VALIDATION FOR MONTE CARLO SIMULATION OF CHARACTERISTICS OF GAMMA SPECTROMETER USING HPGe GMX35P4-70 DETECTOR BY MCNP5 AND GEANT4 CODES

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ABSTRACT

The study used two Monte Carlo simulation codes of MCNP5 and GEANT4 to simulate HPGe detector of GMX35P4-70, then its response spectra and peak efficiencies characteristics were evaluated. The results show that when increasing the inner dead layer thickness of the detector from 1.8mm to 2.2mm, there is a better fit of the response spectra and the peak efficiencies characteristics compared with the measured ones. In general, it is useful to use two these input files to simulate response spectra and calculating the peak efficiency of GMX detector for determination of radionuclide distribution in the soil by in situ or laboratory gamma-ray spectrometry.

Keywords: GMX detector, Monte Carlo, MCNP5, Geant4.

TÓM TẮT

Xác nhận hiệu lực mô hình mô phỏng đặc trưng hệ phổ kế gamma đầu dò bán dẫn siêu tinh khiết GMX35P4-70 với chương trình MCNP5 và GEANT4

Trong công trình này, chúng tôi sử dụng hai chương trình mô phỏng Monte Carlo MCNP5 và GEANT4 để mô phỏng hệ đầu đò HPGe kí hiệu GMX35P4-70, sau đó nghiên cứu đặc trưng phổ và tính toán hiệu suất đỉnh. Kết quả cho thấy khi thay đổi bề dày lớp chết từ 1.8mm đến 2.2mm đáp ứng phổ mô phỏng và hiệu suất đỉnh phù hợp với thực nghiệm hơn. Từ đó có thể sử dụng mô hình mô phỏng để tính toán hiệu suất hoặc cung cấp đáp ứng phổ cho việc phân tích hoạt độ phóng xạ sử dụng hệ phổ kế gamma trong phòng thí nghiệm hay tại hiện trường.

Từ khóa: GMX detector, Monte Carlo, MCNP5, GEANT4.

1. Introduction

Monte Carlo method is based on the seeding of the random number to sample in a set. It was first used by Metropolis (1947) [15]. This method has a very important role in computational physics. There are so many authors who have used the Monte Carlo method to solve problems in the nuclear physics by writing and developing the codes as MCNP [15], Geant [2], EGSnrc [8]. Thereby some authors have applied the codes for evaluation of response spectra of detector and have compared the results with

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experimental spectra [4], [6], [11], [12], [13], [14]. Rodenas et al [10], Ngo Quang Huy et al [9] have used MCNP code to evaluate the dead layer thickness of the HPGe detector based on comparison of the simulated efficiencies and empirical ones. Ashrafi et al [1], Berndt et al [3] have done to scan the detector to have detailed data of detector configuration which is used for simulation. Hau et al [5] have used MCNP code for studying Compton scattering and HPGe detector benchmark with previously validated Cyltran model. Thereby Monte Carlo method has a very important role to study the spectra characteristics of the HPGe detector.

In this work we studied spectra characteristics of HPGe GMX35P4-70 detector by using MCNP5 and GEANT4 codes, the change of sensitive volume of Germanium crystal after a long time of use due to the increased thickness of the inner dead layer. In order to do that, comparison of the simulated spectra response and the empirical ones for point sources of radioactive isotopes at 25cm from detector surface were carried out. It takes our care for peak efficiencies, the valley area, Compton edge, and energy range from 20 keV up to 60 keV in the simulated spectra.

2. Materials and Methods

The studied GMX35P4-70 HPGe detector has its diameter of 55.8 mm, height of 78.1 mm, core hole diameter of 8.6 mm, core hole depth of 69.6 mm, beryllium window thickness of 0.5mm. Reference sources of ²⁴¹Am, ¹³⁷Cs, ⁵⁴Mn, ⁵⁷Co, ⁶⁰Co, ²²Na isotopes of 1µCi (3%) at 25cm from the detector surface were used for spectra response measurements and simulation.

In this work two MCNP5 and Geant4 codes were used to simulate photon transports in studied detector. The information of configuration and materials of the detector which based on data from Ortec industries were used in the input file of detector simulation. The codes was done under Linux operating system with personal computer using i3 core. Number of particle history was selected for efficiency errors below 0.1%. FWHM values were obtained from fitted empirical FWHM values to energies as follows:

 $FWHM = 0.000743405 + 0.0006332324\sqrt{E + 0.8615278178E^2}$ (1)

3. Results and Discussion

3.1. Simulation of GMX spectrometer using MCNP5 and GEANT4 codes

To determine accurately radioactivity of gamma emitted isotopes for HPGe detector, the peak efficiency of detector need to be exactly known. The peak efficiency curve of the detector is dependent on incident gamma energies. However there are no available enough the reference point sources for efficiency calibration, especially in the energy ranges below 120 keV or above 1.5 MeV. It is necessary to use analytical or Monte Carlo method to estimate the peak efficiencies. In this case, Monte Carlo simulation becomes useful and important. In this work, MCNP5 and GEANT4 codes were used to simulate the HPGe detector and to have a validation of the simulated

spectra responses comparing with the empirical ones. However, there are differences of simulated efficiencies from the empirical ones when using data of detector configuration from Ortec Industries in the input file of detector simulation, especially in the high energy as presented in Table 1. It is explained by increasing dead layer of Germanium crystal after long time of use [3]. Therefore study on the increase of inner dead layer of Germanium crystal of the GMX detector was aimed in the work.

To determine the thickness of inner dead layer of GMX detector, peak efficiencies of GMX detector were estimated for many different photon energies of the above reference point sources at 25cm from detector surface using MCNP5 input file of the detector simulation. These peak efficiencies were calculated for many different thicknesses of dead layer in simulation and then were compared with the respectively empirical ones. The dead layer thickness of 2.2mm was selected because there are a good fit of 3% difference between the simulated efficiencies and the empirical ones for the low energies and high energies. The difference of simulated peak efficiencies using dead layer thickness of 1.8mm from Ortec Industries and the predicted value of 2.2mm for many different energies in code of simulation were presented in Table 1.

Gamma energy	Difference %	Difference %	Gamma energy	Difference %	Difference %	
(keV)	(2.2mm)	(1.8mm)	(keV)	(2.2mm)	(1.8mm)	
59.50	0.21	2.97	383.57	1.62	8.30	
88.03	0.21	1.70	661.66	1.49	9.96	
122.06	0.60	2.10	834.84	1.19	10.27	
136.50	1.38	2.18	1115.54	3.30	13.01	
276.32	2.27	6.71	1173.23	2.81	12.29	
302.71	2.23	7.57	1274.54	2.73	12.51	
355.78	1.77	7.72	1332.50	3.06	13.61	

Table 1. The difference of peak efficiencies using the dead layer thicknessof 1.8mm (from Ortec Industries) and of 2.2mm (as predicted)

It is noted that when the inner dead layer thickness of GMX is increased from 1.8mm to 2.2mm, there are less difference of peak efficiencies at the low energies than at the high energies. For example, the peak efficiency difference decreased from 13.6% using the value of 1.8mm to 3% using the value of 2.2mm for 1332.50 keV of 60 Co. The same results also were found in studies of Matsumasa T. et al [7] using scan tecknique for two n – type detectors of JIRO and HNAKO. It could be explained that the dead layer of the used n – type detector exist in the inner side, the low energy gamma from external sources deposited almost its energy in the active germanium volume before going through the inner dead layer. In the meanwhile, the high energy

gammas could pass through it. Then the thickness of dead layer influence on the peak efficiencies for the high energy gamma acquisition.

3.2. Validation of two MCNP5 and GEANT4 codes of GMX detector simulation for calculating the peak efficiencies.

Two MCNP5 and GEANT4 codes were used for GMX detector simulation using data of detector configuration from Ortec producer, with dead layer thickness of 2.2mm estimated in section 3.1. The validation of two codes were estimated for calculating the peak efficiencies in this section. To do that, the simulated peak efficiencies for different gamma energies were calculated by these simulation codes and then compared with the empirical ones respectively and were presented in Table 2.

Energy (keV)	Empirical (1)	MCNP5 (2)	GEANT4 (3)	(2)/(1)	(3)/(1)	(2)/(3)
53.16	0.00223	0.00226	0.00224	1.0134	1.0053	1.0089
59.5	0.00212	0.00211	0.0021	0.9979	0.9935	1.0048
88.03	0.00217	0.00216	0.00213	0.9979	0.9848	1.0141
122.06	0.00207	0.00209	0.00208	1.0060	1.0010	1.0048
136.5	0.00201	0.00204	0.00203	1.0138	1.0101	1.0049
276.32	0.00132	0.00135	0.00134	1.0228	1.0133	1.0075
302.71	0.00122	0.00125	0.00124	1.0223	1.0132	1.0081
355.78	0.00108	0.00110	0.00108	1.0176	1.0019	1.0185
383.57	0.00102	0.00103	0.00099	1.0162	0.9695	1.0404
661.66	0.00067	0.00068	0.00067	1.0150	1.0052	1.0149
834.84	0.00057	0.00058	0.00057	1.0119	1.0072	1.0175
1115.54	0.00046	0.00047	0.00047	1.0328	1.0267	1.0000
1173.23	0.00045	0.00046	0.00045	1.0280	1.0003	1.0222
1274.54	0.00042	0.00043	0.00042	1.0275	1.0081	1.0238
1332.5	0.00040	0.00042	0.00041	1.0307	1.0250	1.0244

Table 2. Comparison of the simulated peak efficiencies and the empirical ones for 50 keV to 1400 keV gamma energies

There are a less 4% difference between the empirical efficiencies and the ones simulated by two input files from codes of MCNP5 and GEANT4 for observed gamma energy ranges of reference point sources. It is useful to use two these input files to have response spectra and peak efficiency calculation of GMX detector for determination of radionuclide distribution in the soil by in situ or laboratory gamma-ray spectrometry.

3.3. Validation of two MCNP5 and GEANT4 codes of GMX detector simulation for evaluation of Compton scattering domain of spectra

The validation of two MCNP5 and GEANT4 codes of GMX detector simulation are continuously estimated when studying Compton scattering domain in the full spectra response. The figures 1a, 1b, 1c, 1d presented the comparison between the empirical full spectra response and the ones simulated by two codes of simulation.

It is noticed from the figures that beside of a good fit for almost spectra domain, there are some bit difference of less than 5% at the low energy range from 20 keV to 50 keV, at Compton valley and at the left heel of photopeak. At the Compton valley, the simulated spectra are underestimated. They are lower than the empirical ones respectively. This difference becomes clearer for MCNP5 simulation than GEANT4 simulation when using the same FWHM function. It is explained by not enough data of multi scattering in library of simulation codes at the low energies.



Figure 1. Comparison between the empirical spectra and the simulated ones using MCNP5 and GEANT4 codes

4. Conclusion

In this work, we have used MCNP5 code to predict and to determine the value of inner dead layer thickness of GMX detector. It increases from 1.8mm to 2.2mm after two years of use. The new vakue of dead layer thickness and detailed information of detector configuration supplied from Ortec Industries were used in the two input files

of detector simulation by MCNP5 and GEANT4 codes. The validation of these two models were verified by comparing the simulated response spectra and the empirical ones for whole photon energy range of spectrometer. There are a difference of below 3% between simulated peak efficiencies and the empirical ones. But there are underestimation or not enough good fit for energy range from 20keV to 60 keV, at the left heel of photopeak and the Compton valley for MCNP5 simulation and GEANT4 simulation. In general, the evaluation of peak efficiencies by simulation could be useful instead of experimental measurements for determination of radioactivity of sources in condition there are not enough the reference sources. It takes our more detailed care to study about full reponse spectra by simulation for further studies.

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