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Comprehensive Modeling of High-Energy Gamma Spectrum using MCNP PTRAC

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1. Introduction

Recent advancements in spatially resolved Prompt Gamma-ray Activation Analysis (PGAA) have significantly influenced the methodologies for gamma ray detection and analysis. Contemporary approaches often involve collimating either the incident neutron beam or the emitted gamma rays [1]. Such a procedure typically necessitates the scanning of the sample or the collimator. Recently, notable advancements have been achieved through the use of pixelated CdZnTe (CZT) detectors for Compton imaging [2]. Utilizing this methodology, researchers have successfully analyzed the 2.2 MeV prompt gamma rays emitted from hydrogen, allowing for a 3D reconstruction of the sample. While Compton cameras traditionally operate within the 250 keV to 3 MeV energy range, the unique demands of Prompt Gamma Imaging (PGI) analyses favor high-energy evaluations to minimize background interference. This shift underscores the necessity to assess the efficiency of Compton imaging across different energy scales and compare it with conventional collimator-based PGI.

Monte Carlo N-Particle (MCNP) simulations, coupled with its PTRAC function, serve as valuable tools in these evaluations. PTRAC enables selective extraction of particle history information, which demands subsequent data processing. As energy levels ascend, the likelihood of pair production becomes predominant, complicating modeling the energy spectrum using the simulated PTRAC data. This study aims to bridge this complexity by presenting a method to process PTRAC output data, effectively capturing the Compton imaging efficiency at high energies. A crucial component of this research is the assessment of the unity between the energy spectrum derived from PTRAC data and the results from the F8 tally.

2. Materials and Methods

2.1 MCNP Simulation Setup

Our MCNP simulations modeled the geometry based on the commercially available H3D's M400 model, representing a single CZT crystal measuring 4.4 cm x 4.4 cm x 0.5 cm. The unique configuration of the H3D enables precise 3D reconstruction of gamma-ray interaction locations within an individual cell, enhancing the energy resolution and facilitating effective Compton imaging. Assuming a practical scenario, the gamma-ray source was positioned 13 cm above the detector, designed to emit single photons isotropically with an energy of 1 or 8 MeV. To ensure the comprehensive capture of particle interactions and reactions, we activated the PTRAC function in its default mode, logging every particle and its associated reactions. To validate the accuracy and integrity of our findings, the energy spectrum, derived from PTRAC outputs, was cross-checked using the F8 tally, subdividing the energy evaluations into precise units of 1 keV for a detailed assessment.

2.2 PTRAC Output Processing

Upon completing the MCNP simulations, the generated PTRAC output files provided a detailed record of individual particle histories, encapsulating every interaction and event throughout the simulation. Python was employed for processing this extensive dataset, as illustrated in Figure 1, which depicts the data processing flow. The primary objectives of the PTRAC results were to calculate the energy deposited in the detector cell and to evaluate the full-energy peak efficiency resulting from Compton scatterings. To determine the deposited energy within the cell, we employed a method similar to the F8 tally by calculating the difference between energies that enter and exit the cell. Notably, in energy regions where pair production occurs, it is essential to account for electrons, positrons, and annihilation photons, as they can exit the cell; thus, they were meticulously tracked in our study.

3. Results and Discussion

Figure 2 presents a comparative analysis of the energy spectrum originating from a 1 MeV gamma-ray source. Two distinct approaches were utilized for the investigation, as represented by PTRAC A and PTRAC B. PTRAC A considers all particles as delineated in Figure 1. It incorporates the electrons, positrons, and annihilation photons potentially exiting the detector cell. On the other hand, PTRAC B calculates the accumulated energy within the cell by only focusing on the net difference between incoming and outgoing gamma ray energies. Although both approaches yielded similar spectra, a complete concordance with the F8 tally results was observed only in the case of PTRAC A.

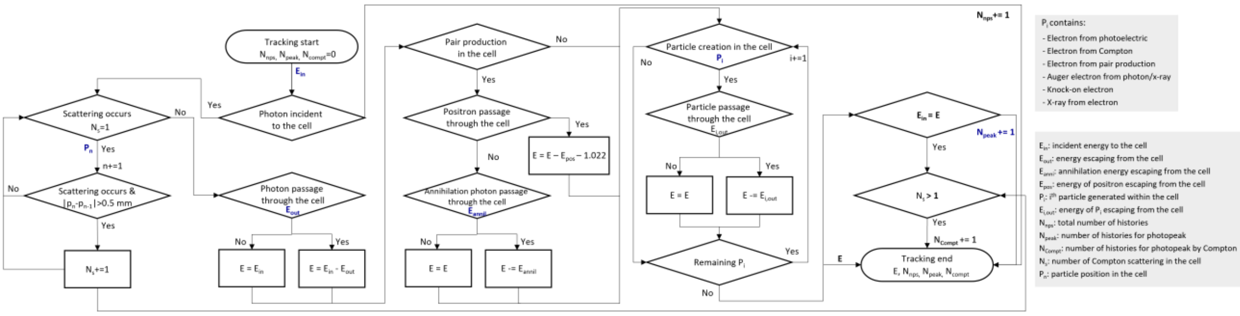

Figure 1. Flowchart illustrating the data processing of PTRAC outputs using Python

For the PTRAC B, although pair production was absent at the 1 MeV energy level, minor discrepancies emerged when compared with the F8 tally results. This divergence can be attributed to secondary electrons generated near the cell's surface that subsequently escape, leading to a measurable energy difference. As evident in Figure 3, this variance becomes more pronounced in energy domains dominated by pair production. Such discrepancies can mainly be attributed to the neglect of annihilation photons resulting from pair production. As one moves to higher energy regions where pair production becomes prevalent, the influence of single or double escape peaks intensifies. Consequently, disregarding these effects can lead to potentially erroneous conclusions when evaluating efficiencies through PTRAC, especially for the high-energy region.

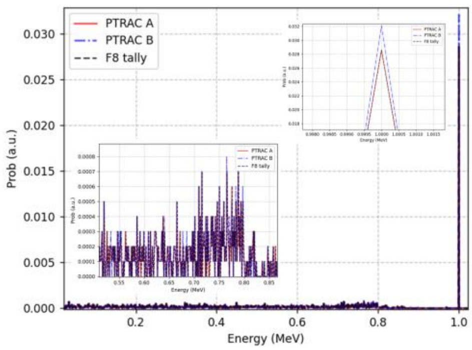

Figure 2. Comparative spectra of PTRAC A, PTRAC B, and F8 tally results for a 1 MeV gamma-ray source.

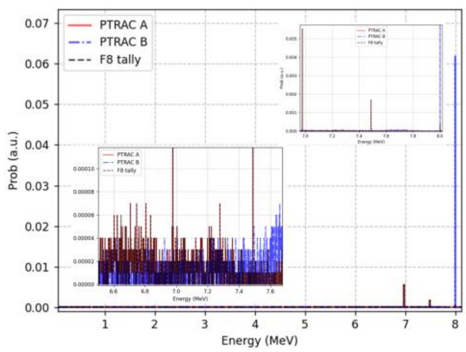

Figure 3. Comparative spectra of PTRAC A, PTRAC B, and F8 tally results for a 8 MeV gamma-ray source.

4. Conclusion

Using the MCNP PTRAC function, our investigation reveals the significance of detailed data processing in modeling high-energy gamma spectra. The study emphasized the criticality of including all particle interactions, especially in high-energy domains where pair production is prevalent. In future work, we intend to evaluate the Compton imaging efficiency concerning varying CZT crystal sizes and energy levels, providing deeper insights into optimization avenues for high-energy gamma spectrum analysis.

REFERENCES

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