i,:) = DET(record_length * (i-1) + 1:record_length * (i-1) + record_length,1);
    baseline(i) = mean(pulse_raw(i,1:baseline_range));
end
mean_baseline = mean(baseline);
for i = 1:number_pulses
    pulse(i,:) = pulse_raw(i,:) - mean_baseline;
end
max_pulse = zeros(number_pulses,1); %maximum of pulses initialization
loc_max_pulse = zeros(number_pulses,1); %location at which max pulse occurs
for i = 1:number_pulses
    [max_pulse(i), loc_max_pulse(i)] = max(pulse(i,:));
end
% Finding the min mean and max of pulses with locations
min_max_pulse = min(max_pulse);
mean_max_pulse = mean(max_pulse);
max_max_pulse = max(max_pulse);
min_loc_max_pulse = min(loc_max_pulse);
mean_loc_max_pulse = mean(loc_max_pulse);
max_loc_max_pulse = max(loc_max_pulse);

%%% Pulses outside the window eliminated
tolerance = 20;
in_window_pulse =
logical(loc_max_pulse<mean_loc_max_pulse+tolerance &
... loc_max_pulse>mean_loc_max_pulse-tolerance);
pulse = pulse(in_window_pulse == 1,:);
[number_pulses, column_pass] = size(pulse);
for i = 1:number_pulses
[max_pulse(i), loc_max_pulse(i)] = max(pulse(i,:));
end

%%% Clipped Pulses eliminated
clip_pulse = 2 * ones(1,number_pulses);
for i=1:number_pulses
    clippedulse(i) = logical(pulse(i,loc_max_pulse(i)) ==
pulse(i,loc_max_pulse(i) + 1));
end
clip_pulse = logical(clippedulse == 0);
clip_pulse = clipulse';
pulse_pass = pulse(clippedulse == 1,:);
[number_pulses_pass, column_pass] = size(pulse_pass);

%%%%%%% Double pulse elimination
double_pulse = zeros(number_pulses_pass,1);
for j = 1:number_pulses_pass
    [max_pulse, loc_max_pulse] = max(pulse_pass(j,:));
    for i=loc_max_pulse+20:record_length-1
        diff = (pulse_pass(j,i)...
        - pulse_pass(j,i-3));
        if diff>1000 %%%%% Number carefully chosen not to
eliminate neutron pulses
            doubleulse(j,1) = 1;
            break
        end
    end
end
doubleulse = logical(doubleulse == 0);
doubleulse = doubleulse';
pulse_pass = pulse_pass(doubleulse == 1,:);
[size_pulses_row, size_pulses_col] = size(pulse_pass);
number_pulses_pass = size_pulses_row;
%% Finding the min mean and max of pulses with locations after elimination
max_pulse_af = zeros(number_pulses_pass,1); %maximum of pulses initialization
loc_max_pulse_af = zeros(number_pulses_pass,1); %location at which max pulse occurs
for i = 1:number_pulses_pass
   [max_pulse_af(i), loc_max_pulse_af(i)] = max(pulse_pass(i,:));
end
min_max_pulse_af = min(max_pulse_af);
mean_max_pulse_af = mean(max_pulse_af);
max_max_pulse_af = max(max_pulse_af);
min_loc_max_pulse_af = min(loc_max_pulse_af);
mean_loc_max_pulse_af = mean(loc_max_pulse_af);
max_loc_max_pulse_af = max(loc_max_pulse_af);

% % % % Filtering & smoothing % % % %
filter_range_init = min_loc_max_pulse_af - 40;
filter_range_fin = max_loc_max_pulse_af + 50;
filter_step = 5;

number_filter_init = floor(filter_range_init/filter_step);
number_filter_fin = floor((record_length-filter_range_fin)/filter_step);
total_number_step = floor(record_length/filter_step);
baseline_pass = zeros(number_pulses_pass,1);
pulse_pass_bsb = pulse_pass;
baseline_filter = zeros(number_pulses_pass,number_filter_init);
for i = 1:number_pulses_pass
   for j = 1:number_filter_init
      baseline_filter(i,j) = ...
      mean(pulse_pass(i,filter_step*(j-1)+1:filter_step*(j-1)+filter_step));
      if abs(baseline_filter(i,j)) >= 100
         % pulse_pass_bsb(i,:) = pulse_pass(i,:);
         break
      end
   end
   pulse_pass_bsb(i,filter_step*(j-1)+1:filter_step*(j-1)+filter_step) = ...
   baseline_filter(i,j);
end
for i = 1:number_pulses_pass
    for j = number_filter_fin:total_number_step
        baseline_filter(i,j) = ...
            mean(pulse_pass(i,filter_step*(j-1)+1:filter_step*(j-1)+filter_step));
        if abs(baseline_filter(i,j)) >= 100
            break
        end
        pulse_pass_bsb(i,filter_step*(j-1)+1:filter_step*(j-1)+filter_step) = ...
            baseline_filter(i,j);
    end
end
baseline_mean = zeros(number_pulses_pass,1);
%%%%%%%%%%%%%%%% Baseline correction
for i = 1:number_pulses_pass
    baseline_mean(i) = mean(pulse_pass_bsb(i,1:baseline_range));
    if abs(baseline_mean(i)) >= 100
    else
        pulse_pass_bsb(i,:) = pulse_pass_bsb(i,:) - baseline_mean(i);
    end
end
%%%%%%%%%%%%%%%% Tail correction
tail_mean = zeros(number_pulses_pass,1);
for i = 1:number_pulses_pass
    tail_mean(i) = mean(pulse_pass_bsb(i,record_length/2:end));
    if (tail_mean(i)) >= 0
    else
        pulse_pass_bsb(i,record_length/2:end) = ...
            pulse_pass_bsb(i,record_length/2:end) - tail_mean(i);
    end
end
%-------------------------------------
tail_range_in = 10;
tail_range_fin = 0;
max_pulse_pass = zeros(number_pulses_pass,1);
loc_max_pulse_pass = zeros(number_pulses_pass,1);
for i = 1:number_pulses_pass
    [max_pulse_pass(i), loc_max_pulse_pass(i)] = max(pulse_pass_bsb(i,:));
end
full_int = zeros(number_pulses_pass,1);
tail_int = zeros(number_pulses_pass,1);
for i = 1:number_pulses_pass
    full_int(i) = sum(pulse_pass_bsb(i,:));
    tail_int(i) = sum(pulse_pass_bsb(i,...
        loc_max_pulse_pass(i)+tail_range_in:record_length-
        tail_range_fin));
end
for i =1:number_pulses_pass
    baseline(i) = mean(pulse_pass_bsb(i,1:10));
    pulse_pass_bsb(i,:) = pulse_pass_bsb(i,:) - baseline(i);
end
% % % % % % % % % % % % % % % % % % % % % % % % % % % % % % % % % % %
% Ringing Elimination % % % % % % % % % % % % % % % % % % %
% % % % % % % % % % % % % % % % % % % % % % % % % % % % % % % % % % %
for j = 1:number_pulses_pass
    [max_pulse_bsb, loc_max_pulse_bsb] =
        max(pulse_pass_bsb(j,:));
    for i=1:50
        diff = (pulse_pass_bsb(j,loc_max_pulse_bsb+i)... - pulse_pass_bsb(j,loc_max_pulse_bsb+i-1));
        if diff>100
            pulse_pass_bsb(j,loc_max_pulse_bsb+i)... = pulse_pass_bsb(j,loc_max_pulse_bsb+i-1);
        end
    end
end
% % % % % % % % % % % % % % % % % % % % % % % % % % % % % % % % % % %
% Pulse shape discrimination % % % % % % % % % % % % % % % % %
% tail_int = tail_int(tail_int>0);
% full_int = full_int(tail_int>0);
% threshold_psd = 0.16;
threshold_removal = 0.38;
threshold_psd = -1.23333E-6*full_int + 0.37;
threshold_psd = 0.22;
threshold_psd = 2.6666666*10^-12*full_int.^2 - 2*10^-7*full_int+0.063333;
tail_to_full = tail_int./full_int;
gamma_pulses =
pulse_pass_bsb(tail_to_full<=threshold_psd,:);
neutron_pulses =
pulse_pass_bsb(tail_to_full>threshold_psd,:);
    % & tail_to_full<threshold_removal,:);
%other_pulses =
pulse_pass_bsb(tail_to_full>threshold_removal,:);
gamma_full_int = full_int(tail_to_full<=threshold_psd);
neutron_full_int = full_int(tail_to_full>threshold_psd);
% & tail_to_full<threshold_removal);
%other_full_int = full_int(tail_to_full>threshold_removal);
gamma_tail_int = tail_int(tail_to_full<=threshold_psd);
neutron_tail_int = tail_int(tail_to_full>threshold_psd);
% & tail_to_full<threshold_removal);
%other_tail_int = tail_int(tail_to_full>threshold_removal);
gamma_tail_to_full = gamma_tail_int./gamma_full_int;
neutron_tail_to_full = neutron_tail_int./neutron_full_int;
%other_tail_to_full = other_tail_int./other_full_int;

figure
%subplot(1,2,1)
scatter(gamma_full_int,gamma_tail_to_full,'.');
hold on;
scatter(neutron_full_int,neutron_tail_to_full,'.', 'r');
xlabel('Full Integral (Arbitrary Units)')
ylabel('PSD Parameter')
legend('gamma','neutron')
%hold on;
%scatter(other_full_int,other_tail_to_full,'g');
ylim([0 0.5]);
% subplot(1,2,2)
% scatter(gamma_full_int,gamma_tail_int,'.');
% hold on;
% scatter(neutron_full_int,neutron_tail_int,'.', 'r');
% xlabel('Full Integral (Arbitrary Units)')
% ylabel('Tail Integral (Arbitrary Units')
% legend('gamma','neutron')
%ylim([0 3*10^4]);
%hold on;
%scatter(other_full_int,other_tail_to_full,'g');

% Histogram for FOM %%%%%%%%%%%%%%%%%
limit_hist = 0.6;
step_hist = 400;
bin = linspace(0,limit_hist,step_hist);
number_of_neutrons = histc(neutron_tail_to_full,bin);
number_of_gammas = histc(gamma_tail_to_full,bin);
%number_of_others = histc(other_tail_to_full,bin);
figure
bar(bin,number_of_gammas)
hold on;
bar(bin,number_of_neutrons,'r')
hold on;
%bar(bin,number_of_others,'g');

fwhm_of_gammas = fwhm(bin,number_of_gammas);
fwhm_of_neutrons = fwhm(bin,number_of_neutrons);
[max_gamma_count, loc_max_gamma_count] =
max(number_of_gammas);
[max_neutron_count, loc_max_neutron_count] =
max(number_of_neutrons);
loc_max_gamma_count = loc_max_gamma_count * limit_hist/step_hist;
loc_max_neutron_count = loc_max_neutron_count * limit_hist/step_hist;
distance = loc_max_neutron_count - loc_max_gamma_count;
FOM = distance/(fwhm_of_gammas + fwhm_of_neutrons)
size(neutron_pulses)

% channel

max_neutron_int = max(neutron_full_int);
min_neutron_int = min(neutron_full_int);
ch = 100;
integ = max_neutron_int/ch;
if min_neutron_int<integ
    min_neutron_int = integ;
end

full_int_number = zeros(1,ch);
full_int_x = zeros(1,ch);
for i = round(min_neutron_int/integ):max_neutron_int/integ
    fnd = find(neutron_full_int>=(i-1)*integ)... & neutron_full_int<=(((i-1)*integ+integ));
    [row_full_int, column_full_int] = size(fnd);
    full_int_number(i) = row_full_int;
    column_full_int(i) = i;
    full_int_x(i) = (i-1)*integ;
end
figure
plot(full_int_x,full_int_number);
[a b] = max(full_int_number);
a
b * max_neutron_int / ch
size(gamma_pulses)
Appendix B - PTRAC Code for Neutron Energy Spectrum at the Time of Capture by $^6$Li with a Sample MCNP6 Input File

PTRAC Code

```matlab
load ptraq
tp = ptrar;
[m n] = size(tp);
tpp = ones(m,9);
S = 0;
%bb = ones(500,1);
for i=1:m
    b = sqrt(tp(i,1)^2+tp(i,2)^2+tp(i,3)^2);
    if b>99 && b<101
        tpp(i,:) = 1;
    else
        tpp(i,1) = tp(i,1);
        tpp(i,2) = tp(i,2);
        tpp(i,3) = tp(i,3);
        tpp(i,4) = tp(i,4);
        tpp(i,5) = tp(i,5);
        tpp(i,6) = tp(i,6);
        tpp(i,7) = tp(i,7);
        tpp(i,8) = tp(i,8);
        tpp(i,9) = tp(i,9);
    end
end
RM1 = tpp(:,1) == 1;
tpp(RM1,:) = [];
RM2 = tpp(:,3)>0.055 | tpp(:,3)<0.005;
tpp(RM2,:) = [];
MINE =floor(10^9* min(tpp(:,7)));
MAXE =floor(10^9* max(tpp(:,7)));
d = 1
    for i = 1:1:MAXE
        FINDER = find(d*(i-1)*10^-9<tpp(:,7) & d*(i-1)*10^-9+d*10^-9>=tpp(:,7));
        [aaa bbb] = size(FINDER);
        a(i) = aaa;
        bb(i) = i;
    end
    bb = d * 10^-3 * bb;
    for i=1:1:200
        S = S + a(i)*bb(i);
    end
Smean = S/MAXE;
plot(bb,a)
xlim([0 200*10^-3]);
[maxn maxp] = max(a)
```
MCNP6 Input

1 1 -2.635 -1   $LiF spherical volume
2 2 -4.09 1 -2   $ZnS thickness
3 4 -0.93 2      $Binder volume
4 0 3 -4 5 -6 7 -8  $Lattice construction
5 0 -9 10 -11 12 -13 14  $Detector sheet construction
6 3 -0.93 -15 16 -17 18 -19 20  $Polyethylene Moderator
7 0 #5 #6 -21  $Vacuum
8 0 21  $Outside of the geometry

1 so 19e-4  $LiF radius
2 so 20e-4  $ZnS radius
3 px -50e-4  $Pitch
4 px 50e-4
5 py -50e-4
6 py 50e-4
7 pz -50e-4
8 pz 50e-4
9 px 5  $Sheet dimensions
10 px -5
11 py -0.5
12 py -5.5
13 pz 0.055
14 pz 0.005
15 px 5  $Moderator dimensions
16 px -5
17 py 5.5
18 py -5.5
19 pz 0.005
20 pz -9.595
21 so 100

mode n a t  $Simulation of alpha triton and neutron
imp:n,a,t 1 1 1 1 1 1 0  $importance of each cell
u 2 2 2 1 j j j j  $universe number
fill j jj 2 1 jj j $fill the cell with
lat j jj 1 jj jj $lattice number
vol j j 7.52e-7 jj jj j $Volume of the irregular cell
PHYS:N 20 0 0 jj j 5 -1 $Neutron Physics
PHYS:A 100 jj j 0 j 1 jj jj $Alpha Physics
PHYS:T 100 jj j 0 j 1 jj jj $Triton Physics
CUT:a j 0.001 $Alpha cut
CUT:t j 0.001 $Triton Cut
nps 5e6 $number of histories
SDEF ERG d2 DIR d1 VEC 0 0 1 PAR 1 POS -5.5 0 -9.6 $Source definition
SI1 0 1 $Direction cosine in +z direction
SP1 -21 0
SP2 -3 1.025 2.926 $Cf-252 source
PTRAC FILE=ASC EVENT=TER TYPE=n CELL=1& $PTRAC cards
WRITE=ALL
c PTRAC FILE=ASC EVENT=SRC TYPE=t&
c WRITE=ALL
F1:t 1 $Number of tritons crossing surface 1
c
m1 3006 0.475 3007 0.025 9019 0.5 $materials
m2 30064 0.246 30066 0.1385 30067 0.02 30068 0.0925 16032 0.5
m3 1001 2 6012 1
m4 11023 1 14028 1 8016 1
Appendix C – Numerical Calculation of Range and SRIM Results

Numerical Integration for Alpha and Triton Range in LiF and ZnS Using Trapezoid Integration

```matlab
n=3.34*10^29;
T=2.75;
Z2=8;
mcsquare=938;
gamma=T/mcsquare+1;
betasq=1-(1/gamma)^2;
betasq1=1-(1/(T/mcsquare+1))^2;
beta=sqrt(betasq);
lnI=(2*1*log(19)+1*8*log(11.2+11.7*Z2))/10;%h20
I=exp(lnI);
F=(log(1.02*10^6*beta^2/(1-beta^2)))-beta^2;
Na=0.602*10^24;
%z=input('atom number of particle=');
z=1;
if z==2
    mcsquare=3727.4;
elseif z==1
    mcsquare=2808.7;
else
    disp('enter another 1 or 2');
z=0;
end
%N=input('neutron number of particle=');
N=2;
%Z1=input('atom number of first element in medium=');
Z1=16;
%Z2=input('atom number of second element in medium=');
Z2=30;
%ZZ1=input('Amount of first element in the compound=');
ZZ1=1;
%ZZ2=input('Amount of second element in the compound=');
ZZ2=1;
%rho=input('density of the material (g/cm^3)=');
rho=4.09;
%M=input('total mass of compound=');
M=97;
```
if \( Z_1 = 1 \)
    \( I_1 = 19 \);
elseif \( 2 \leq Z_1 \leq 13 \)
    \( I_1 = 11.2 + 11.7 \cdot Z_1 \);
else
    \( I_1 = 52.8 + 8.71 \cdot Z_1 \);
end

if \( Z_2 = 1 \)
    \( I_2 = 19 \);
elseif \( 2 \leq Z_2 \leq 13 \)
    \( I_2 = 11.2 + 11.7 \cdot Z_2 \);
else
    \( I_2 = 52.8 + 8.71 \cdot Z_2 \);
end

\( nn = ZZ_1 \cdot Z_1 + ZZ_2 \cdot Z_2 \);

\( \ln I = ZZ_1 \cdot Z_1 / nn \cdot \log(I_1) + ZZ_2 \cdot Z_2 / nn \cdot \log(I_2) \);

\( I = \exp(\ln I) \);

\% mcsquare=z*1.0073*1.66054*10^-24*0.001*(299792458)^2*6.242*10^12+N*1.0078*1.66054*10^-24*0.001*(299792458)^2*6.242*10^12; \% fix this

\( n = Na \cdot (nn) \cdot \rho \cdot 10^6 / M \);

\( h = 1 / 10000 \);

\% mdxde2=1/((5.08*10^-31*z^2*n/(1-(1/(T/mcsquare+1))^-2))\*(\log(1.02*10^6*(1-(1/(T/mcsquare+1))^-2))/(1-(1-(1/(T/mcsquare+1))^-2))))-(1-(1/(T/mcsquare+1))^-2)-lnI));

\( a_0 = 1/((5.08*10^-31*z^2*n/(1-(1/(0/mcsquare+1))^-2))\*(\log(1.02*10^6*(1-(1/(0/mcsquare+1))^-2))/(1-(1-(1/(0/mcsquare+1))^-2))))-(1-(1/(0/mcsquare+1))^-2)-lnI));

\( a_1 = 1/((5.08*10^-31*z^2*n/(1-(1/(1/mcsquare+1))^-2))\*(\log(1.02*10^6*(1-(1/(1/mcsquare+1))^-2))/(1-(1-(1/(1/mcsquare+1))^-2))))-(1-(1/(1/mcsquare+1))^-2)-lnI));

\( i = h / T; \)

\( a = 1/((5.08*10^-31*z^2*n/(1-(1/(i./mcsquare+1)).^-2))\*(\log(1.02*10^6*(1-(1/(i./mcsquare+1)).^-2))/(1-(1-(1./(i./mcsquare+1)).^-2))))-(1-(1./(i./mcsquare+1)).^-2)-lnI));

\( d = h / 2 * (2 * \text{sum}(a) + a_1 + a_0); \)
SRIM RESULTS

H (10) into Layer 1

**ION RANGES**

**ION STAT**s:
- **Range**:
  - 5.56 um
- **Straggles**:
  - 2355 A
- **Kurtosis**:
  - 77,769

Calculation Parameters:
- Backscattered Ions: 0
- Transmitted Ions: 0
- Vacancies/Atom

Stopping Power Version: SRIM-2008

**SPLINTERING YIELD**

**TOTAL**

<table>
<thead>
<tr>
<th>Atom/Ion</th>
<th>dV/Atom</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li</td>
<td>0.000000</td>
</tr>
<tr>
<td>F</td>
<td>0.000000</td>
</tr>
</tbody>
</table>

2839 Ions Calculated
- Ion Type = He
- Ion Energy = 2.05 MeV
- Ion Angle = 0

H (10) into Layer 1

**ION RANGES**

**ION STAT**s:
- **Range**:
  - 0.65 um
- **Straggles**:
  - 1855 A
- **Kurtosis**:
  - 153,365

Calculation Parameters:
- Backscattered Ions: 0
- Transmitted Ions: 0
- Vacancies/Atom

Stopping Power Version: SRIM-2008

**SPLINTERING YIELD**

**TOTAL**

<table>
<thead>
<tr>
<th>Atom/Ion</th>
<th>dV/Atom</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li</td>
<td>0.000000</td>
</tr>
<tr>
<td>F</td>
<td>0.000000</td>
</tr>
</tbody>
</table>
2415 Ions Calculated
Ion Type = H
Ion Energy = 2.75 MeV
Ion Angle = 0

Calculation Parameters:
Backscattered Ions 0
Transmitted Ions 0
Vacancies/Ion 66.7

ION STATs
Range 32.3 um
Longitudinal 32.3 um
Lateral Proj. 1.16 um
Radial 1.82 um

Type of Damage Calculation
Quick: Kinchin-Pease

Stopping Power Version
SRIM-2008

% ENERGY LOSS
Ions 99.74 0.04
Vacancies 0.00 0.00
Phonons 0.04 0.17

SPUTTERING YIELD
TOTAL
0.000000 0.00

2805 Ions Calculated
Ion Type = H
Ion Energy = 2.75 MeV
Ion Angle = 0

Calculation Parameters:
Backscattered Ions 0
Transmitted Ions 0
Vacancies/Ion 61.2

ION STATs
Range 34.1 um
Longitudinal 34.1 um
Lateral Proj. 9209 A
Radial 1920 A

Type of Damage Calculation
Quick: Kinchin-Pease

Stopping Power Version
SRIM-2008

% ENERGY LOSS
Ions 99.73 0.07
Vacancies 0.00 0.00
Phonons 0.04 0.16

SPUTTERING YIELD
TOTAL
0.000000 0.00
Appendix D – GEANT4 codes

Sample Detector Construction Code

Some information on the materials is excluded on the request of the manufacturers.

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// ............................................................................


/// file B1DetectorConstruction.cc
/// brief Implementation of the B1DetectorConstruction class

#include "B1DetectorConstruction.hh"

#include "G4RunManager.hh"
#include "G4NistManager.hh"
#include "G4Box.hh"
#include "G4Cons.hh"
#include "G4Orb.hh"
#include "G4Sphere.hh"
#include "G4Trd.hh"
#include "G4Tubs.hh"
#include "G4Ellipsoid.hh"
#include "G4LogicalVolume.hh"
#include "G4PVPlacement.hh"
#include "G4SystemOfUnits.hh"
#include "G4LogicalBorderSurface.hh"
#include "G4LogicalSkinSurface.hh"
#include "G4OpticalSurface.hh"
#include "G4PVReplica.hh"
#include "G4Track.hh"

B1DetectorConstruction::B1DetectorConstruction()
    : G4VUserDetectorConstruction()
    , fScoringVolume(0), fLiF_phys(0), fZnS_phys(0)
{
}

B1DetectorConstruction::~B1DetectorConstruction()
{
}
G4VPhysicalVolume* B1DetectorConstruction::Construct()
{
    // Get nist material manager
    G4NistManager* nist = G4NistManager::Instance();

    G4double RZnS=20*um;
    G4double RLiF=19*um;
    G4double xpoly=30*um, ypoly=30*um, zpoly=30*um;
    G4double abundance, A, Z, a, z, density;
    G4int ncomp, ncomponent;
    G4String symbol;

    //
    a=1.*g/mole;
    G4Element* elH=new G4Element("Hydrogen", "H", z=1, a);
    a=12.*g/mole;
    G4Element* elC=new G4Element("Carbon", "C", z=6, a);
    a=16.*g/mole;
    G4Element* elO=new G4Element("Oxygen", "O", z=8, a);

    density=0.93*g/cm3;
    G4Material* mat_Polyethylene=new G4Material("Polyethylene", density, ncomp=2);
    mat_Polyethylene->AddElement(elH, ncomponent=2);
    mat_Polyethylene->AddElement(elC, ncomponent=1);
    mat_Polyethylene->AddElement(elO, ncomponent=3);

    a=23*g/mole;
    G4Element* elNa=new G4Element("Soduium", "Na", z=11, a);
    a=28*g/mole;
    G4Element*elSi= new G4Element("Silicon", "Si", z=14,a);

    a=64*g/mole;
    G4Isotope* isoZn64=new G4Isotope("Zn64", Z=30, A=64, a);
    a=66*g/mole;
    G4Isotope* isoZn66=new G4Isotope("Zn66", Z=30, A=66, a);
    a=68*g/mole;
    G4Isotope* isoZn68=new G4Isotope("Zn68", Z=30, A=68, a);
    G4Element* elZn = new G4Element("Zinc", symbol = "Zn", ncomp = 3);
    elZn->AddIsotope(isoZn64, abundance=49.2*perCent);
    elZn->AddIsotope(isoZn66, abundance=27.7*perCent);
    elZn->AddIsotope(isoZn68, abundance=18.5*perCent);
    a=32*g/mole;
    G4Element*elS= new G4Element("Sulphur", "S", z=16,a);

    density=4.09*g/cm3;
    G4Material* mat_ZnS= new G4Material("ZincSulphide", density, ncomp=2);
    mat_ZnS->AddElement(elZn, ncomponent=1);
    mat_ZnS->AddElement(elS, ncomponent=1);

    a=6*g/mole;
    G4Isotope* isoLi6= new G4Isotope("Li6", Z=3, A=6, a);
    a=7*g/mole;
    G4Isotope* isoLi7= new G4Isotope("Li7", Z=3, A=7, a);

    G4Element* enrichedLi= new G4Element("enrichedLi", symbol="Li", ncomp=2);
    enrichedLi->AddIsotope(isoLi6, abundance=95.*perCent);
    enrichedLi->AddIsotope(isoLi7, abundance=5.*perCent);

    a=19*g/mole;
    G4Element* elF=new G4Element("Flourine", symbol="F", z=9, a);

    density=2.635*g/cm3;
    G4Material*mat_LiF= new G4Material("LithiumFluoride", density, ncomp=2);
    mat_LiF->AddElement(enrichedLi, ncomponent=1);
mat_LiF->AddElement(eF, ncomponent=1);

// density = 0.8203*g/cm3; // 7.5 grain size
density = 1.0597*g/cm3; // 8
// density=1.17*g/cm3; // 8.2
// density=1.6059*g/cm3;
G4Material* mat_hom= new G4Material("Hom", density, ncomp=5);
mat_hom->AddElement(enrichedLi, ncomponent=1);
mat_hom->AddElement(eF, ncomponent=1);
mat_hom->AddElement(eNa, ncomponent=1);
mat_hom->AddElement(eSi, ncomponent=1);
mat_hom->AddElement(eO, ncomponent=1);
// mat_hom->AddElement(eH, ncomponent=2);
// mat_hom->AddElement(eC, ncomponent=5);
// mat_hom->AddElement(eO, ncomponent=3);
density=0.93*g/cm3;
G4Material* mat_binder=new G4Material("binder", density, ncomp=3);
mat_binder->AddElement(eNa, ncomponent=1);
mat_binder->AddElement(eSi, ncomponent=1);
mat_binder->AddElement(eO, ncomponent=1);
a=207*g/mole;
G4Element* elPb=new G4Element("Pb", symbol="Pb", z=82, a);
density=11.34*g/cm3;
G4Material* mat_Pb=new G4Material("lead", density, ncomp=1);
mat_Pb->AddElement(ePb, ncomponent=1);
density=1.38*g/cm3;
G4Material* mat_Polyester= new G4Material("Polyester", density, ncomp=3);
mat_Polyester->AddElement(eO, ncomponent=2);
mat_Polyester->AddElement(eC, ncomponent=5);
mat_Polyester->AddElement(eH, ncomponent=4);

// Envelope parameters
//
G4Material* env_mat = nist->FindOrBuildMaterial("G4_WATER");
G4Box* solidWorld = new G4Box("World", 200*cm, 200*cm, 200*cm);

G4Material* world_mat = nist->FindOrBuildMaterial("G4_AIR");

////////////ZNS///////////
///AIR///////////

// World
//
G4double world_sizeXY = 1.2*env_sizeXY;
G4double world_sizeZ = 1.2*env_sizeZ;
G4Box* solidWorld = new G4Box("World", 200*cm, 200*cm, 200*cm);
30*cm, 30*cm, 30*cm); //its size

G4LogicalVolume* logicWorld =
    new G4LogicalVolume(solidWorld, //its solid
    world_mat, //its material
    "World"); //its name

G4VPhysicalVolume* physWorld =
    new G4PVPlacement(0, //no rotation
    G4ThreeVector(), //at (0,0,0)
    logicWorld, //its logical volume
    "World", //its name
    0, //its mother volume
    false, //no boolean operation
    0, //copy number
    checkOverlaps); //overlaps checking

G4ThreeVector pos30 = G4ThreeVector(0*cm, -0.23*cm, 0.071*cm);
G4Tubs* solidDet = new G4Tubs("Det", 0*cm, 1.27*cm, 0.016*cm, 0*deg, 360*deg);
G4LogicalVolume* logicDet = new G4LogicalVolume(solidDet, world_mat, "Det");
G4VPhysicalVolume* Det_phys = new G4PVPlacement(0, pos30, logicDet, "Det", logicWorld, false, 0, checkOverlaps);

G4ThreeVector pos35 = G4ThreeVector(0*cm, 6.0*cm, -3.055*cm);
G4Box* solidMod = new G4Box("Mod", 7.5*cm, 7.5*cm, 3*cm);
G4LogicalVolume* logicMod = new G4LogicalVolume(solidMod, mat_Polyethylene, "Mod");
G4VPhysicalVolume* Mod_phys = new G4PVPlacement(0, pos35, logicMod, "Mod", logicWorld, false, 0, checkOverlaps);

G4ThreeVector pos37 = G4ThreeVector(0*cm, 0*cm, -0.0425*cm);
G4Box* solidPolyester1 = new G4Box("Polyester1", 1.5*cm, 1.5*cm, 0.0125*cm);
G4LogicalVolume* logicPolyester1 = new G4LogicalVolume(solidPolyester1, mat_Polyester, "Polyester1");
G4VPhysicalVolume* Polyester1_phys = new G4PVPlacement(0, pos37, logicPolyester1, "Polyester1", logicWorld, false, 0, checkOverlaps);

G4ThreeVector pos38 = G4ThreeVector(0*cm, 0*cm, 0.0425*cm);
G4Box* solidPolyester2 = new G4Box("Polyester2", 1.5*cm, 1.5*cm, 0.0125*cm);
G4LogicalVolume* logicPolyester2 = new G4LogicalVolume(solidPolyester2, mat_Polyester, "Polyester2");
G4VPhysicalVolume* Polyester2_phys = new G4PVPlacement(0, pos38, logicPolyester2, "Polyester2", logicWorld, false, 0, checkOverlaps);

// // Envelope //

G4ThreeVector posEnv = G4ThreeVector(0*cm, 0, 0);

G4Box* solidEnv =
    new G4Box("Envelope", //its name
    1.5*cm, 1.5*cm, 0.03*cm); //its size

G4LogicalVolume* logicEnv =
    new G4LogicalVolume(solidEnv, //its solid
    mat_binder, //its material
    "Envelope"); //its name

G4VPhysicalVolume* Poly_phys = new G4PVPlacement(0, //no rotation
    posEnv, //at (0,0,0)
    logicEnv, //its logical volume
    "Envelope", //its name
    logicWorld, //its mother volume
    false, //no boolean operation
    0, //copy number
    checkOverlaps); //overlaps checking

G4Box* solidEnvz =
    new G4Box("Envz", //its name
    1.5*cm, 1.5*cm, 0.030*cm); //its size

G4LogicalVolume* logicEnvz =
    new G4LogicalVolume(solidEnvz, //its solid
    mat_binder, //its material
    "Envz"); //its name
G4VPhysicalVolume* Poly_phys1 = new G4PVReplica("Envz",                   //no rotation
       logicEnvz, //at (0,0,0)
logicEnv, //its logical volume
kZAxis, //its name
1, //its mother volume
0.06*cm); //no boolean operation
//overlaps checking

G4Box* solidEnvy =
new G4Box("Envy", //its name
1.5*cm, 10*ypoly, 0.03*cm); //its size

G4LogicalVolume* logicEnvy =
new G4LogicalVolume(solidEnvy, //its solid
   mat_binder, //its material
   "Envy"); //its name

G4VPhysicalVolume* Poly_phys2 = new G4PVReplica("Envy",                   //no rotation
       logicEnvy, //at (0,0,0)
logicEnvz, //its logical volume
kYAxis, //its name
50, //its mother volume
0.06*cm); //no boolean operation
//overlaps checking

//G4ThreeVector pos3 = G4ThreeVector(0, 0, 0);

// ZnS
//G4Material* shape1_mat = nist->FindOrBuildMaterial("G4_A-150_TISSUE");
//G4ThreeVector pos1 = G4ThreeVector(0, 0, 0);

// LIF
//G4Material* shape2_mat = nist->FindOrBuildMaterial("G4_BONE_COMPACT_ICRU");
G4ThreeVector pos0 = G4ThreeVector(0, 0, 0);
G4ThreeVector pos3 = G4ThreeVector(-12.5*um, 0, 0);

G4Box* solidPoly =
new G4Box("Poly", //its name
10*xpoly, 10*ypoly, 10*zpoly); //its size

G4LogicalVolume* logicPoly =
new G4LogicalVolume(solidPoly, //its solid
   mat_binder, //its material
   "Poly"); //its name

G4VPhysicalVolume* Poly_phys0 =
new G4PVReplica("Poly", logicPoly, logicEnvy, kXAxis, 50, 0.06*cm);

const G4int n = 1000;
G4Ellipsoid* solidZnS[n] = {};
G4LogicalVolume* logicZnS[n] = {};
G4VPhysicalVolume* ZnS_phys[n] = {};
G4Ellipsoid* solidLiF[n] = {};
G4LogicalVolume* logicLiF[n] = {};
G4VPhysicalVolume* LiF_phys[n] = {};
G4int cnt = 0;
G4ThreeVector pos[n] = {};

for (G4int i=0; i<10; i++){
for (G4int j=0; j<10; j++){
for (G4int k=0; k<10; k++){
pos[cnt] = G4ThreeVector((16*G4UniformRand()+(60*i-278))*um, (16*G4UniformRand()+(60*j-278))*um, (16*G4UniformRand()+(60*k-278))*um);
cnt = cnt + 1;
}
}
G4double ksi1;
G4double psi1;
G4double ksi2;
G4double psi2;
G4double ksi3;
G4double psi3;
G4RotationMatrix rotmpos = G4RotationMatrix();

for (G4int w=0; w<n; w++){
  G4double ksi10 = G4UniformRand();
  if (ksi10<=0.33)
  {
    rotmpos.rotateX(90*G4UniformRand()*deg);
  }
  else if (ksi10<=0.66 && ksi10>0.33)
  {
    rotmpos.rotateY(90*G4UniformRand()*deg);
  }
  else if (ksi10<=1 && ksi10>0.66)
  {
    rotmpos.rotateZ(90*G4UniformRand()*deg);
  }
  G4Transform3D transformpos = G4Transform3D(rotmpos,pos[w]);
  //
  ksi1 = 2*(G4UniformRand()+10)*um;
  psi1 = 2*(G4UniformRand()*um+((ksi1/2)-1.1*um));
  ksi2 = 2*(G4UniformRand()+10)*um;
  psi2 = 2*(G4UniformRand()*(ksi2/2)-1.1*um));
  ksi3 = 2*(G4UniformRand()+10)*um;
  psi3 = 2*(G4UniformRand()*(ksi3/2)-1.1*um));

solidZnS[w] =
new G4Ellipsoid("ZnS", ksi1, ksi2, ksi3);
logicZnS[w] =
new G4LogicalVolume(solidZnS[w], //its solid
mat_ZnS, //its material
"ZnS"); //its name

ZnS_phys[w] =
new G4PVPlacement(0,
pos[w],
logicZnS[w], //its logical volume
"ZnS", //its name
logicPoly, //its mother volume
false, //no boolean operation
0, //copy number
checkOverlaps); //overlaps checking

solidLiF[w] =
new G4Ellipsoid("LiF", psi1, psi2 ,psi3);
logicLiF[w] =
new G4LogicalVolume(solidLiF[w], //its solid
mat_LiF, //its material
"LiF"); //its name

LiF_phys[w] =
new G4PVPlacement(0,
pos0, //no
logicLiF[w],    // its logical volume
"LiF",        // its name
logicZnS[w],    // its mother volume
false,      // no boolean operation
0,          // copy number
checkOverlaps);  // overlaps checking

} // ----------- Surfaces -----------

G4OpticalSurface* LiFZnSSurface = new G4OpticalSurface("LiFZnSSurface");
LiFZnSSurface->SetType(dielectric_metal);
LiFZnSSurface->SetFinish(polished);
LiFZnSSurface->SetModel(unified);

G4LogicalBorderSurface* ZnSLiFSurface =
    new G4LogicalBorderSurface("ZnSLiFSurface",
Polyester2_phys,Det_phys,LiFZnSSurface);

G4OpticalSurface* opticalSurface = dynamic_cast <G4OpticalSurface*>(
    (ZnSLiFSurface->GetSurface(Polyester2_phys,Det_phys)->
     GetSurfaceProperty()));

if (opticalSurface) opticalSurface->DumpInfo();

}//....oooOO0OOooo........oooOO0OOooo........oooOO0OOooo........oooOO0OOooo......

Sample Particle Tracking Code

// ********************************************************************
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// ********************************************************************

// $Id: B1SteppingAction.cc 74483 2013-10-09 13:37:06Z gcosmo $
B1SteppingAction::B1SteppingAction(B1DetectorConstruction* det, B1EventAction* evt, HistoManager* histo) : G4UserSteppingAction(), fHistoManager(histo), fScoringVolume(0), fDetector(det), fEventAction(evt) {}

B1SteppingAction::~B1SteppingAction() {}
G4Track* thetrack = step->GetTrack();

if (!thetrack->GetNextVolume())
  thetrack->SetTrackStatus(fStopAndKill);

if (edepstephist != 0)
{
  if (thePrePVname == "LiF") fEventAction->AddLiF(edepstephist, stepstephist);
  if (thePrePVname == "ZnS") fEventAction->AddZnS(edepstephist, stepstephist);
}
if (!fScoringVolume) {
  const B1DetectorConstruction* detectorConstruction =
      static_cast<const B1DetectorConstruction*>(G4RunManager::GetRunManager()->
        GetUserDetectorConstruction());
  fScoringVolume = detectorConstruction->GetScoringVolume();
}
G4double saystep=0;
G4double saystepn=0;
G4double saystepp=0;

//G4String name;
//name=step->GetTrack()->GetDefinition()->GetParticleName();
// get volume of the current step
G4LogicalVolume* volume = step->GetPreStepPoint()->GetTouchableHandle()->
    GetVolume()->GetLogicalVolume();
G4StepPoint* point = step->GetPostStepPoint();
G4StepPoint* point2 = step->GetPreStepPoint();
G4VPhysicalVolume* thepostpv = point->GetPhysicalVolume();
G4VPhysicalVolume* theprepv = point2->GetPhysicalVolume();
G4Track* atrack = step->GetTrack();
//point->GetStepStatus() == fGeomBoundary &&
//theprev->GetName() == "Poly"
if (name == "opticalphoton")
{
  // if (step->GetTrack()->GetKineticEnergy()<=0.044*eV)
  //}
  if (theprev->GetName() == "Polyester2" && thepostpv->GetName() == "Det")
    fEventAction->Addposx(pos_z_1_p);
  fEventAction->Addposy(pos_y);
  // fHistoManager->Fill2D(0, pos_x, pos_y);
  fHistoManager->FillHisto(4, pos_z_1_p);
  fHistoManager->Fill3D(0, pos_z_1_p, pos_x_1_p, pos_y_1_p);
}
if (name == "opticalphoton")
{
  if (theprevv->GetName() == "Polyester2")
  {
    if (thepostpv->GetName() == "World" || thepostpv->GetName() == "Det")
    { fHistoManager->Fill2D(0, pos_x, pos_y); fHistoManager->FillHisto(4, pos_z_1_p); }
  }
}
if (name == "triton")
{
  if (theprevv->GetName() == "LiF")
  {
    if (thepostpv->GetName() == "ZnS")
    { fHistoManager->FillHisto(3, pos_z); }
  }
}
if (name == "alpha")
{
    if (theprev->GetName() == "LiF")
    {
        if (thepostv->GetName() == "ZnS")
        {
            fHistoManager->FillHist(2, pos_z);
        }
    }
}
if (name == "opticalphoton")
{
    if (theprev->GetName() == "Polyester2" && thepostv->GetName() == "Det")
    {
        saystep=1;
    }
} //fEventAction->Addposx(pos_x);
//fEventAction->Addposx(saystep);
if (name == "neutron")
{
    if (step->GetTrack()->GetKineticEnergy()<=0.044*eV)
    {
        if (theprev->GetName() == "Mod" && thepostv->GetName() == "Polyester1")
        {
            saystepn=1;
        }
    }
}

G4String namer = atrack->GetVolume()->GetName();
if ((namer == "Det")&&name == "opticalphoton")
    atrack->SetTrackStatus(fStopAndKill);

fEventAction->AddSay(saystep);
fEventAction->AddSayn(saystepn);
// fEventAction->AddSayy(saystepp);

G4double edepStep=0.0;
// G4int trackID;
// G4ParticleDefinition* parDef;

G4double tracklstep=0.0;
//const G4double parDef=0;
//check if we are in scoring volume
//if (volume != fScoringVolume) return;

//Particle id
//if (step->GetTrack()->GetParentID() != 0)
if (name=="alpha"||name=="triton")
{
    edepStep=step->GetTotalEnergyDeposit();
    tracklstep=step->GetTrack()->GetTrackID();
    //charge=step->GetTrack()->GetDefinition()->GetParticleName();
}
G4int ab=0;
if (name=="opticalphoton")
    tracklstep=step->GetStepLength();
if (name == "triton")
{
if (ab->GetTrack()->GetCurrentStepNumber() == 1)
{ saystepp=1.1; }
}
G4cout<<name<<","<<tracklstep<<G4endl;

// collect energy deposited in this step
// G4double edepStep = step->GetTotalEnergyDeposit();
// fEventAction->AddEdep(edepStep);
// fEventAction->AddTrackl(tracklstep);
// fEventAction->AddSayy(saystepp);
} //....oooOO0OOooo........oooOO0OOooo........oooOO0OOooo........oooOO0OOooo......
Appendix E – Additional Figures

Figures to Compare the Pitch and ZnS Thickness

Figure A-0-1 Comparison of the pitch and ZnS thickness for 0.032cm detector
Figures to Compare the Detector Thickness

Figure A-0-2 Figures for comparing detector thickness