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Automated Parametric Optimization of a High-Purity Germanium Monte Carlo Neutral-Particle Model (December 2017)

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*Abstract*—One Hundred fiftey – 250 words

*Index Terms*—Enter key words or phrases in alphabetical order, separated by commas. For a list of suggested keywords, send a blank e-mail to [keywords@ieee.org](mailto:keywords@ieee.org) or visit <http://www.ieee.org/organizations/pubs/ani_prod/keywrd98.txt>

# INTRODUCTION

G

amma-ray spectroscopy using high-purity germanium (HPGe) detectors is a leading method for obtaining high-energy resolution spectra in both the laboratory setting and in the field. These detectors have the ability to obtain energy resolutions as low as 0.15 keV for the Full-Width-Half-Maximum (FWHM), at incident photons around 5.9 keV. [1] The tradeoff for such high energy resolution, is an overall lower detection efficiency compared to other types of nuclear instrumentals, such as sodium iodide NaI scinitllators. The advancement of radiation transport codes, such as Monte Carlo Neutral-Particle (MCNP), allows researchers to accurately model the detection response of HPGe detectors at various geometries, source energies, and environments. Radiation transport modeling provides insight to potential anomalies that could occur during an experiment, and enables the user to intelligently modify experiments which could improve results, conserve resources, and ensure safety requirements are followed. Unfortunately, creating a detector MCNP model that accurately represents reality can be difficult and time consuming, and so by applying a systematic or computational approach the process can be streamlined. Rather than manually performing trial-and-error adjustments to match experimental data, the development of an automated parametric optimization code will simplify the enhancement of a rudimentary HPGe detector model. Ideally, an optimized HPGe MCNP model should accurately predict the detection efficiency curves at various source positions, which can then be applied to developing an adjoint flux model representing the detection efficiency over all space.

# Problem Description

The development of an MCNP model that accurately resembles a detectors experimental response is not an elementary task. Factors to consider when modeling are: the type and position of the radiation source, the properties, both geometrical and compositional of the detector being modeled, and the characteristics of primary and secondary incident radiation. Published literature has stated relative differences between the experimental and Monte Carlo simulated full-energy peak absolute efficiencies for HPGe detectors have reached as low as 0.2%. [2] There has also been studies showing discrepancies between the manufacturer-provided detector specifications of internal components compared to measured values, such as the crystal length and dead layers. [3]

Experimental measurements of gamma-ray emissions using a standard Canberra p-type HPGe detector were provided by Lieutenant Colonel Buckley O’Day using a multi-nuclide source. The multi-nuclide source covered photon energies ranging from 0.06 to 1.836 MeV, which allowed for a full representation of the absolute efficiency curve. The numerical values listed for the energies in Table 1 follow the rounding format listed on the source specifications sheet provided by Eckert & Ziegler Isotope Products for consistency, and the documentation also states the source uncertainty to be 3.1% for each energy.

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| TABLE 1  Multi-nuclide Source Information | | | |
| Gamma-Ray Energy [keV] | Nuclide | Activity [µCi] | Gammas per Second |
| 60 | Am-241 | 0.02941 | 391.7 |
| 88 | Cd-109 | 0.2707 | 363.6 |
| 122 | Co-57 | 0.01019 | 322.7 |
| 159 | Te-123 | 0.01403 | 436.1 |
| 320 | Cr-51 | 0.3389 | 1236 |
| 392 | Sn-113 | 0.05109 | 1227 |
| 514 | Sr-85 | 0.06171 | 2247 |
| 662 | Cs-137 | 0.04325 | 1362 |
| 898 | Y-88 | 0.09633 | 3347 |
| 1173 | Co-60 | 0.05101 | 1885 |
| 1333 | Co-60 | 0.05101 | 1887 |
| 1836 | Y-88 | 0.09622 | 3539 |

A labeled diagram of the various source positions with respect to the HPGe detector are shown in Figure 2. At each position, a 24-hour count was performed to minimize uncertainty. For positon 1, the source was placed centered on the Al casing, position 2 was resting on the front face and flush with the edge of the casing, position 3 was centered 7 cm above the front face, position 4 was placed 3 cm down the side of the casing, and positon 5 was offset 13 cm above the detector.

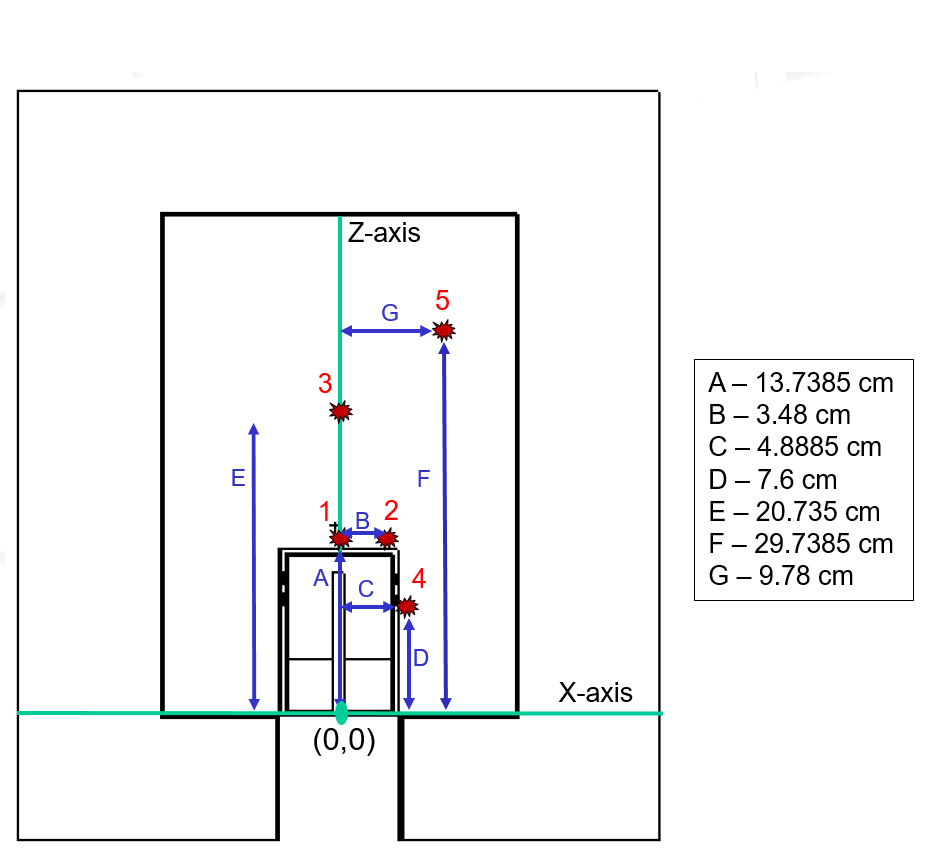


Fig. 1. Experimental setup diagram, displaying each source position on a Cartesian coordinate system, where the origin is centered at the base of the Al casing of the detector

A plot of the spectra, and the calculated absolute efficiencies as a function energy were also provided by Lt Col O’day, for comparison with the simulated results. The absolute efficiency was calculated using equation 1.

Equation 1

Where Nc is the total number of counts under the full-energy peak, Ag is the amount of gammas emitted per second which is listed in column 4 of Table 1, multiplied by the live time, tl (seconds). And the source decay is accounted for by multiplying the denominator by the decay exponential where t1/2 is the half-life (seconds), and td (seconds) is the age of the source.

# Description of Work

First, an HPGe detector model was created using MCNP, and then an optimization code was produced in Python. After the model was optimized: Efficiency curves were plotted for a quantitative analysis, and then ADVANTG weight windows were implemented to generate the adjoint flux response for a qualitative representation of the results.

## HPGe MCNP Model

The MCNP model was designed based off the manufacturer provided detector diagram labeling various dimensions, and materials. Unfortunately, some dimensions were not labeled, including information about the internal contact pin, gap widths between the Ge crystal and the inner Al holder, and the insulation materials. For higher energy photons, these features are not as important, but for the lower energies, attenuation is more probable to occur which might affect the results. Knowing that the overall goal of the generic MCNP model was to have easily adjustable parameters, the decision was made to only use right circular cylinders (RCC) and planes. This would allow the model to be very generic, and simple where the only adjustments needed would be to raise or lower heights, and widen or compress widths. The final design of the generic HPGe MCNP model, generated in VisEd can be seen in Figure 2.

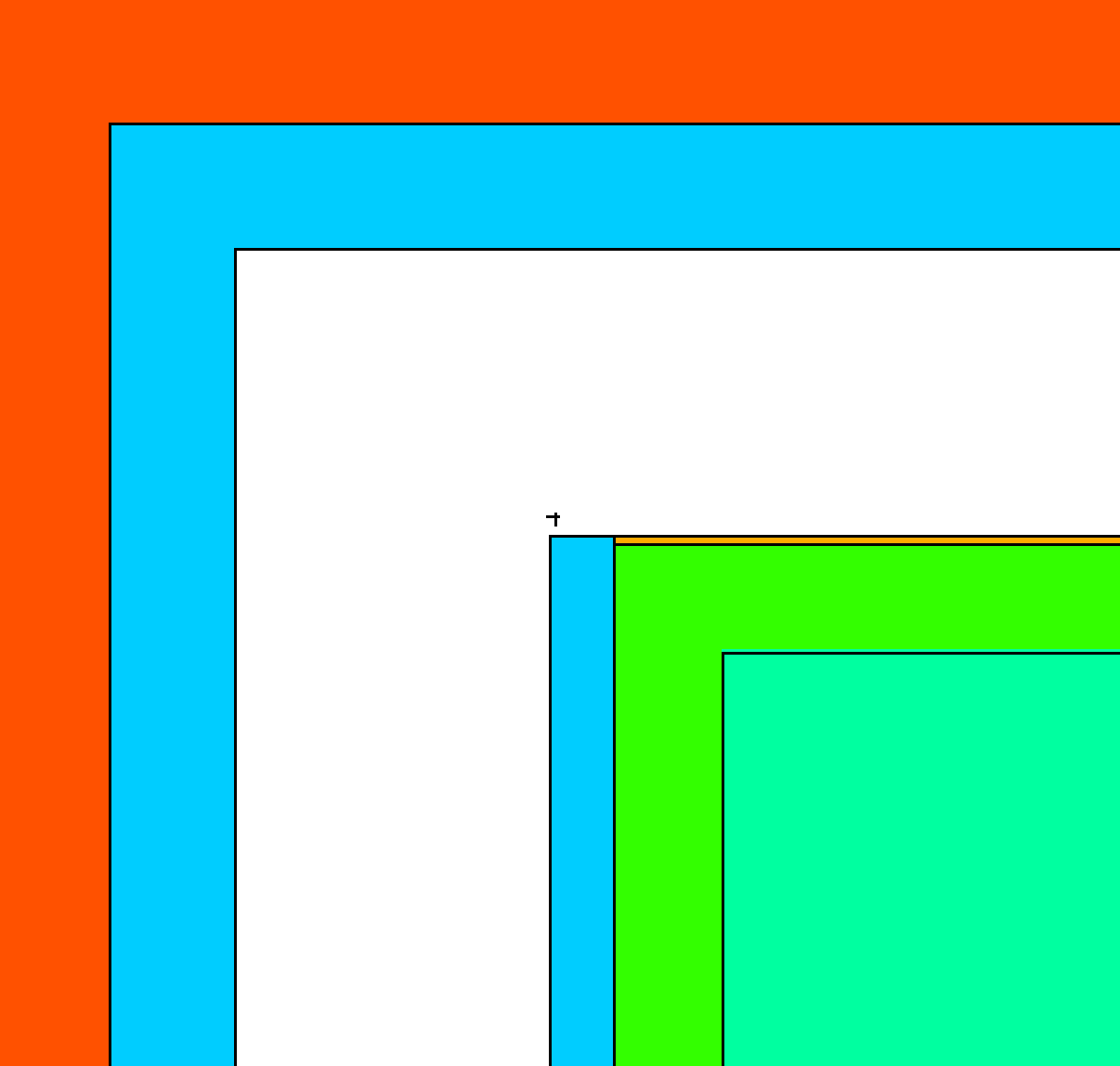
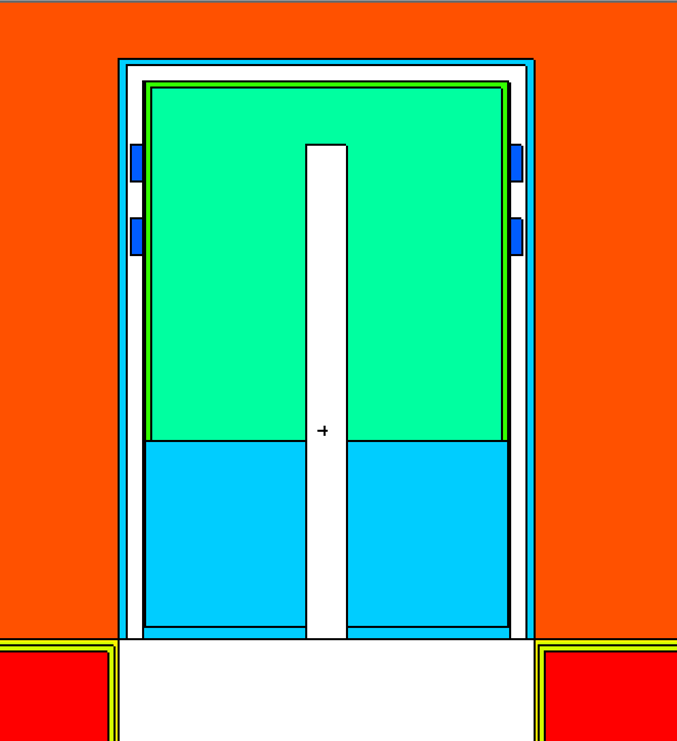


Fig. 2. Generic HPGe Model, displayed using VisEd. A zoomed in view of the top edge of the Ge crystal is shown, where the IR window is placed on top of the outer deadlayer, flush with the top of the Al holder.

Air

Al Casing

Vacuum

IR Window

Ge Crystal

Outer Deadlayer

Al Holder

Air

Metal Clasps

Inner Deadlayer

The IR window placed directly on top of the top deadlayer is composed of a thin 0.01016 cm Kapton tape window and a 0.000847 cm Al Mylar layer. Both the Ge crystal top edges, and the top of the inner coaxial were assumed to be squared, rather than rounded, the manufacture did not specify these features. In the left image of Figure 2, the outer deadlayer can be seen, and it was assumed to be a lithium drifted surface. The inner deadlayer contact, was assumed to be boron implanted contact. Neither of these materials were explicitly stated in the detector schematic, and the compositional assumptions were based on previous knowledge of p-type HPGe detectors. [1] The materials used for other components in the MCNP model were standard for HPGe detectors, and a full list can be found in Table 4. All material composition data was found in Los Alamos National Laboratory’s (LANL) ACE Data Tables or Pacific North Western National Laboratory’s (PNNL) Compendium of Material Composition Data for Radiation Transport Modeling. [4] [5] The cross-sectional data library used was mcplib84 (.84p), for photon transport and which was composed of 278 energy groups.

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| TABLE 2  MCNP Material Compositions | | |
| Material | Density [g/cm3] | Component(s) |
| Mylar | 1.38 | IR Window |
| Brass | 8.41 | Metal Clasps |
| Aluminum | 2.7 | Detector Housing and Casing |
| Germanium | 5.32 | Ge Crystal |
| Lithium | 0.534 | Outer Deadlayer |
| Boron | 2.73 | Inner Deadlayer |
| Copper | 8.96 | Shield Lining |
| Tin | 7.31 | Shield Lining |
| Kapton Film | 1.42 | IR Window |
| Air | 0.001224 | Shielding Chamber |
| Lead | 11.34 | Shielding |
| Acrylic Glass | 1.19 | Source Encapsulation |
| Vacuum | --- | Coaxial Space |

The Data Block of the MCNP model also consisted of information about the photon transport, physics, tallies and the source definition. Only photons were tracked in the simulation, because only the absolute efficiency was desired. And so a full energy spectrum that accounts for secondary radiation was not required, and the Gaussian Energy Broadening Card (GEB) was not utilized. The default Physic Card settings were used where Bremsstrahlung, coherent scattering, and photo-fission were ignored. The source card created an isotropic point source that emitted 12 discrete photon energies, each with the same probability distribution, actual energies are displayed in Table 1. The F8, energy deposition, tally was used to track each particle’s interaction with the Ge crystal, and 106 source particles were used to reduce uncertainties.

After the model was created, research into which parameters have the largest effect on an HPGe detection efficiency was performed, and it was found that: The deadlayers, entrance windows, and the Ge crystal length and radius played the largest role in photon attenuation. [2] Understanding that lower energy photons will be more affected by attenuating layers between the source and physical Ge crystal, and that higher energy photon interactions depend more on the length and radius of the crystal, a list of parameters that were optimized can be found in Table 3.

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| TABLE 3  HPGE MCNP Model Parameters to Optimize | | | |
| Parameter | Initial Value | Lower Bound | Upper Bound |
| Outer Top Deadlayer [cm] | 0.13 | 0.013 | 0.73899333 |
| Outer Sides Deadlayer [cm] | 0.13 | 0.03 | 0.23 |
| Ge Crystal Length [cm] | 8.32 | 7.474993997 | 9.165002 |
| Kapton Window [cm] | 0.01016 | 0.00516 | 0.11016 |
| Inner Top Coaxial Deadlayer [cm] | 3.00E-05 | 5.67E-06 | 0.00013 |
| Inner Sides Coaxial Deadlayer [cm] | 3.00E-05 | 1.00E-05 | 1.00E-04 |
| Top Al Casing Thickness [cm] | 0.15 | 0.05 | 0.25 |
| Sides Al Casing Thickness [cm] | 0.15 | 0.05 | 0.25 |
| Ge Crystal Density [g/cm] | 5.32 | 5.29 | 5.32 |

## Automated Parametric Optimization Code

Describe how/what/all details about the code and what it does. Along with Chi-square, etc. ( Try and match my equation 1 format, but I can always edit it, just use the equation editor to start) OR TYPE you section on a separate word doc, and I can copy and paste it in.

# Results

What are the optimal parameters at each source position?ficiency plots/total relative difference

Fig. 3. Experimental

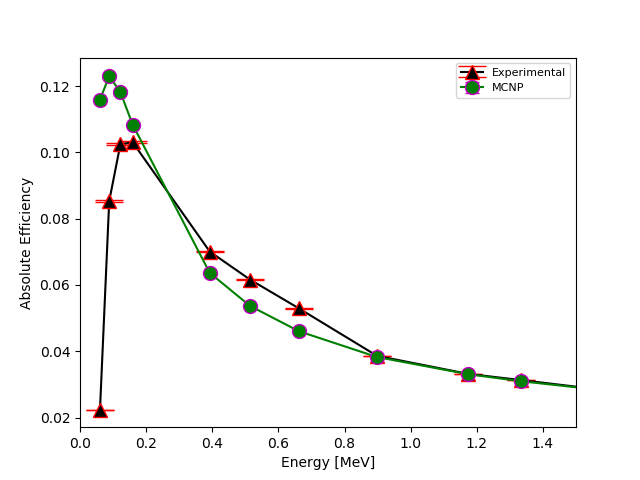


Fig. 4. Experimental

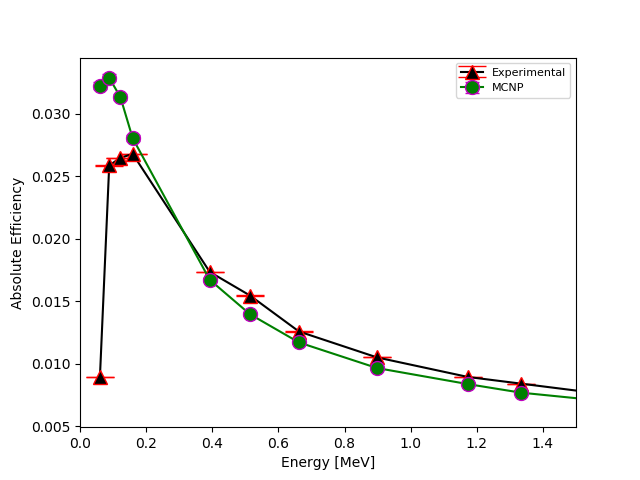


Fig. 5. Experimental

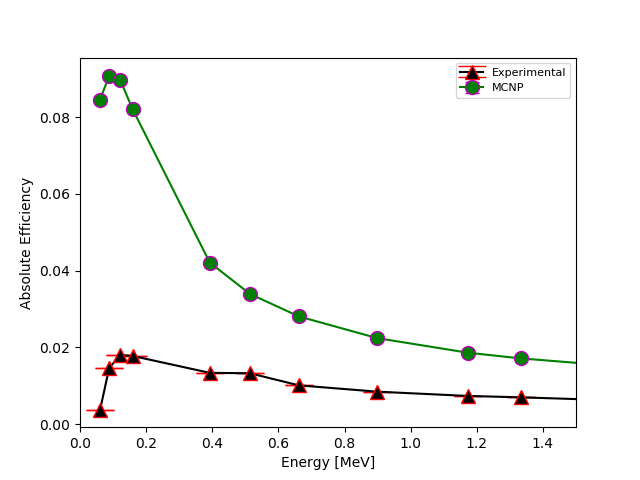


Fig. 6. Experimental

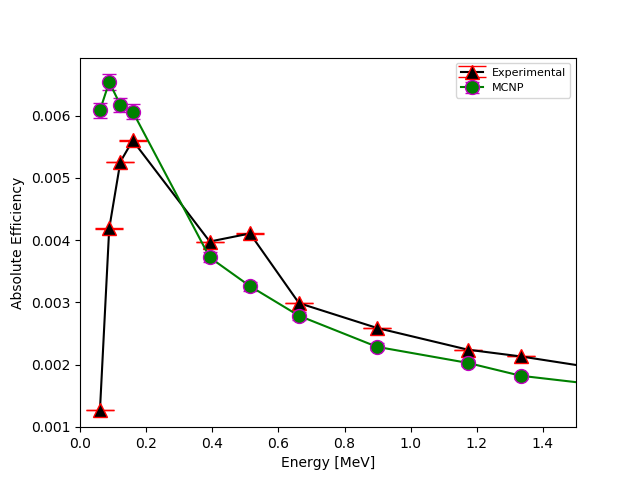


Fig. 7. Experimental

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| --- | --- | --- | --- | --- | --- | --- |
| TABLE 4  Optimized Detector Parameters | | | | | | |
| Parameter | Initial Value | Position: | | | | |
| 1 | 2 | 3 | 4 | 5 |
| Outer Top Deadlayer [cm] | 0.13 | 0.7389 | 0.7389 | 0.7389 | 0.7389 | 0.7389 |
| Outer Sides Deadlayer [cm] | 0.13 | 0.23 | 0.23 | 0.23 | 1.35 | 0.23 |
| Ge Crystal Length [cm] | 8.32 | 7.6627 | 7.4749 | 7.4749 | 7.4749 | 7.4749 |
| Kapton Window [cm] | 0.01016 | 0.1101 | 0.1101 | 0.1101 | 0.0576 | 0.1101 |
| Inner Top Coaxial Deadlayer [cm] | 0.00003 | 0.0001 | 6E-05 | 6E-05 | 0.0001 | 6E-05 |
| Inner Sides Coaxial Deadlayer [cm] | 0.00003 | 2E-05 | 6E-05 | 7E-05 | 0.001 | 7E-05 |
| Top Al Casing Thickness [cm] | 0.15 | 0.25 | 0.25 | 0.25 | 0.05 | 0.25 |
| Sides Al Casing Thickness [cm] | 0.15 | 0.05 | 0.05 | 0.05 | 0.27 | 0.25 |
| Ge Crystal Density [g/cm3] | 5.32 | 5.32 | 5.32 | 5.35 | 5.32 | 5.3425 |

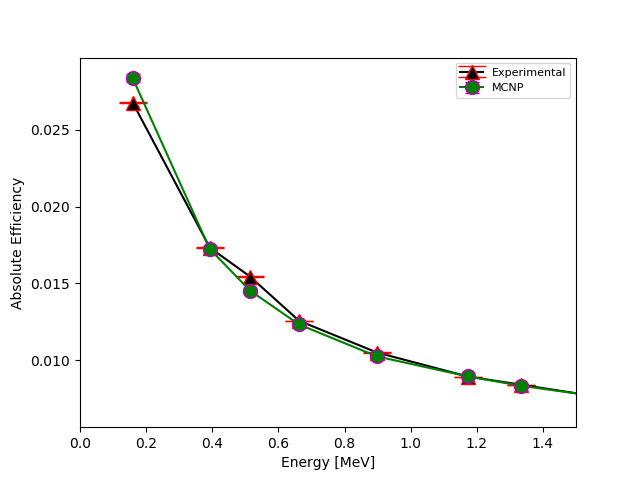


Fig. 8. Experimental

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| --- | --- | --- | --- |
| TABLE 5  Optimized Detector Parameters for Position 3 | | | |
| Parameter | Initial Value | Position | |
| 3 | 3 Adjusted |
| Outer Top Deadlayer [cm] | 0.13 | 0.73899 | 0.97535 |
| Outer Sides Deadlayer [cm] | 0.13 | 0.23 | 0.13 |
| Ge Crystal Length [cm] | 8.32 | 7.47499 | 8.60166 |
| Kapton Window [cm] | 0.01016 | 0.11016 | 0.13016 |
| Inner Top Coaxial Deadlayer [cm] | 0.00003 | 6E-05 | 50E-05 |
| Inner Sides Coaxial Deadlayer [cm] | 0.00003 | 7E-05 | 5E-05 |
| Top Al Casing Thickness [cm] | 0.15 | 0.25 | 0.18333 |
| Sides Al Casing Thickness [cm] | 0.15 | 0.05 | 0.25 |
| Ge Crystal Density [g/cm3] | 5.32 | 5.35 | 5.35 |

# Conclusion

## What do your findings mean? How does that relate to the goal you laid out in the introduction?

Appendix

Appendixes, if needed, appear before the acknowledgment.

Acknowledgment

We are grateful for the inspiration and mentorship of Captain James Bevins (AFIT/ENP), whom taught NENG 685 during the fall 2018 Quarter at the Air Force Institute of Technology (AFIT). We are appreciative of Lt Col O’Day (AFIT/ENP) for providing experimental data, and Mr. Will Kable (LLNL) and Capt Bevins for providing a template HPGe MCNP model.

# References

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| [5] | C. G. R. P. R. R. R. W. I. R. M. Jr, "Compendium of Material Composition Data for Radiation Transport Modeling," Pacific North Western National Laboratory, Richland, WA, 2011. |

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