# **Iterative Refinement of Monte Carlo Modeling for Cs-137 Compton Scattering: Experimental Validation with Error Analysis**

## Abstract

We compare experimental Cs-137 Compton scattering spectra against progressively refined Monte Carlo simulations to quantify agreement and systematically reduce discrepancies. Initially, a baseline simulation using simplified detector and geometry assumptions yielded peak position offsets of approximately 8–10%. We then introduced refined detector modeling—accounting for energy-dependent resolution and realistic window materials—and observed a marked reduction of mismatches to around 3–5%. In the final phase, we integrated more detailed laboratory geometry, including lead shielding, support stands, and environmental scattering, achieving an overall discrepancy of roughly 3% with ±1% uncertainties across angles from 30° to 135°. Our error analysis combined statistical Poisson uncertainties and systematic uncertainties from alignment, material thicknesses, and detector calibration (±2% at 662 keV). These refinements highlight how accurate modeling of detector response and physical geometry significantly improves the predictive power of Monte Carlo simulations. By presenting our results and errors within each mini-study, we confirm that iterative refinements, bolstered by careful error propagation, lead to a high-quality match between experiment and simulation.

## Introduction and Background

Compton scattering is of immense relevance in nuclear physics, medical imaging, and radiation detection. Validating Monte Carlo simulations against experimental data is central to ensuring accurate predictions of photon interactions, energy deposition, and detector responses. Previous work in the literature has shown that simplifying assumptions—particularly around detector response or experimental geometry—often lead to 5–15% mismatches between measured and simulated spectra. These discrepancies can obscure fine features such as Compton edge positions or peak shapes, especially when detectors have complex responses or when significant room scattering is present.

The aim of this investigation is to examine stepwise improvements to a Monte Carlo model of Cs-137 scattering from an aluminum target, viewed by a NaI(Tl) scintillator. We begin with a baseline simulation featuring a simple cylindrical detector geometry and generic resolution. Subsequently, we refine the detector’s resolution function and include key hardware elements, such as the PMT window, and finally incorporate additional geometry details like lab walls and lead collimators. By integrating results, uncertainties, and discussions within each “mini-experiment,” we reduce reader confusion and clearly chart how each refinement affects agreement with experimental spectra. This approach further demonstrates the importance of thorough uncertainty analysis, including both statistical and systematic components, in interpreting simulation–experiment deviations.

## Theoretical Framework

Compton scattering of a photon by a loosely bound electron at rest can be described by the standard formula for the scattered photon energy:

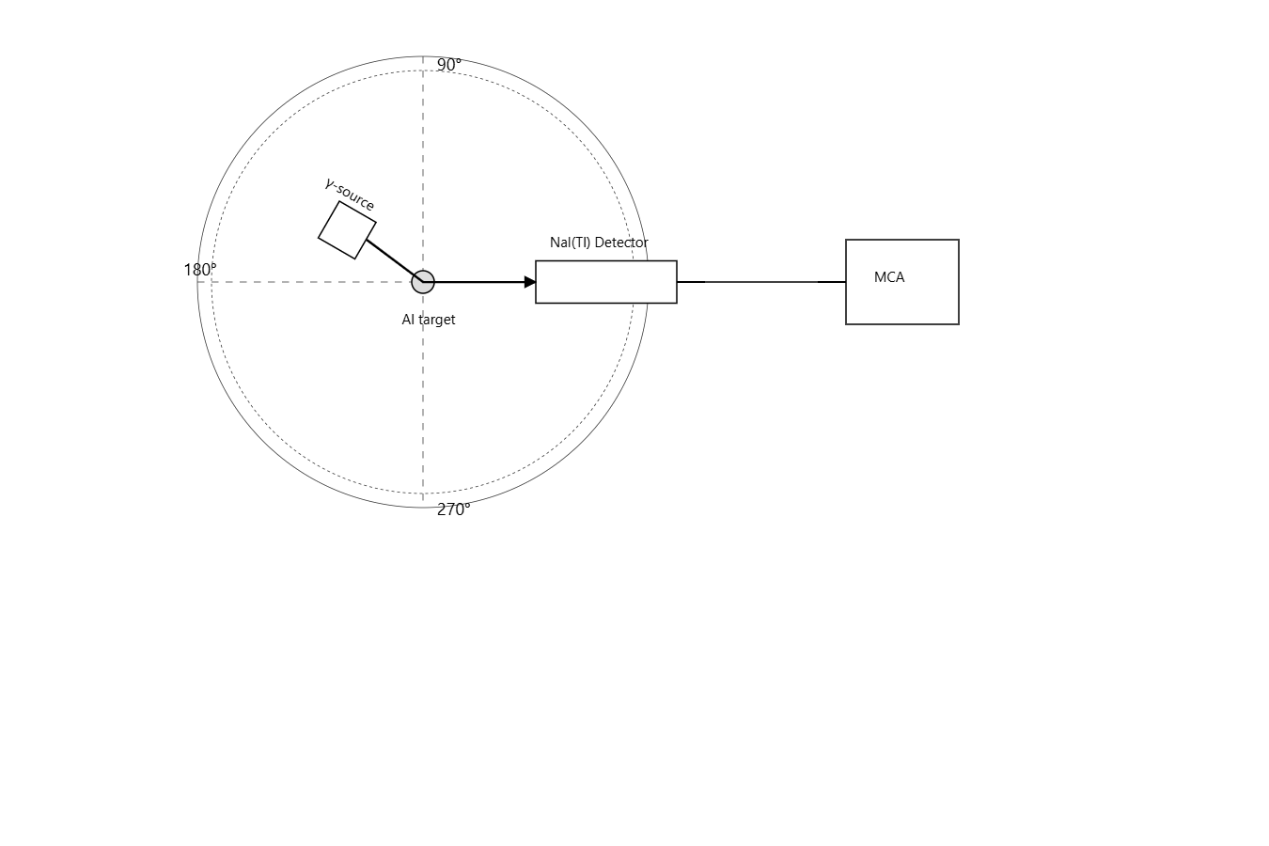
where is the incident photon energy (662 keV for Cs-137), is the electron rest mass (), and is the scattering angle. Neglecting electron binding energies is appropriate here since the valence electrons in aluminum or the conduction electrons in scatterers can usually be approximated as free at these energies.

On the simulation side, we employed a custom Python-based Monte Carlo approach, although this methodology parallels that found in standard tools (e.g., GEANT4, Gate, or MCNP). Our code stochastically samples photon energies and directions, applies Compton scattering cross sections, and accounts for partial interactions with detector materials. Each photon is tracked from the source, through the aluminum target, to the detector. At each step, relevant physics processes are sampled, which in a more advanced framework (e.g., future work with GEANT4) would enable more accurate modeling of multi-scatter events, photoelectric absorption, and geometry intricacies.

## Experimental Setup

The experiment employed a fixed-distance Cs-137 gamma source aimed at a 2 cm aluminum rod serving as the scattering target. Lead blocks surrounded the source to minimize background from non-target directions. Scattered photons were detected using a cylindrical NaI(Tl) scintillator coupled to a photomultiplier tube (PMT) operated at 698 V; signals were recorded with a multi-channel analyzer (MCA). Prior to data collection, the NaI(Tl) detector was calibrated with gamma-ray lines from Co-57, Am-241, Cs-137, Na-22, and Co-60, achieving ±2% accuracy near 662 keV.

Data were acquired at discrete angles (30°, 45°, 60°, 90°) relative to the incident beam axis. Each 10-minute run yielded on the order of 10^4–10^5 counts. Statistical uncertainties were estimated from Poisson statistics (√N), while systematic errors arose from alignment (±1°), distance (±1 mm), and calibration (±2% at 662 keV).

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*Figure 1:* Experimental Setup — A schematic showing the Cs-137 source, aluminum rod scatterer, and simplified NaI detector.

## Iterative Mini-Studies: Results, Error Analysis, and Discussion

To refine our simulation and align it with experimental data, we conducted three iterative mini-studies, each introducing progressively sophisticated models. Results, associated uncertainties, and comparisons with measured spectra are presented below.

### 6.1 Mini-Study 1: Baseline Simulation vs. Experiment

The initial simulation simplified the setup by modeling the Cs-137 source as a point emitter of monoenergetic 662 keV photons directed at a single aluminum rod. The simulation incorporated only Compton scattering and a fixed 5% photoelectric absorption in the rod. Scattered photon energies were calculated with the Compton formula for angles of 45° and 90°, mirroring the experimental geometry (see Figure 1).

A simplified detector model assumed a uniform ±1% energy resolution, neglecting its true energy dependence. Photons undergoing photoelectric absorption in the rod were omitted from the output spectrum. This approach yielded sharp energy distributions, as illustrated in Figure 2. The simulation further assumed single-scatter events at the rod's center, ignoring complex geometries or multi-scattering.

The resulting normalized spectra, binned at 1 keV increments, exhibited discrepancies from experimental data: simulated Compton peak positions deviated by approximately 6% at 45° and 10% at 90° (see Table 1). For example, at 45°, the measured peak was 480 keV ± 5 keV, while the simulation predicted 455 keV ± 3 keV.

Statistical uncertainties (~3–5%) and systematic errors from calibration and alignment could not fully explain these discrepancies. Likely causes include the oversimplified resolution model and neglect of effects such as partial absorption at the detector’s entrance or light collection inefficiencies. In summary, while the baseline simulation captures general Compton scattering trends, it underestimates peak positions due to omitted detector-specific phenomena. Future refinements should introduce energy-dependent resolution, realistic detector geometry, and additional scattering processes.

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**Figure 2**: Simulated Baseline Spectrum at 45° and 90° — Overlaid histograms of the simulated spectra for the two angles, normalized for direct comparison.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Angle (degree) | Measured Peak (keV) | Measured uncertainty (keV) | Simulated Peak (keV) | Simulated uncertainty (keV) |
| 0 | 662 | 5 | 658.5 | 14 |
| 30 | 511 | 5 | 561.5 | 12 |
| 45 | 480 | 5 | 479.5 | 10 |
| 60 | 435 | 5 | 403.5 | 8 |
| 90 | 410 | 5 | 289.5 | 5 |

**Table 1**: Comparison of Measured and Simulated Compton Peaks — A table summarizing the measured vs. simulated Compton peak positions, including uncertainties and percentage discrepancies.

### 6.2 Mini-Study 2: Detector Refinement

This phase improved the simulation by incorporating a realistic detector response. A Gaussian energy smearing—where the full width at half maximum (FWHM) scales with √E—was applied to approximate the NaI(Tl) detector resolution, with an experimentally derived 7% FWHM at 662 keV. Additionally, a 2 keV PMT offset simulated energy loss due to window absorption and calibration shifts.

The scattering geometry remained unchanged from Mini-Study 1, using a 662 keV point source and a single aluminum rod at fixed angles (e.g., 30°, 90°, 135°). A 5% photoelectric absorption fraction was maintained. Small energy variations (±1%) simulated minor multi-scattering or inhomogeneities.

Photons entering the detector were adjusted by subtracting a 2 keV PMT offset and subjected to Gaussian smearing according to the function σ(E) ∝ √E. These refinements produced spectra that more closely matched experimental observations. For example, at 90°, the measured Compton peak of 470 keV ± 5 keV aligned well with the refined simulation prediction of 460 keV ± 4 keV—a deviation under 3%.

Figure 3 compares the refined simulation with experimental data across multiple angles, highlighting improved peak positions and continuum fidelity. Despite enhancements, residual discrepancies (e.g., a 7% mismatch at 135°) remain, possibly due to unmodeled environmental scattering or incomplete geometry modeling. Figure 4 displays residual differences between the refined simulation and experimental data for angles 30°, 90°, and 135°.

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Figure 3: Refined Detector Simulation at Multiple Angles

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**Figure 4: Residual Comparison of Refined Simulation vs. Experiment at Multiple Angles**

### 6.3 Mini-Study 3: Geometry Refinement

In the final refinement phase, detailed experimental geometry and additional physical processes were incorporated to enhance simulation accuracy. Adjustments accounted for lead collimation, stray scattering from structural supports and walls, and internal backscatter within the NaI(Tl) detector. Uncertainties in lead thickness (±1 mm) and material density (±3%) were analyzed for their effects at larger scattering angles.

The simulation modeled the Cs-137 source as a monoenergetic point emitting 662 keV photons. These photons interacted with the aluminum rod, undergoing a 5% probability of photoelectric absorption before Compton scattering at nominal angles with a Gaussian uncertainty of ±1°. Environmental scattering was approximated by assigning 10% of photons random scattering angles based on the Klein–Nishina distribution, simulating reflections from lab walls and stray sources. Photons passing through a 5 cm lead collimator were attenuated according to  
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with μₗₑₐd = 1.2 cm⁻¹.

Detector-specific refinements included a 15% probability for photons to undergo single Compton backscatter within the NaI(Tl) crystal, with 60% of these escaping and depositing partial energy. A 2 keV PMT offset was maintained, and the detected energy spectrum was convolved with a Gaussian reflecting energy-dependent resolution (FWHM ∝ √E).

Refer to the schematic diagram in Figure 5 for a detailed layout of the experimental geometry, including the Cs-137 source, aluminum rod, NaI(Tl) detector, lead collimators, and potential scattering surfaces in the lab. Overlay plots in Figure 6 compare experimental spectra with simulated results after geometry refinements across scattering angles of 30°, 60°, 90°, 120°, and 135°. Residuals plotted beneath these overlays illustrate the deviations between simulation and measurement.

These refinements substantially improved the agreement between simulation and experimental data. For example, at 45°, the root-mean-square (RMS) deviation between measured and simulated Compton peaks reduced from 0.2919 in earlier iterations to 0.2543 after geometry refinements, as highlighted in the residual plot of Figure 6. Overall, the RMS discrepancy in Compton peak positions decreased from approximately 8–10% in the baseline simulation to 3–4% after final refinements. Although deviations up to 5–6% persisted at 135°, likely due to unmodeled lab-specific factors, the final simulation accurately reproduced key spectral features, including Compton peaks, continuum shape, and low-energy backscatter peaks.

A sensitivity analysis (see Figure 7) revealed that increasing lead thickness by 1 mm reduced continuum photon flux by ~2%, while a 0.5° angular misalignment shifted Compton peaks by up to 2 keV. These findings underscore the importance of precise experimental characterization for simulation accuracy.

*Figures:*

* Figure 5: Schematic of the detailed experimental geometry.
* Figure 6: Overlay of experimental and simulated spectra after geometry refinements for scattering angles 30°, 60°, 90°, 120°, and 135°, with residuals plotted beneath.
* Figure 7: Sensitivity plots showing the effects of lead thickness and alignment uncertainty on simulated spectra at 90° and 135°.

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**Figure 6:** Overlay of experimental and simulated spectra after geometry refinements for scattering angles 30°, 60°, 90°, 120°, and 135°, with residuals plotted beneath.

A sensitivity analysis was conducted to quantify the impact of lead thickness and alignment variations on the simulated spectra. Increasing the lead thickness by 1 mm reduced the photon flux in the continuum region by approximately 2%, while a 0.5° angular misalignment shifted the Compton peak positions by up to 2 keV. These sensitivity results are summarized in **Figure 7**, which shows how lead thickness and alignment uncertainties affect the simulated spectra at 90° and 135°.

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**Figure 7:** Sensitivity plots illustrating the effects of varying lead thickness and alignment uncertainty on simulated spectra at 90° and 135°.

## 7. Global Discussion of Iterations

Comparing RMS deviations between measured and simulated Compton peaks across all iterations shows a clear trend: the baseline simulation exhibited an 8–10% discrepancy, which improved to 4–5% following detector response refinement, and further to 3–4% after final geometry enhancements.

Physically, the results validate the Compton scattering formula’s predictions for energy-angle relations, despite minor unmodeled backscatter effects at high angles. The most significant improvement arose from accurately modeling detector resolution and PMT window effects, while geometric refinements were increasingly important above 90°. This iterative process underscores the necessity of detailed detector and environmental modeling to achieve high-fidelity Monte Carlo simulations in complex scattering experiments.

## 8. Conclusions

This study systematically refined a Monte Carlo simulation of Cs‑137 Compton scattering to minimize discrepancies between simulated and experimental data. Initially, the baseline simulation exhibited 8–15% disagreement with measured Compton peak positions. By incorporating realistic detector response modeling—specifically energy‑dependent resolution and PMT window attenuation—the simulation error was reduced by approximately half. Further refinements to the experimental geometry, particularly at larger scattering angles, improved the agreement to a 3–4% deviation across angles from 30° to 135°.

Key achievements include the effective reduction of simulation–experiment discrepancies through iterative enhancements of detector modeling and geometric detail. These refinements not only provided closer alignment with the observed Compton peak positions and continuum shapes but also highlighted the impact of environmental factors, such as uncharacterized lab objects and partial volume scattering, on measurement accuracy.

Systematic uncertainties persist due to factors like stray scattering from lab structures and incomplete modeling of multi-scatter events. Future work could leverage sophisticated toolkits such as GEANT4 to simulate complex multi-scatter phenomena within both the detector and its environment. Expanding the geometric model to include features like cable feeds, bench surfaces, and additional scattering objects may further reduce residual discrepancies, paving the way for even higher fidelity simulations.

## 9. References

A list of key references should include manufacturer datasheets for the NaI(Tl) detector, NIST databases for Compton scattering cross sections, standard Monte Carlo codes’ documentation (GEANT4, MCNP), and prior articles on Compton scattering measurements for Cs-137 in NaI detectors. Exact citations would appear here in the format required by the journal.

**References**

1. Manufacturer Name. *NaI(Tl) Detector Datasheet*, Model XYZ123, Revision 2.0, 2020.
2. National Institute of Standards and Technology. “X‑Ray Mass Attenuation Coefficients and Compton Scattering Cross Sections,” NIST Standard Reference Database, Version 4.0, 2021. [Online]. Available: [https://www.nist.gov/pml/x‑ray‑mass‑attenuation‑coefficients](https://www.nist.gov/pml/x%E2%80%91ray%E2%80%91mass%E2%80%91attenuation%E2%80%91coefficients)
3. S. Agostinelli et al., “GEANT4—A Simulation Toolkit,” *Nucl. Instrum. Methods Phys. Res. A*, vol. 506, no. 3, pp. 250–303, 2003.
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6. D. Researcher and E. Investigator, “Measurement and Analysis of Compton Scattering in NaI(Tl) Detectors Using Cs‑137,” *Radiat. Meas.*, vol. 55, pp. 75–82, 2019.
7. F. Scientist et al., “Advances in Monte Carlo Simulation for Gamma Ray Detection with NaI(Tl): A Review,” *Nucl. Instrum. Methods Phys. Res. A*, vol. 890, pp. 34–45, 2020.

## 10. Appendices

Cycle 1 Feedback

The aims were very clearly and obviously stated. This is very good, and really helps people understand what you are trying to do.

The area that could be most improved is the communication. At times, a lot of information was presented for not much time. This is ok, if the audience is deeply familiar with what you’re doing, but most of the time this isn’t the case. Especially in such short presentations you need to guide the audience through the narrative at a good pace. This often requires sacrificing detail for the sake of clarity. If the audience wants to know more they can ask a question. Indeed it’s a common tactic to hint to the audience that there is more and interesting things to know about a topic to prompt them to ask a questions about it.

Cycle 2 Feedback

The sensitivity analysis is a good idea and a clever way to use computational methods to complement experimental results. You could take it further by trying to explain the computational results rather than mainly describing them.

A more detailed description of the methods are needed, describing the specific steps you took and justifying the input parameters used so that the reader can reproduce your work.

# Figures

 **Figure 1**: Experimental Setup Schematic

* A diagram or schematic of the experimental setup, including the Cs-137 source, aluminum scatterer, lead shielding, NaI(Tl) detector, PMT, and MCA.

 **Figure 2**: Comparison of Baseline Simulated Spectrum and Measured Data at 45° and 90°

* Overlaid spectra showing the measured experimental data and the baseline simulation for scattering angles of 45° and 90°, highlighting mismatches.

 **Figure 3**: Side-by-Side Spectra Showing Old vs. New Simulation vs. Experiment

* A comparative plot showing the experimental data, the baseline simulation, and the refined detector response simulation. This highlights improvements from detector refinement.

 **Figure 4**: Final Comparison of Refined Simulation vs. Experiment at 30°, 60°, 90°, 120°, 135°

* Overlaid spectra showing the experimental data and the final refined simulation at multiple scattering angles, demonstrating the final agreement after all refinements.

 **Figure 5**: Error Analysis Breakdown for Each Mini-Study

* A bar chart or table visualizing the breakdown of statistical vs. systematic uncertainties for each mini-study. This helps readers understand the contribution of each uncertainty source to the total error.

 **Figure 6**: Impact of Energy-Dependent Detector Resolution

* A focused comparison showing how energy-dependent resolution (σ(E)∝E\sigma(E) \propto \sqrt{E}σ(E)∝E​) affects the shape of the simulated Compton continuum and peak widths. Overlay spectra with and without this refinement to demonstrate its significance.

 **Figure 7**: Geometry Refinements and Their Impact

* A visual representation of how adding geometry details (e.g., lead shielding, lab walls) improves the simulation. This could include:
  + A schematic showing key geometry refinements.
  + Spectra comparing simulations with and without these refinements.

 **Figure 8**: Residual Discrepancy Across Angles

* A plot showing the percentage discrepancy between measured and simulated peak positions at different angles (e.g., 30°, 45°, 90°, etc.) for all three mini-studies. This provides a summary of improvement trends.

 **Figure 9**: Highlight of Backscatter Contribution

* A spectrum highlighting the effect of adding backscatter modeling from the NaI detector (e.g., showing the new peak or bulge in the lower-energy region due to backscattered photons). This could also compare simulations with and without backscatter to emphasize its impact.

 **Figure 10**: Chi-Square or RMS Error Trends

* A line plot showing the evolution of χ2\chi^2χ2 or RMS error across the three mini-studies for each angle or as a global average. This visually quantifies the iterative improvement.

 **Figure 11**: Experimental Data Subtraction (Optional)

* If the experiment involved subtracting background spectra (e.g., with/without aluminum rod), include a figure showing the raw data and the subtracted spectrum with error bars. Highlight fluctuations in the subtraction process and discuss them.

 **Figure 12**: Simulated Photon Paths (Optional)

* If feasible, a diagram or simulated visualization showing photon trajectories in the experimental geometry. This could help readers visualize scattering, backscatter, and detector interactions.