Energy Deposition in Polymers

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Todo list

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1 Introduction

A typical day in 2011 saw 932,456 people cross into the U.S. (258,191 by air 48,073 by sea, and 621,874 by land) [2]. In addition there was 64,483 truck, rail and sea containers with 253,821 privately-owned vehicles [2]. As shown in Figure 1 there are numerous entry points into the U.S. that are interconnected by a networks of rail and highways. In the interdiction of special nuclear material it is desirable to detect and seize the material before it enters into this complex network. Radiation Portal Monitors (RPMs) are passive radiation detection systems implemented at over a thousand border crossings, designed to determine if cargo contains any nuclear material in a safe, nondestructive and effective manner[3]. The Department of Homeland Security (DHS) continues to fund research through the Domestic Nuclear Detection Office (DNDO) in order to develop replacement technologies for the current ^{3}He RPMs as ^{3}He cannot be economically replaced. There are several alternatives to ^{3}He being considered and all, with the exception of gas filled proportional detectors involve the detection of neutrons from scintillation events of the energy deposited in the material from the neutron absorption reaction. These detectors (among other requirements outline in Table 1) must be able to effectively discriminate between gamma (which can occur in medical isotopes) and neutrons (which are likely to be a signature of special nuclear material).

Table 1: Replacement Detector Requirements [1]

Parameter	Specification
Absolute neutron detection efficiency	2.5 cps/ng of ^{252}Cf (in specified test configuration)
Intrinsic gamma-neutron detection efficiency	$\epsilon_{int,\gamma n} \leq 10^{-6}$
Gamma absolute rejection ratio for neutrons (GARRn)	$0.9 \leq$ GARRn ≤ 1.1 at 10 mR/h exposure
Cost	\$ 30,000 per system

Neutron detectors often utilize a material doped with an isotope of large thermal cross section for absorption such as ^{6}Li or ^{10}B. When these materials absorb a neutron the nucleus of the isotope becomes unstable and fissions into reaction products. These reaction products (having an initial kinetic energy from the Q-value of the neutron absorption reaction) travel through the material, transferring their kinetic energy to the material. Photon interactions in the detector occur when a photon scatters of a single electron in a Compton scattering event (Table 2). This Compton electron then produces a cascade of secondary electrons in the material, which depending upon the energy may or may not deposit a majority of it's energy in the detector. The difference in the transfer of kinetic energy from charged particle to electrons and from photon interactions (Compton scattering) to electrons introduces an opportunity to exploit the difference in energy deposition in order to maximize the discrimination between neutron and photon interactions in a detector.

Table 2: Maximum Energy of Secondary Electrons from Compton Scattering

	Photon Energy (MeV)	Maximum Compton Energy (MeV)
^{137}Cs	0.662	0.478
^{60}Co	1.17, 1.33	0.960, 1160

This document is organized as follows. A brief overview of the interaction of charged particles in matter will be provided in Section 2, as well as some preliminary experiments demonstrating the range of secondary electrons to aid in neutron-gamma discrimination. The GEANT4 toolkit was used for the modeling of the energy deposition. Section 3 will provide an overview of the GEANT4 toolkit. Section 4 will provide details on how the GEANT4 toolkit was implemented for this particular simulation, as well as providing validation of the calculations preformed by the GEANT4 toolkit in Section 5. In the 6 the results of this model applied to a single film will demonstrate the enhanced ability of neutron-gamma discrimination through secondary electrons.

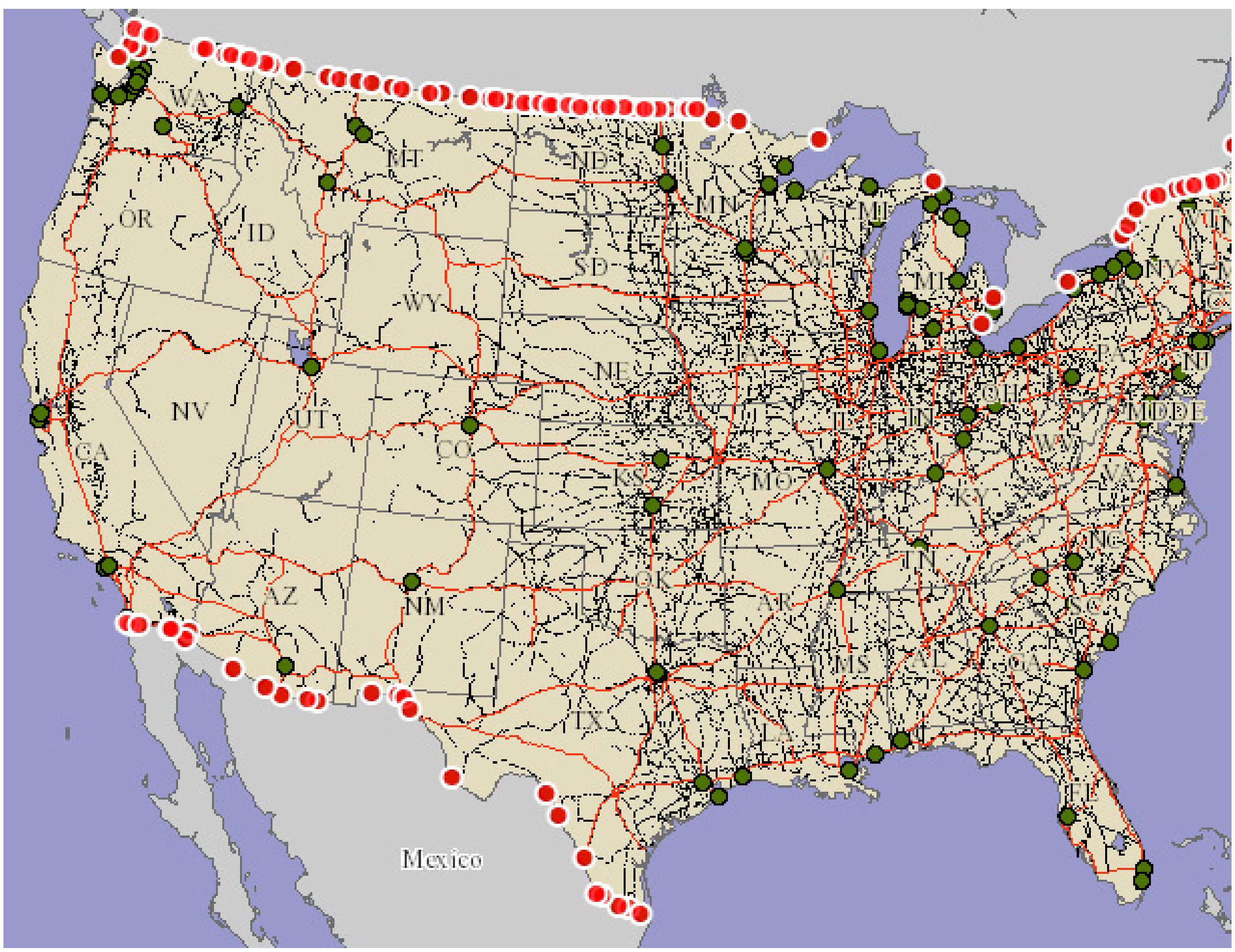


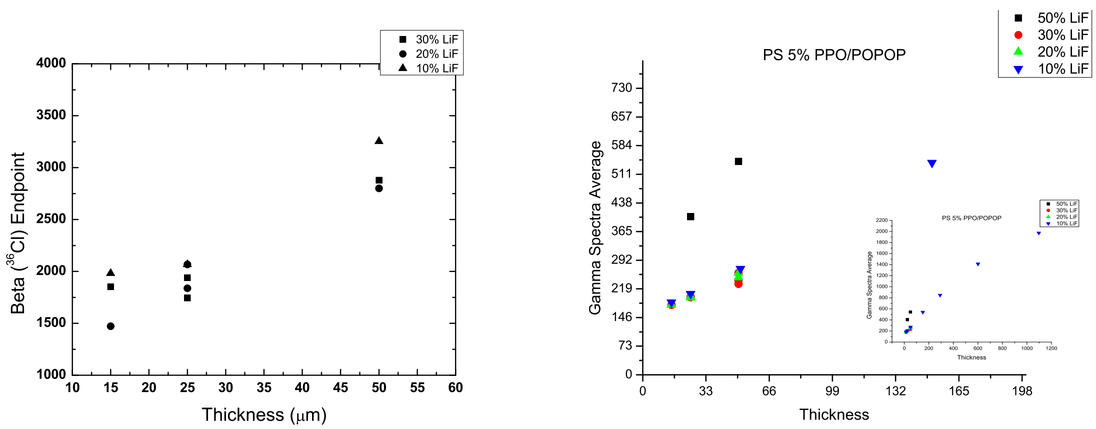
Figure 1: Portal Entry Points into the U.S.

2 Previous Work

Previous work on the energy deposition of thin focused on spectra measurements from fabricated films as wells as single collision energy loss spectra. A sequence of 10% ^{6}LiF, 5% PPOPOPOP films in a PS matrix cast to thickness between 15 and 600 μm where fabricated and the response was measured from a gamma source as well as a neutron source. These experiment results are shown in 2.1.

2.1 Spectra Measurements

Evidence that the secondary electrons contribute to energy loss can be seen in Figure 2 where there is an increase in the endpoint of the spectra as films become thicker. This increase in the spectra endpoint is indicative of the film producing more light, and as the light collection geometry remained constant the increase in the endpoint is attributed to a larger energy deposition in the 50 μm film compared to the 15 μm or 25 μm film. Figure 3 shows the intrinsic efficiency of these film (from spectra obtained from a ^{60}Co



(a) Beta Spectra Endpoints for a 5% PS film

(b) Gamma Spectra Averages for PS films

Figure 2: Spectra properties as a function of film thickness

source). As the film thickness increases the pulse height discriminator at which an intrinsic efficiency of one in a million ($\epsilon_{int,\gamma} \leq 10^{-6}$) is reached also increase. The neutron spectra (shown in the solid lines) does not increase in light yield with increasing thickness, further providing an indication that the thickness of the films can be optimized to maximize the neutron count rates[1] while minimizing the response of the detector to photons.

2.2 Single Collision Energy Loss

Single collision energy loss spectra provide the probability that that a given collision will result in an energy loss of Q. Provided a spectra of secondary electrons from either the Compton scattered electron or the ^{6}Li reaction products it is then possible to determine the average energy loss per collision. A single collision energy loss spectra for water is shown in Figure 4. For low electron energies (< 50 eV) it is very probable that the electron will lose a majority of its energy in a single collision. For higher electron energies, however, the electrons tend to lose a lower fraction of there total energy. A Compton scattered photon, with an energy in the MeV range, will then lose far less energy per collision than an electron (in the low keV range) liberated from the passage of a neutron reaction product through the material. When the average and median energy transfer are plotted as a function of incident electron energy (Figure 5) the difference in the energy loss spectra becomes more apparent. For low energies (up to an incident electron energy of 100 eV) the average and median energy transfer are roughly equal to each other, about half of the incident electron. Past 100 eV

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[1]The neutron count rate is increased with thickness by the increased mass of the detector

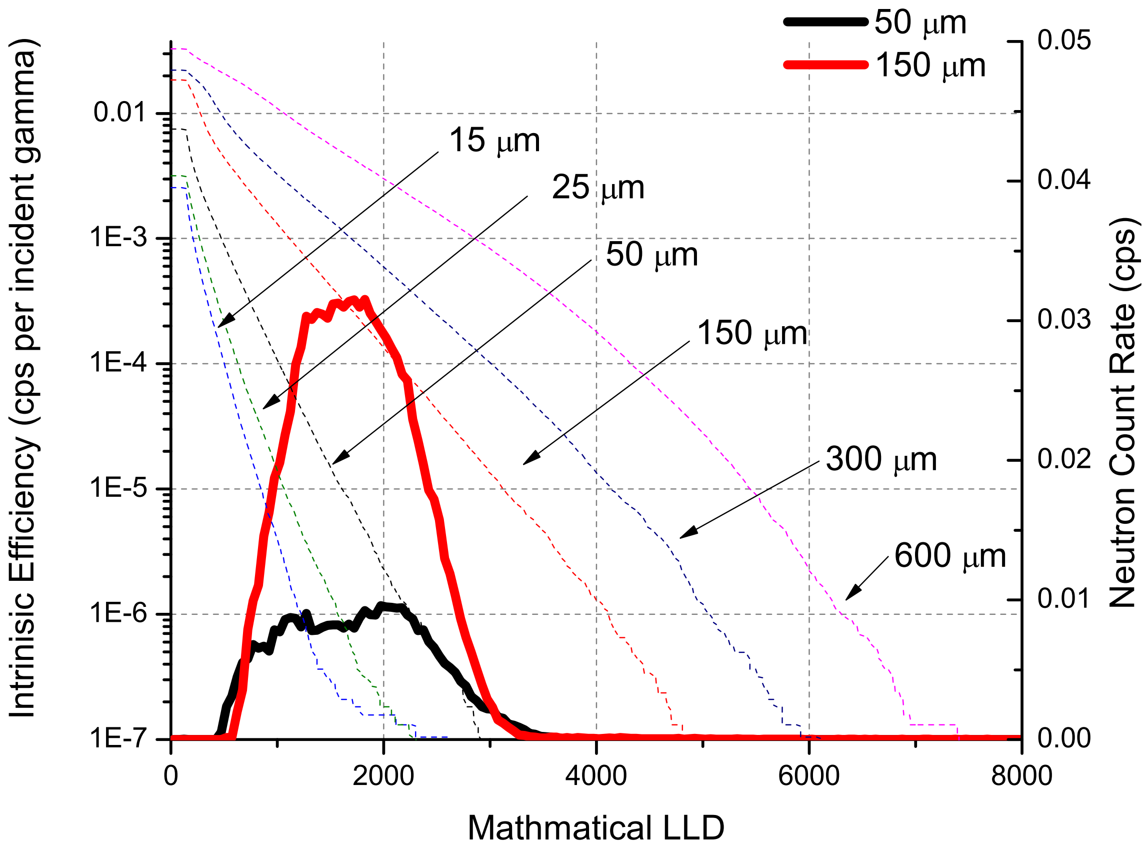


Figure 3: Gamma intrinsic efficiency (dashed lines) plotted against neutron counts (solid)

average energy increases faster than the median energy transfer implying that while a few collisions result in large energy transfers most of the collisions do not. It is also interesting to note that the average and median do not increase linearly with the incident energy past 100 eV (the ordinate axis is a log scale). In fact, the average energy transferred per collision is mostly bounded by 60 eV even for incident electron energies of $\tilde{1}0$ keV. This is significant because it implies that high energy electrons from photon events will deposit a small fraction of their energy in the material.

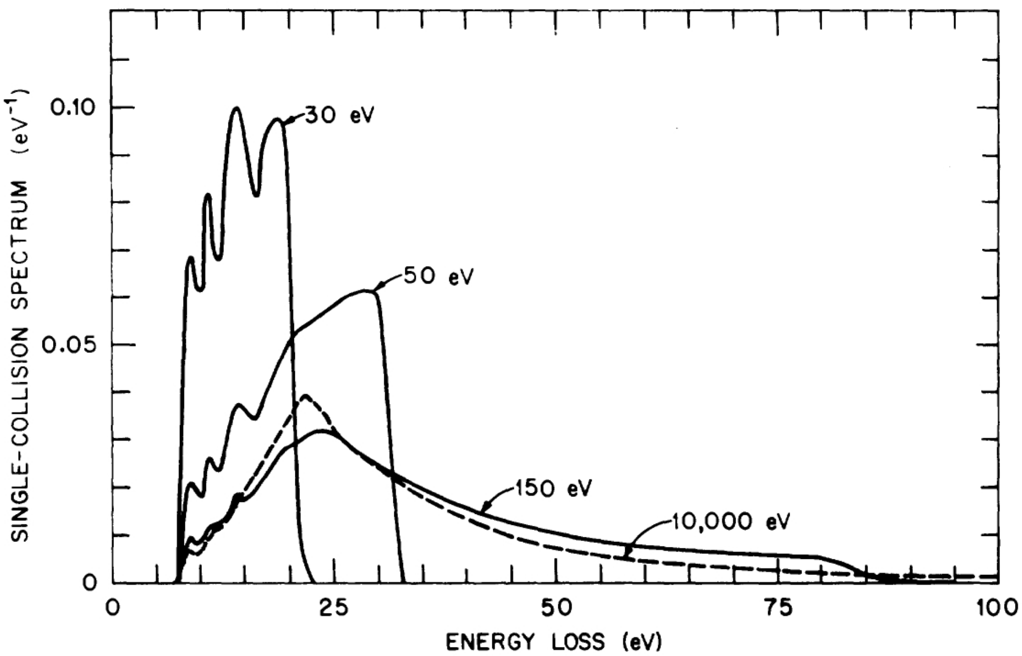


Figure 4: Single-collision energy loss spectra for electrons in water [?]

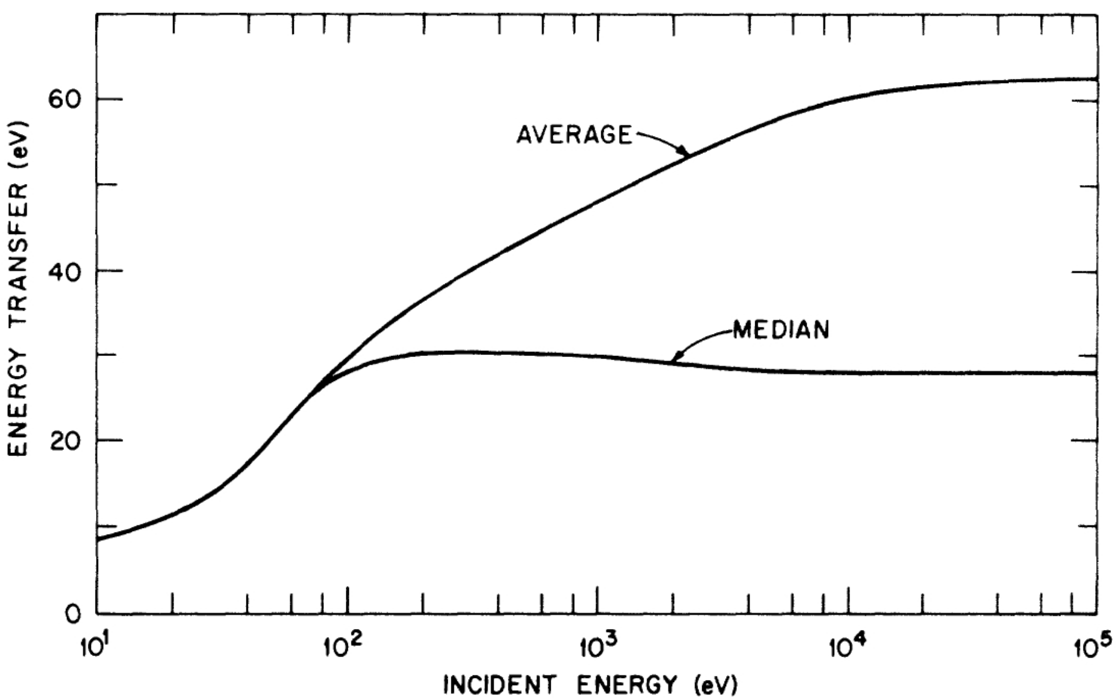


Figure 5: Average and median energy transfer in liquid water as functions of incident-electron energy [?]

3 Introduction to GEANT4

GEANT4 (GEomentry ANd Tracking) is a free, open source Monte Carlo based physics simulation toolkit developed and maintained at CERN widely used in the physics community. A GEANT4 simulation starts with a run which contains a set number of events. An event is particular process of interest to the user, such as shooting a single particle at a detector. Typical usage might be to have a run be firing 1,000 neutrons at a detector, were each neutron is a single event. Each particle transported in GEANT4 is assigned a unique track ID and a parent ID. The particle that initiates the event is given a parent ID of 0 and a track ID of 1. If the parent particle has a collision and produces a secondary particle this secondary particle is then given a parent ID of 1 (corresponding to the first secondary) and a track ID of 2. Secondaries are tracked in GEANT4 utilizing a stack tracking the most recent secondary (and its cascade) first. Listing 1 provides an example from the verbose output of GEANT4 of the tracking in which only secondaries are not shown for the secondaries. The initial particle in the event is the neutron because it has a parent ID of 0. The alpha and triton are the secondaries produced by this collision. The alpha is assigned a parent ID of 1 (corresponding to the first generation) with a track ID of 3. The triton is also assigned a parent ID of 1, but with a track ID of 2.

Listing 1: Tracking Example

```
*********************************************************************************************
* G4Track Information:   Particle = neutron,   Track ID = 1,   Parent ID = 0
*********************************************************************************************

Step#    X(mm)    Y(mm)    Z(mm) KinE(MeV)  dE(MeV) StepLeng TrackLeng  NextVolume ProcName
    0        0        0    -6.59   2.5e-08        0        0         0    Absorber initStep
    1        0        0    -3.64         0        0     2.95      2.95    Absorber NeutronInelastic
    :----- List of 2ndaries - #SpawnInStep=  2(Rest= 0,Along= 0,Post= 2), #SpawnTotal=  2 ---------------
    :          0        0    -3.64      2.73                   triton
    :          0        0    -3.64      2.05                   alpha
    :------------------------------------------------------------------- EndOf2ndaries Info ---------------

*********************************************************************************************
* G4Track Information:   Particle = alpha,   Track ID = 3,   Parent ID = 1
*********************************************************************************************

Step#    X(mm)    Y(mm)    Z(mm) KinE(MeV)  dE(MeV) StepLeng TrackLeng  NextVolume ProcName
    0        0        0    -3.64      2.05        0        0         0    Absorber initStep
    1 -0.000201 0.000128   -3.64      2.01   0.0491 0.000266  0.000266    Absorber ionIoni
    2 -0.00049 0.000312    -3.64      1.93   0.0705 0.000381  0.000647    Absorber ionIoni

*********************************************************************************************
* G4Track Information:   Particle = triton,   Track ID = 2,   Parent ID = 1
*********************************************************************************************

Step#    X(mm)    Y(mm)    Z(mm) KinE(MeV)  dE(MeV) StepLeng TrackLeng  NextVolume ProcName
    0        0        0    -3.64      2.73        0        0         0    Absorber initStep
    1 0.000339 -0.000215   -3.64      2.71   0.0116 0.000447  0.000447    Absorber hIoni
```

3.0.1 Organization of the GEANT4 Toolkit

The GEANT4 toolkit is divided into eight (8) class categories:

- Run and Event - generation of events and secondary particles.
- Tracking and Track - transport of a particle by analyzing the factors limiting the step size and by applying the relevant physics models.
- Geometry and Magnetic Field - the geometrical definition of a detector (including the computation of the distances to solids) as wells as the management of magnetic fields.
- Particle Definition and Matter - definition of particles and matter.
- Hits and Digitization - the creation of hits and their use for digitization in order to model a detectors readout response.
- Visualization - the visualization of a simulation including the solid geometry, trajectories and hits.
- Interface - the interactions between the toolkit and graphical user interfaces and well as external software.

There are then three classes which must be implemented by the user in order use the toolkit. These classes are:

- `G4VuserDetectorConstruction` which defines the geometry of the simulation,
- `G4VUserPhysicsList` which defines the physics of the simulation, and
- `G4VUserPriamryGeneratorAction` which defines the generation of primary events.

Five additional classes are available for further control over the simulation:

- `G4UserRunAction` which allows for user actions

As GEANT4 is a toolkit primarily developed for high energy physics particles are designated according the the `PDG` (Particle Data Group) encoding. In addition, the physics processes are referenced according to the standard model. In the standard model particles are divided into two families, bosons (the force carriers such as photons) and fermions (matter). The fermions consist of both hadrons and leptons. Hadrons are particles composed of quarks which are divided into two classes: baryons (three quarks) and mesons (two quarks). Typical baryons include the neutron and the proton, while an example of a meson is the pion. An example of a lepton is the electron.

4 Methods

4.1 GEANT4 Implemenation

A large focus of this work was on creating a working simulation of the GEANT4 toolkit. Prelimary attemps were made to install GEANT4 on a windows based machine linking to Microscoft Visual Studio. While these attempts were sucessful, a larger scale computing enviroment was desired. GEANT4 was then installed on the University of Tennessee's nuclear engineering computing cluster, along with the necessary visualation drivers and data files. Brief documenation on compiling simple examples on the cluster are aviable at `necluster.engr.utk.edu/wiki/index.php/Geant4`[2]. For convince a subversion repository was created to manage the developed code base, and all source code is available by anonymous checkout from `http://www.murphs-code-repository.googlecode.com/svn/trunk/layeredPolymerTracking`. Revision 360 was the code base used to generate the results shown in 6. The following section provides implemenation specific details of the code base used to simulate the energy deposition in thin films. It is organzied according to the three base classes that a user must implement in GEANT4, namely `G4VUserDetectorConstruciton`, `G4VUserPhysicsList`, and `G4VuserPrimaryGeneratorAction`.

Get URL to work

4.1.1 Detector Geometry

A detector geometry in GEANT4 is made up of a number of volumes. The largest volume is the `world` volume which contains all other volumes in the detector geometry. Each volume (an instance of `G4VPhysicalVolume`) by assigning a position, a pointer to the mother volume and a pointer to its mother volume (or `NULL` if it is the `world` volume). A volume's shape is described by `G4VSolid` which has a shape and the specific values for each dimension. A volume's full properties is described by a logical volume. A `G4LogicalVolume` includes a pointer to the geometrical properties of the volume (the solid) along with physical characteristics including:

- the material of the volume,
- sensitive detectors of the volume and,
- any magnetic fields.

Listing 2 provides the implementation of the world physical volume. The geometry was setup such that it is possible to define multiple layers of detectors, as shown in Figure 6.

Listing 2: World Physical Volume

```
// World
worldS = new G4Box("World",worldSizeXY, worldSizeXY, worldSizeZ*0.5);
worldLV = new G4LogicalVolume(worldS,defaultMaterial,"World");
worldPV = new G4PVPlacement(0,G4ThreeVector(),worldLV,"World",0,false,0,fCheckOverlaps);
```

The detector was described by creating creating a single layer of neutron absorber and gap material and placing it in another volume (the calorimeter). The containing volume (calorimeter) was placed inside of the the physical world (Listing 3).

Listing 3: Calorimeter Volume

```
// Calorimeter (gap material)
caloS = new G4Tubs("Calorimeter",iRadius,oRadius,caloThickness/2,startAngle,spanAngle);
caloLV = new G4LogicalVolume(caloS,gapMaterial,"Calorimeter");
caloPV = new G4PVPlacement(0,G4ThreeVector(),caloLV,"Calorimeter",worldLV,false,0,
    fCheckOverlaps);
```

The `calorimeter` was the mother volume for each layer. The code was developed such that the simulation of multiple layers can be easily set at compile time or by utilizing a run macro through the `DetectorMessenger` class. Multiple repeated volume can be achieved in GEANT4 through `G4PVReplica` or `G4PVParameterised`. As each of the layers had the same geometry, `G4PVReplica` was chosen as the implementation (Listing 4.

[2] It should be noted that this example uses the CMAKE build system (as per the GEANT4 recommendation) but a large majority of the examples still use GNUMake for building. This can be accomplished by adding `source /opt/geant4/geant4-9.5p1/share/Geant4-9.5.1/geant4make/geant4make.sh` to the user's `.bashrc`.

Listing 4: Layer Volume

```
// Layer (Consists of Absorber and Gap)
layerS = new G4Tubs("Layer",iRadius,oRadius,layerThickness/2,startAngle,spanAngle);
layerLV = new G4LogicalVolume(layerS,defaultMaterial,"Layer");
if (nofLayers > 1){
    layerPV = new G4PVReplica("Layer",layerLV,caloLV,kZAxis,nofLayers,layerThickness,-
        caloThickness/2);
}else{
    layerPV = new G4PVPlacement(0,G4ThreeVector(0.0,0.0,0.0),layerLV,"Layer",caloLV,
        false,0,fCheckOverlaps);
}
```

Finally, the neutron absorber and gap material were defined as single cylinders which were then placed in the layer mother volume (Listing 5). The size of these solids (and the materials) could be set either at compile time through `DetectorConstruction` constructor or by using the `DetectorMessenger` in the run macro.

Listing 5: Absorber and Gap Volumes

```
// Absorber
absS = new G4Tubs("Abso",iRadius,oRadius,absThickness/2,startAngle,spanAngle);
absLV = new G4LogicalVolume(absS,absMaterial,"Absorber",0);
absPV = new G4PVPlacement(0,G4ThreeVector(0.0,0.0,-gapThickness/2),absLV,"Absorber",
    layerLV,false,0,fCheckOverlaps);

// Gap
gapS = new G4Tubs("Gap",iRadius,oRadius,gapThickness/2,startAngle,spanAngle);
gapLV = new G4LogicalVolume(gapS,gapMaterial,"Gap",0);
gapPV = new G4PVPlacement(0,G4ThreeVector(0.0,0.0,absThickness/2),gapLV,"Gap",layerLV,
    false,0,fCheckOverlaps);
```

Figure 6 shows a rendering of the 10 layers of the detector with the trajectories from a gamma event.

4.1.2 Physics Lists

The user of the GEANT4 toolkit is responsible for selecting the proper physics processes to model in the `PhysicsList`. This is unlike other transport codes (such as MCNPX) where basic physics are enabled by default and the user only has select the appropriate cards. However, GEANT4 does provide examples of implemented `PhysicsLists` as wells as modular physics lists which provide a way to construct a physics list by combing physics list. Thus, extensive use of `G4ModularPhysicsList` was employed to handle the assigning of the physics processes to each particle in the correct order. The physics lists chosen for this simulation are listed below:

- `G4EmStandardPhysics`
- `G4EmLivermorePhysics`
- `HadronPhysicsQGSP_BERT_HP` Hadronic physics are
- `G4IonPhysics` Finally, to handle the transport of the charged ions resulting from an $^6\mathrm{Li}((n),\alpha)^3\mathrm{H}$ interaction the `G4IonPhysics` list was used.

Listing 6: Implemented Physics List

```
/**
 * PhysicsList
 *
 * Constructs the physics of the simulation
 */
PhysicsList::PhysicsList() : G4VModularPhysicsList() {
    currentDefaultCut   = 10*nm;

    // Adding Physics List
    //RegisterPhysics( new G4EmDNAPhysics());
    RegisterPhysics( new G4EmStandardPhysics());
```

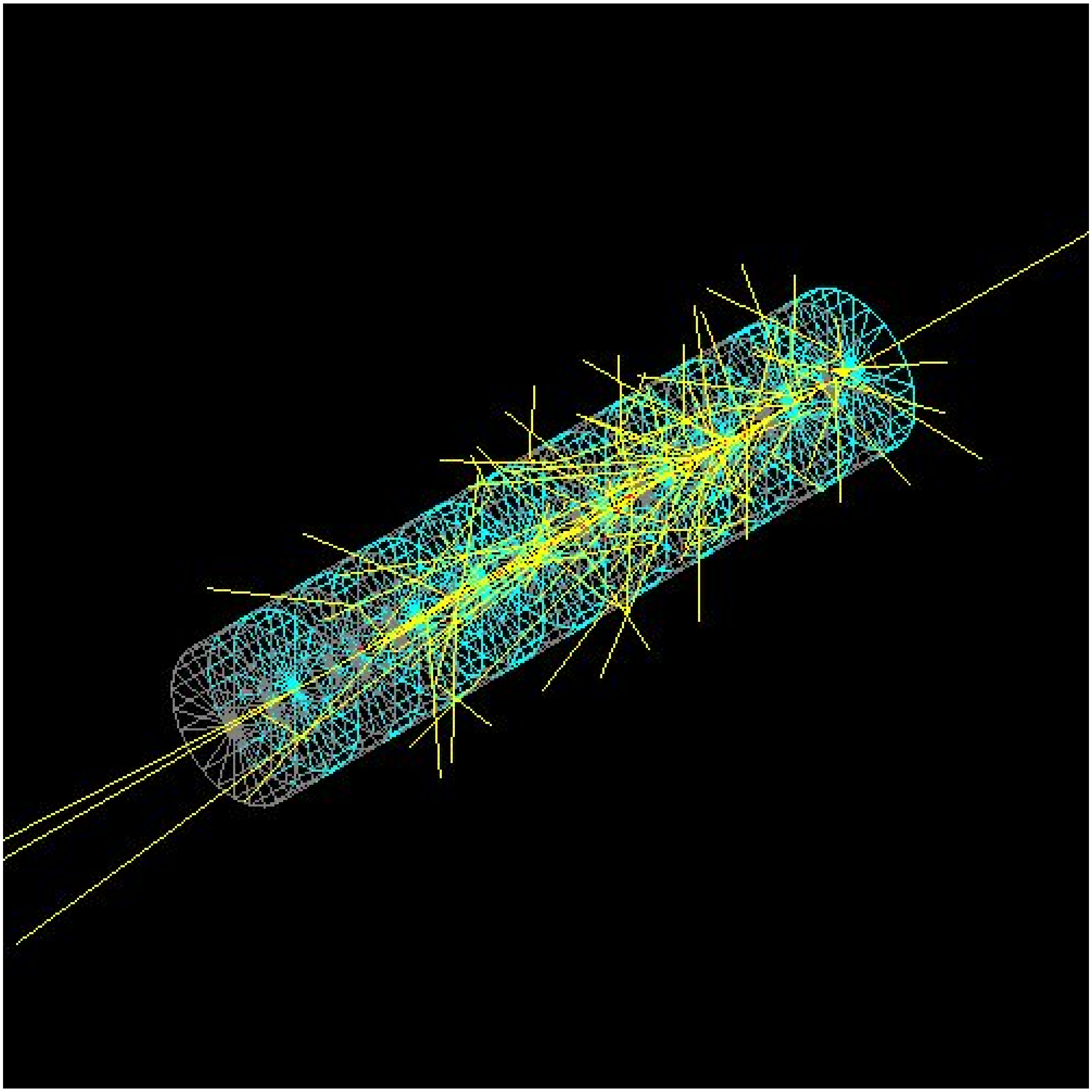


Figure 6: 10 Layer Detector with a simulated gamma event

```
    RegisterPhysics( new G4EmLivermorePhysics());
    RegisterPhysics( new HadronPhysicsQGSP_BERT_HP());
    RegisterPhysics( new G4IonPhysics());
}
```

Finally, the default cut range was decreased from 1 cm to 1 nm in `SetCuts()` (Listing ??)

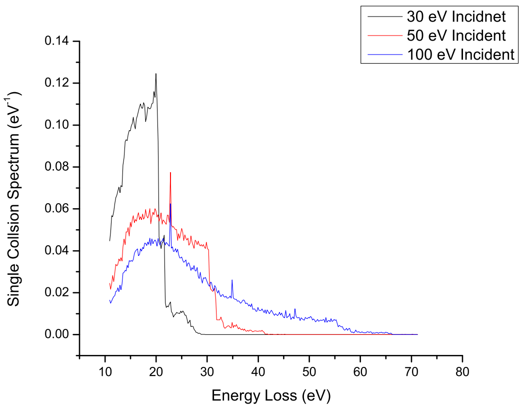
Listing 7: Implemented Physics List

```
}
```

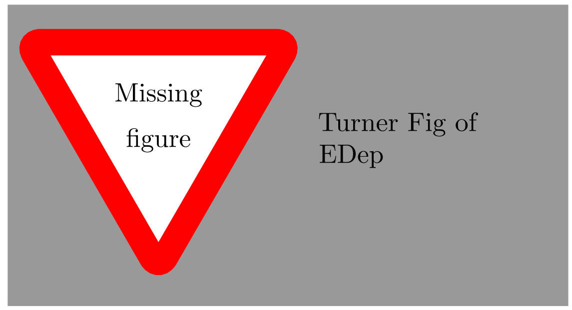
4.2 Determination of Single Collision Energy Loss Spectra

4.3 Determination of Energy Deposition

Figure 7: Single Collision Energy Loss of Water



(a) Simulated



(b) Turner

5 Simulation Validation

5.1 Energy Deposition Validation

The energy deposition was tested by reproducing the single collision energy loss spectra in water[3]. The `PhysicsList` was extended to include `G4DNAPhysics` and the detector material was set to the NIST definition contained in the toolkit with `G4Material* H2O = man->FindOrBuildMaterial("G4_WATER")`. In general there was excellent agreement between the simulated energy spectra and that of [?]. The simulated spectra had much better resolution at fine energies (corresponding to discrete states) of which Turners did not.

5.2 Spectra Validation

The simulation was validated by computing the weighted average of the energy deposition 5.1 and comparing it to the spectra average defined in 5.2.

$$< E >= \frac{\int_0^\infty \phi(E) E dE}{\int_0^\infty \phi(E) dE} \text{where} \tag{5.1}$$

$$< \mu >= \frac{\int_0^\infty f(x) x dx}{\int_0^\infty x(x) dx} \text{where} \tag{5.2}$$

[3] An analysis class was not written for this simulation. Instead the verbosity of the simulation was set to `verbose=1` in the run macro. The first ionisation collision (`e-_G4DNAIonisation`) was then extracted with `sed -n '/ParentID = 0/,/e-_G4DNAIonisation/p' G4OutputFileName.txt` `grep` and `awk` were then used to extract the actual energy, `| grep "e-\_G4DNAIonisatioin" | awk '${print $5}'`

Figure 8: Gamma Simulation Agreement

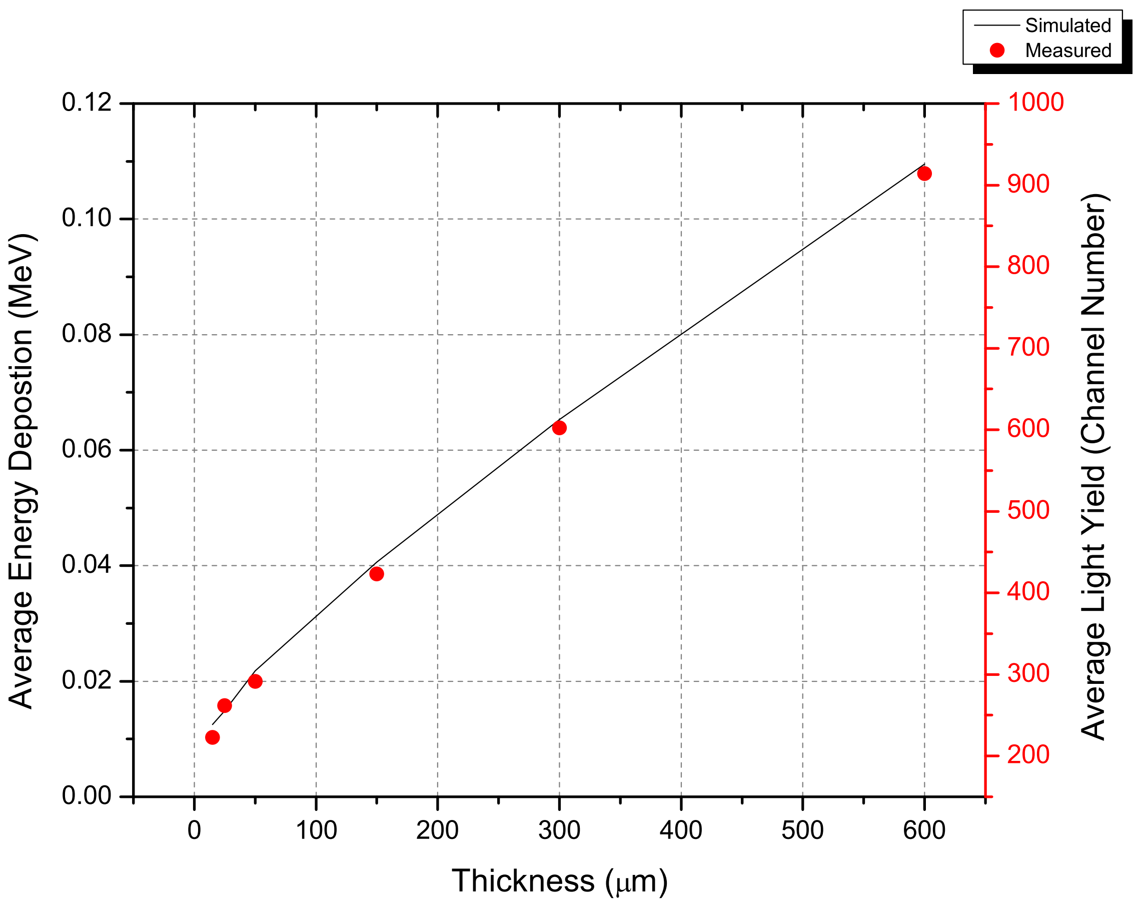
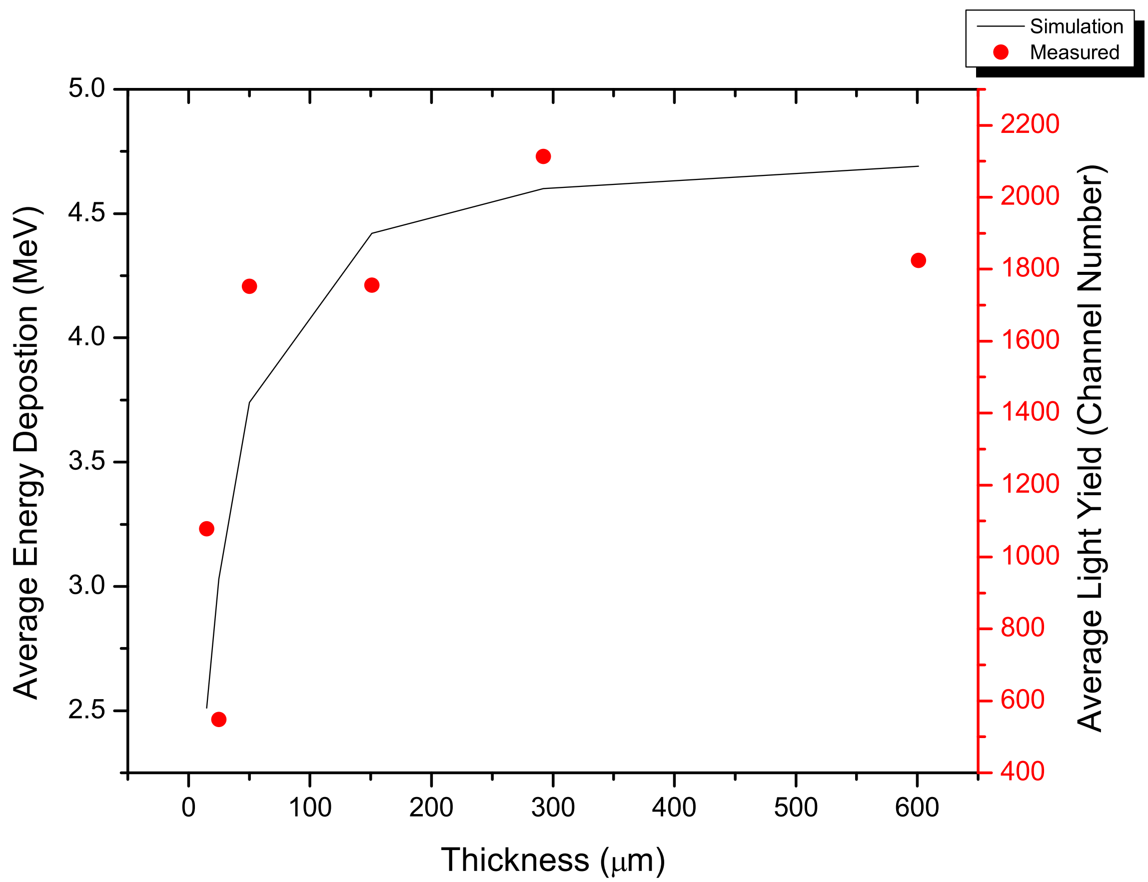


Figure 9: Neutron Simulation Agreement



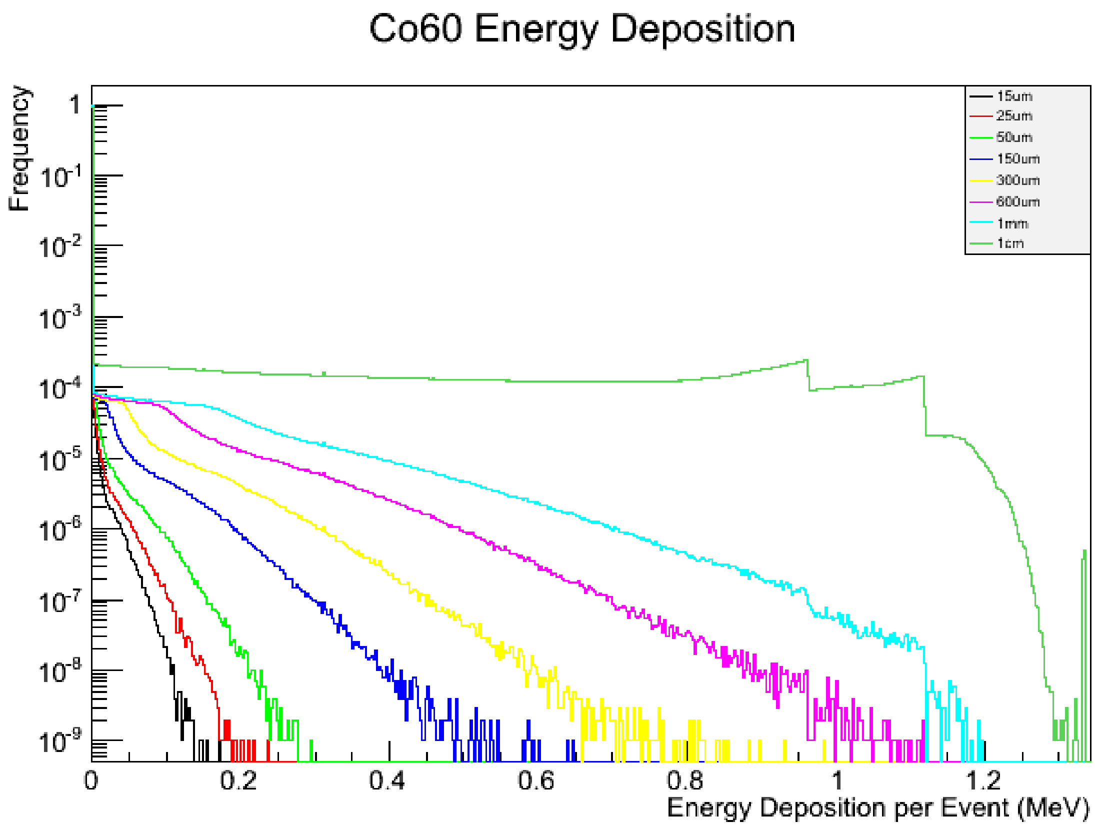


Figure 10: Simulated Energy Depositon for a Single Film (gammas)

6 Results

Write Results Section

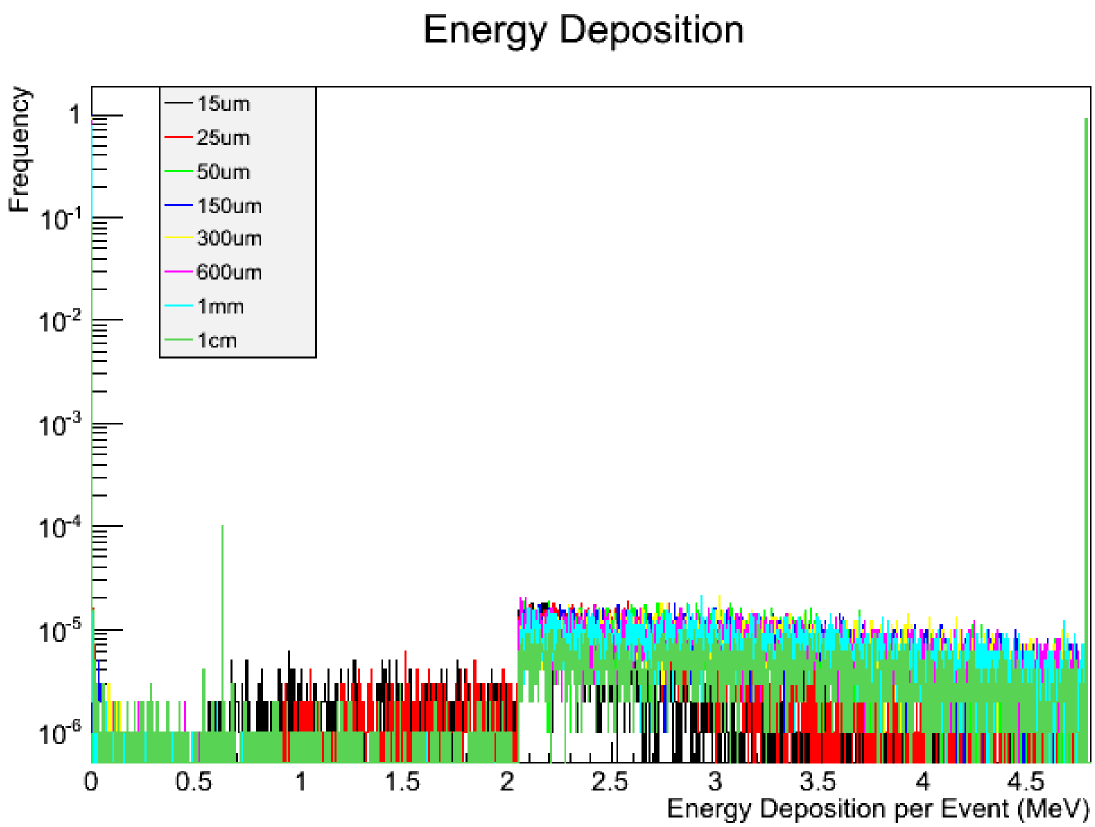


Figure 11: Simulated Energy Depositon for a Single Film (neutrons)

References

[1] R. Kouzes, J. Ely, A. Lintereur, and D. Stephens, "Neutron detector gamma insenstivity criteria," *PNNL 18903*, 1999.

[2] CPB, "On a typical day in fiscl year 2011 CBP." http://www.cbp.gov/xp/cgov/about/, 2012.

[3] R. T. Kouzes, J. H. Ely, L. E. Erikson, W. J. Kernan, A. T. Lintereur, E. R. Siciliano, D. L. Stephens, D. C. Stromswold, R. M. Van Ginhoven, and M. L. Woodring, "Neutron detection alternatives to 3He for national security applications," *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, vol. 623, pp. 1035–1045, Nov. 2010.

.1 GEANT4 Implementation

Visible light in GEANT4 is known as an optical photon. An optical photon has momentum ($\vec{p} = \hbar\vec{k}$), corresponding to the energy and direction of the photon, as well as a polarization ($\vec{e}$). The GEANT4 toolkit breaks up light transport into two parts; the creation of the optical photon an the transport of the optical photon through the material. Each of these are material dependent properties which need to be supplied by the user. This done by creating a material properties table G4MaterialPropertyTable, of which the following properties are available:

- `RINDEX`
- `ABSLENGTH`

.1.1 Scintillation Process

The number of optical photons generated by GEANT4 is proportional to the energy lost during the step, determining the energy from the empirical emission spectra of the material. In GEANT4 this is accomplished by creating a `G4Scintillation` process.[4]

```
#include "G4Scintillation.hh"

G4Scintillation* theScintProcess = new G4Scintillation("Scintillation");

theScintProcess->SetTrackSecondariesFirst(true);
theScintProcess->SetScintillationYield(7500.0/MeV);
theScintProcess->SetResolutionScale(1.0);
theScintProcess->SetScintillationTime(45.*ns);
```

.1.2 Optical Photon Transport

There are three classes of optical photon interactions in GEANT4:

- Refraction and reflection
- Bulk Absorption
- Rayleigh scattering

Of these only refraction and reflection are necessary. [?]

[?]

[4] As the scintillation properties are attached to the process and not the material GEANT4 is incapable of more than one scintillation material in any given application.