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Evaluating coincidence summing factor using marinelli beaker on coaxial HPGe detector by Monte Carlo simulation and calculating

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Abstract: This investigation aims to compare the full energy peak efficiencies in the energy range of 46-1836 keV on a type-p coaxial HPGe and estimate the coincidence summing factor for the case of Marinelli Beaker samples used by two general Monte-Carlo simulation software MCNP and PENELOPE. The radioactive nuclides used in determining the coincidence summing factor include ^{22}Na, ^{60}Co, ^{88}Y, ^{133}Ba, ^{134}Cs, ^{154}Eu, and ^{208}Tl, which are prepared in HCl 2M solution and contained in a Marinelli beaker with the source's volume of 3000 ml. The results demonstrate there is a good agreement between the two simulation software with an average discrepancy of 1.3%. On the other hand, the simulation coincidence summing factor values are also compared with the results from the calculating software ETNA with an average discrepancy of approximately 3.1%.

Keywords: *Coaxial HPGe detector, coincidence summing factor, Monte Carlo simulation.*

I. INTRODUCTION

Gamma-ray spectrometry using High Pure Germanium (HPGe) detector has been utilized extensively, keeps an essential role in many applications such as multi-elements analysis, non-destructive testing, radionuclide activities determination. One of the main factors that could affect the accuracy of the measurements is the full energy peak efficiency (FEPE), which is always requested for the efficiency calibration. In the case of low activity sample measurement like the environmental sample, the close distance between the sample and the detector is the possible method to gain more signals that reach the detector, therefore, enhance the values of the FEPE.

However, the more decreasing distance to the detector, the more increasing the coincidence summing effect, which is known as the simultaneous detection of two or more gamma rays from the same decay scheme within the time resolution of the detector [1]. The coincidence summing can causes the loss (called as summing out effect) or the acquisition (called as summing in effect) of counts under the peak areas of the interest nuclei influences the precision of the measurement. Hence, a suitable correction must be performed to compensate for the FEPE. The coincidence summing factor (CSF) can be determined by using two methods consist of efficiency transfer calculated by ETNA software [2], and Monte Carlo simulation such as MCNP-CP [3] and PENNUC [4] software.

The aim of this study is a validation of the FEPE as well as the true summing coincidence factor of a point and the volume source in the type of Marinelli beaker on the HPGe detector.

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Both the FEPE and CSF are obtained by ETNA calculation along with MCNP-CP and PENNUC simulation, then the results will be compared at the end.

II. CONTENT

A. Materials and Methods

Coaxial HPGe detector

In this work, the gamma-ray spectrometry system with an ORTEC p-type HPGe coaxial detector, model GEM50P4-83 was used for constructing the Monte Carlo simulation configuration. The HPGe detector has a relative efficiency of 50%; a Peak-to-Compton ratio is 66:1 at 1332 keV (^{60}Co); a FWHM of 0.9 keV at 122 keV (^{57}Co) and 1.9 keV at 1332 keV (^{60}Co). The detailed parameters of the germanium crystal are provided by the manufacturer, as given in Table I. Outside of the germanium crystal are the holder and the housing, both are made from aluminum with the thickness of 0.8 mm and 1 mm, respectively. The HPGe detector is placed inside the shielding model HPLBS1F, which consists of four layers from inside to outside: 1.6 mm soft-copper sheet liner, 0.5 mm tin sheet liner, 101 mm reprocessed lead, and 12.7 mm low-carbon steel casing.

Table I. Coaxial HPGe detector parameters

Parameter	Value (mm)
Crystal diameter	65.90
Crystal length	77.00
Crystal nomial radius	8.00
Hole diameter	11.50
Hole depth	64.90
Hole nomial radius	8.00
Outer dead layer	0.70
Inner dead layer	0.30×10^{-3}
Crystal-window distance	4.00
Window thickness	1.03 (aluminum)

Source definition

Firstly, a point source placed at a distance of 15 cm far from the window, was used to validate the Monte Carlo simulation configuration of the coaxial HPGe detector. In these cases, the energies of this point source are twelve mono-energy levels from 46 to 1836 keV. Secondly, the point source is substituted by the Marinelli beaker located right above the detector, with the height and diameter of the beaker is 17.8 cm and 20.1 cm, the height and diameter of the groove is 7.6 cm and 8.5 cm, respectively. The Marinelli beaker contains of 3000 ml HCl 2M solution with a density of 1.033 g/cm^3. The configuration of Marinelli beaker are used for both efficiency and CSF determination.

Monte Carlo simulation

There is two main simulation software in this research, which are MCNP and PENELOPE. MCNP (Monte Carlo N-Particle) software with the latest version MCNP6 was created by Los Alamos National Laboratory, can describe the physical interactions of many types of particles such as photon, neutron, electron,

alpha [5]. MCNP software allows users to establish the geometric structure of the simulation configuration with high intricacy as well as illustrating the interaction of particles with substance, nuclear decay process, neutron flux calculation, and dose distribution. All the information that need for the simulation is united in one input text file (*.txt), which includes the definition of cell card, surface card, and data card. The extensive software MCNP-CP was developed by Berlizov from the MCNP4c version [3], which could enable the coincidence summing effect through the optional CPS (Correlated Particle Source) value in the data card. In case the value of CPS is -1, this card specifies an uncorrelated source. On the contrast, to enable default mode of correlation source, user can hide the CPS card. The output of MCNP consists of the information about the efficiencies and their relative uncertainties corresponding to the energy of interest. The efficiency is defined as the ratio between the number of events recorded in the corresponding energy bin N(E) and the number of photons that emitted by the source N_{sim}:

$$\varepsilon(E) = \frac{N(E)}{N_{sim}} \quad (1)$$

On the other hand, PENELOPE (PENetration and Energy LOss of Positrons and Electrons) firstly launched by Salvat in 1996, is a set of subroutines written in the Fortran-77 language [6]. The PENELOPE software bases on the Monte Carlo method to simulate the transport of positrons, electrons, and photons in the matter with energy in a range from 100 eV to 1 GeV. The simulation process can be started by two subprograms: PENCYL or PENMAIN. While the PENCYL can only be used to model the cylindrical geometry, the PENMAIN permits users to construct arbitrary geometries with many types of quadric surfaces [7]. There must be two separate files prepared for the simulation: one is the geometrical model with the extension ".geo" contains surfaces and cells of the configuration, and the other is the input with the extension ".in" contains information about the source, the substance, and geometry. The PENNUC is the extensive subroutine that could link directly to other subroutine packages of PENELOPE, enable the coincidence summing effect mode. In the PENNUC subroutine, if the DETTIME value is 5.10^{-6} , the coincidence mode is activated; inversely the value is -5.10^{-6}. The output of PENELOPE consists of the information about the probability distribution function p(E) and their uncertainties $u_p(E)$ corresponding to the energy of interest. The efficiency can be gained by the product of p(E) and the energy width bin ΔE [8]:

$$\varepsilon(E) = p(E) \times \Delta E \quad (2)$$

The simulation process can be summarised by the following steps:

Step 1: Constructing the HPGe detector with the shielding configuration as given above, using MCNP6 and PENMAIN to execute the simulation for point source with 100 million events was considered.

Step 2: Replacing the point source by the Marinelli beaker (see Fig.1), MCNP6 and PENMAIN are still exploited in this progression. Nevertheless, the started events reduce to 10 million due to the larger simulation time consumption in the case of volume source.

Step 3: Utilising the Marinelli beaker configuration in step 2 for CSF determination. In this stage, the MCNP-CP and PENNUC were taken place. The radioactive nuclide was studied include ^{22}Na, ^{60}Co, ^{88}Y, ^{133}Ba, ^{134}Cs, ^{154}Eu, and ^{208}Tl. Moreover, the CSF are also calculated by ETNA software [9].

Fig.1 illustrates the longitudinal section of the coaxial HPGe with 3000 ml Marinelli beaker on PENELOPE's Gview2D and MCNP's interface viewer.

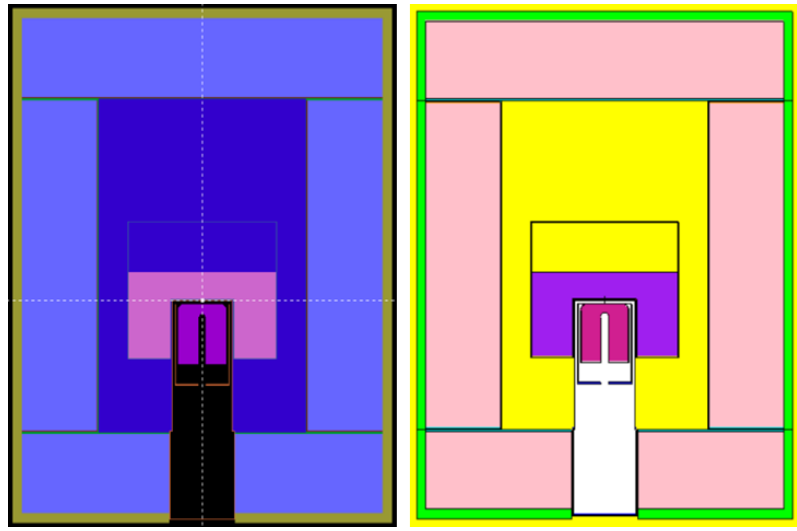

Fig. 1. 2-D representation of the coaxial HPGe with 3000 ml Marinelli beaker on PENELOPE and MCNP

Coincidence summing factor calculation

For each radionuclide, the simulation was accomplished in two cases: one is the configuration called as "With" mode that the coincidence summing effect is regarded, and another is the "Without" mode that the coincidence summing effect is completely neglected. The CSF at each energy is the ratio between the FEPEs in "Without" mode $\varepsilon_{Wo}(E)$ and "With" mode $\varepsilon_{W}(E)$ as defined by the equation [10]:

$$CSF = \frac{\varepsilon_{Wo}(E)}{\varepsilon_{W}(E)} \quad (3)$$

And the relative uncertainty of the CSF:

$$u_{CSF}(E) = \sqrt{\left(u_{\varepsilon_{Wo}(E)}\right)^2 + \left(u_{\varepsilon_{W}(E)}\right)^2} \quad (4)$$

B. Results

The output from both MCNP and PENELOPE simulation are loaded into Microsoft Excel for the convenient calculation of the FEPE and CSF. Table II represents the FEPE and TE values of point source and Marinelli beaker on MCNP as well as PENELOPE simulation in step 1 and 2. The relative discrepancy between PENNUC and MCNP-CP of each energy level is less than 2%.

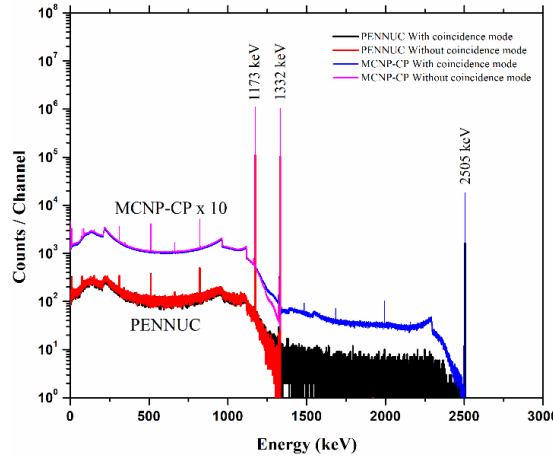

Fig.2: Simulation spectrum of ^{60}Co on PENNUC and MCNP-CP

Table II. Coaxial HPGe detector parameters

Energy (keV)	Point source				Marinelli 3000 ml			
	PENNUC		MCNP-CP		PENNUC		MCNP-CP	
	FEPE	TE	FEPE	TE	FEPE	TE	FEPE	TE
46.5	1.73×10^{-3}	1.85×10^{-3}	1.71×10^{-3}	1.81×10^{-3}	3.87×10^{-3}	6.03×10^{-3}	3.87×10^{-3}	5.90×10^{-3}
59.5	3.92×10^{-3}	4.21×10^{-3}	3.89×10^{-3}	4.16×10^{-3}	1.18×10^{-2}	2.02×10^{-2}	1.19×10^{-2}	1.99×10^{-2}
88.0	6.59×10^{-3}	7.26×10^{-3}	6.58×10^{-3}	7.25×10^{-3}	2.60×10^{-2}	5.07×10^{-2}	2.62×10^{-2}	5.05×10^{-2}
122.1	7.28×10^{-3}	8.39×10^{-3}	7.29×10^{-3}	8.42×10^{-3}	3.22×10^{-2}	6.94×10^{-2}	3.24×10^{-2}	6.95×10^{-2}
159.0	7.05×10^{-3}	8.68×10^{-3}	7.03×10^{-3}	8.69×10^{-3}	3.29×10^{-2}	7.73×10^{-2}	3.32×10^{-2}	7.75×10^{-2}
391.7	4.14×10^{-3}	8.18×10^{-3}	4.15×10^{-3}	8.20×10^{-3}	2.16×10^{-2}	7.73×10^{-2}	2.16×10^{-2}	7.72×10^{-2}
661.7	2.87×10^{-3}	7.69×10^{-3}	2.87×10^{-3}	7.70×10^{-3}	1.56×10^{-2}	7.09×10^{-2}	1.57×10^{-2}	7.08×10^{-2}
898.0	2.34×10^{-3}	7.35×10^{-3}	2.34×10^{-3}	7.35×10^{-3}	1.30×10^{-2}	6.66×10^{-2}	1.30×10^{-2}	6.64×10^{-2}
1173.2	1.96×10^{-3}	7.02×10^{-3}	1.96×10^{-3}	7.02×10^{-3}	1.11×10^{-2}	6.24×10^{-2}	1.11×10^{-2}	6.23×10^{-2}
1332.5	1.79×10^{-3}	6.85×10^{-3}	1.80×10^{-3}	6.85×10^{-3}	1.02×10^{-2}	6.06×10^{-2}	1.03×10^{-2}	6.05×10^{-2}
1836.1	1.42×10^{-3}	6.45×10^{-3}	1.42×10^{-3}	6.45×10^{-3}	8.27×10^{-3}	5.63×10^{-2}	8.24×10^{-3}	5.65×10^{-2}

After that, the simulation process is continued with the step 3 using MCNP-CP and PENNUC for seven radionuclides on "With" and "Without" mode. Fig.2 describes the appearance of the 2505 keV peak (sum of 1173 keV and 1332 keV) in the "With" mode simulation spectrum of ^{60}Co (Note: The result of MCNP is multiplied by ten). The CSF values as given in Table III are calculated by equation (3) from the simulation outcome.

Table III. CSF values for seven nuclides

Nuclide	**Energy (keV)**	**MCNP-CP (1)**	**PENNUC (2)**	**ETNA (3)**	**RD(%) (2)/(1)**	**RD(%) (3)/(1)**
^{22}Na	511.00	1.090	1.092	1.073	0.14	1.56
	1274.54	1.218	1.219	1.175	0.10	3.56
^{60}Co	1173.23	1.092	1.086	1.063	0.56	2.69
	1332.49	1.094	1.094	1.064	0.03	2.71
^{88}Y	898.04	1.079	1.078	1.058	0.08	1.93
	1836.07	1.089	1.094	1.065	0.47	2.20

^{133}Ba	53.16	1.143	1.140	1.345	0.26	17.69
	79.61	1.153	1.133	1.354	1.73	17.39
	81.00	1.131	1.134	1.229	0.26	8.63
	160.60	1.049	1.102	1.065	5.06	1.51
	223.20	1.040	1.034	1.115	0.59	7.18
	276.40	1.055	1.042	1.101	1.16	4.43
	302.90	1.029	1.029	1.051	0.04	2.12
	356.00	1.025	1.023	1.041	0.13	1.65
	383.80	0.967	0.973	0.953	0.70	1.37
^{134}Cs	475.37	1.201	1.202	1.192	0.14	0.72
	563.25	1.213	1.197	1.199	1.30	1.19
	569.33	1.231	1.226	1.197	0.39	2.80
	604.72	1.133	1.124	1.111	0.78	1.95
	795.86	1.135	1.130	1.110	0.37	2.17
	801.90	1.198	1.195	1.171	0.26	2.23
	1038.61	1.018	1.148	1.040	12.71	2.16
	1167.97	0.949	0.939	0.940	1.14	1.02
	1365.19	0.867	0.879	0.889	1.44	2.60
^{154}Eu	123.07	1.127	1.127	1.140	0.04	1.22
	247.93	1.193	1.202	1.226	0.74	2.72
	591.76	1.176	1.224	1.178	4.12	0.23
	723.30	1.134	1.129	1.114	0.43	1.80
	756.80	1.187	1.218	1.224	2.58	3.10
	873.18	1.140	1.155	1.134	1.38	0.51
	996.25	1.063	1.037	1.042	2.45	1.96
	1004.70	1.061	1.069	1.060	0.84	0.04
	1274.40	1.054	1.046	1.050	0.77	0.36
	1596.48	0.823	0.832	0.858	1.11	4.28
^{208}Tl	277.37	1.197	1.198	1.191	0.09	0.48
	510.74	1.208	1.191	1.172	1.42	2.99
	583.19	1.132	1.127	1.102	0.44	2.64
	860.53	1.047	1.066	1.029	1.77	1.74
	2614.51	1.151	1.140	1.105	0.95	4.01

$$RD = \frac{|CSF - CSF_{MCNP-CP}|}{CSF_{MCNP-CP}} \times 100\%$$

C. Discussions

Table II shows a good agreement between MCNP6 and PENELOPE simulation with the relative discrepancy of each energy is less than 2%. The configurations of two simulations are then used for calculating the CSF by MCNP-CP and PENNUC, the results are presented in Table III, with an average relative discrepancy of approximately 1.3%, the average relative uncertainty of CSF is 0.14% and 1.3%, respectively.

Furthermore, the CSF values from the MCNP-CP simulation are compared with the CSF calculated by ETNA software with an

average relative discrepancy of approximately 3.1%. For some cases that the relative discrepancy between two software is higher than 5% for example at 160.60 keV of ^{133}Ba and 1038.61 keV of ^{134}Cs, the reason is mainly because of the low intensity of gamma-rays in the decay schemes.

Moreover, the summing out effect is illustrated by the CSF that is higher than 1, which means the loss rate equals the CSF minus 1. Conversely, the summing in effect is illustrated by the CSF that is lower than 1, which means the acquisition rate equals 1 minus the CSF.

III. CONCLUSIONS

The purpose of this study is to evaluate the FEPEs in the energy range of 46-1836 keV on a type-p coaxial HPGe and estimate the CSF basing on two general Monte Carlo simulation software are MCNP and PENELOPE. Each radionuclide is stored in HCl 2M solution and contained in a 3000 ml Marinelli beaker. The results demonstrate there is a good agreement between the two simulation software with an average discrepancy of 1.3%; the average discrepancy between MCNP-CP and ETNA is approximately 3.1%. Therefore, the CSF values of this configuration from MCNP are recommended to be used as a reference for further experimental investigations.

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