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True coincidence summing corrections in HPGe detectors

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Abstract   The true coincidence effect is studied in two High Purity Germanium (HPGe) detectors for a variety of isotopes, source geometries and source to detector configurations, via computational tools based on Monte–Carlo simulations. The upgraded patch of MCNP code MCNP–CP and the 2018 version of PENELOPE, which take into account the decay scheme of each cascade emitter, are used to calculate the Full Energy Peak Efficiency (FEPE) for the corresponding gamma–ray energies. The true coincidence correction (TCC) factor is calculated as the ratio of the FEPE derived for each nuclide taking into consideration the true coincidence effect, to the FEPE estimated without considering the phenomenon. In all cases, a satisfactory agreement is observed between the TCC factors calculated using MCNP–CP and PENELOPE 2018. Moreover, the results of the calculations are compared against experimentally derived efficiency values. The correction factors obtained using the TrueCoinc software are applied on experimentally determined FEPE curves, based on measurements performed using reference sources, and consequently the corrected data are compared against the simulations for the "non–coincidence" case. The results of this work contribute to the validation of the computational tools and codes used to study the true coincidence effect and determine the corresponding correction factors, providing useful data for gamma–spectrometry studies of cascade emitters.

Keywords   gamma-spectrometry, true coincidence, Germanium detectors, correction factors, Monte-Carlo simulations

INTRODUCTION

The true coincidence effect occurs in gamma spectrometry, when two or more gamma rays (or a γ–ray and an X–ray) are emitted in cascade from an excited nucleus and they are detected "simultaneously", namely within the resolution time of the gamma–ray detector. The coincident photons are registered as a single photon, with energy equal to the sum of the energies of the detected photons. As a result, "summing in" and "summing out" effects are observed in the gamma–ray spectrum. The latter describes the "loss" of counts under the full energy peak of the coincident photons while the former expresses the summation or "gain" of those counts under the resulting sum peak. The true coincidence phenomenon can lead to significant under–estimation or over–estimation of the net area of the corresponding peaks, since it causes either reduction or increase of the counts registered, and thus, it can result to inaccurate determination of the radionuclide activity, unless corrections are performed.

In order to take into account coincidence summing and correct for its effect on the gamma spectrometry results, different methods have been suggested. Andreev et al. [1], [2] have proposed analytical–theoretical methods, which take into consideration the decay scheme, the full energy peak efficiency and the total efficiency. Moreover, empirical and semi–empirical techniques, combining analytical equations and experimental validation, have been used for true coincidence corrections [3]. Furthermore, simulation codes, based on Monte–Carlo methods, are used to account for the true coincidence effect and consequently derive the required correction factors [4].

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In this work, the Monte–Carlo codes PENELOPE and MCNP are employed to study the true coincidence effect and derive the corrections needed. In particular, the 2018 version of PENELOPE [5] and the upgraded patch MCNP–CP [6] in conjunction to the fifth version of MCNP [7] are used in order to calculate correction factors for different gamma–spectrometry configurations. The results of the two codes are compared against each other, as well as against values obtained by the TrueCoinc software [8]. The calculations are also compared against experimentally determined values corrected using TrueCoinc derived factors.

EXPERIMENTAL

Gamma spectrometry systems

In the present work, two Germanium (Ge) detector based spectrometry systems were studied (Fig. 1), all belonging to the Nuclear Engineering Laboratory, Nuclear Engineering Department of National Technical University of Athens (NED–NTUA):

(a) a High Purity Germanium Detector, with relative efficiency of 33.8% (Ge33), surrounded by a stainless steel shielding

(b) a Low Energy Germanium Detector (LEGe), provided with a stainless steel shielding.

Additional Tin (Sn) and Copper (Cu) layers have been also placed inside the shielding of the two detectors, for X–ray absorption purposes. LEGe system has a Beryllium (Be) window that allows the detection of low energy gamma and X–rays.

Figure 1. *Ge33 (left) and LEGe (right) detectors in NED–NTUA lab*

Experimental measurements

A series of cascade emitters and single–energy radionuclides were used for experiments in different configurations:

(i) ^{60}Co and ^{22}Na reference point sources were measured in source to detector distances (sdd) of ~1cm and 10 cm, in the Ge33 system, with either open or closed shielding,

(ii) a reference mixed nuclide surface source, containing ^{133}Ba, ^{57}Co, ^{65}Zn, ^{54}Mn and ^{137}Cs isotopes, was measured in contact with both the Ge33 and LEGe detectors with closed shielding,

(iii) a ^{57}Co reference point source was measured in contact with the LEGe detector with closed shielding.

The duration of the measurements varied between 0.5 hours and 6.8 days in order to obtain

counting statistics of uncertainty lower than 5%. The acquired spectra were collected using the Genie software and afterwards were converted and analyzed using the Gamma Vision software.

SIMULATIONS

Detector models

In order to obtain reliable simulation results, it is crucial to develop high accuracy models of the spectrometry systems of interest, describing in detail the geometrical features and characteristics of the detectors used.

For the purpose of simulations, two models were developed for each of the two Germanium detectors studied: one with the PENELOPE code and the other with the MCNP code. The PENELOPE model for the Ge33 detector was developed based on the detector certificate, which is provided by the manufacturer. It is noted that the nominal dimensions of the germanium crystal of the Ge33 detector were validated through the comparison of simulations against experiments, in order to confirm that they have not been changed over the course of time. The PENELOPE model used for the LEGe detector was developed and validated in a previous study [9]. In terms of the MCNP code, the models for the two detectors were developed from scratch using the same parameters as in the PENELOPE models.

For the requirements of this work, additional modifications had to be implemented in the models in order to describe the exact configuration used in each case, regarding the shielding (open or closed), the source geometry (point, surface, volume) and source to detector distance, other parts of equipment that were used (i.e. plexiglass mountings etc). The detector models developed for PENELOPE and MCNP codes, are shown in Fig. 2, as plotted using the gview2d (first series) and Vised (second series) software, respectively.
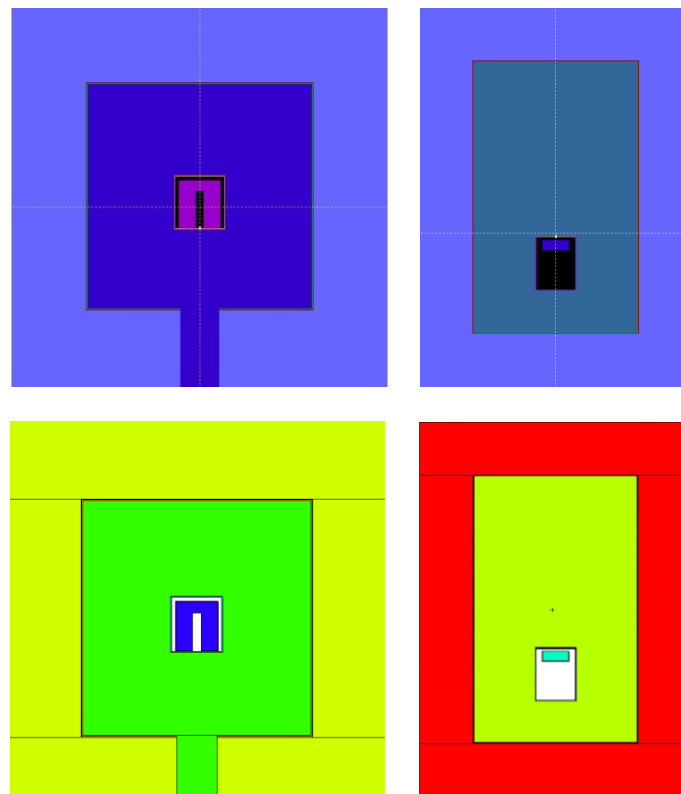

Figure 2. *Ge33 model (left), LEGe model (right) developed for PENELOPE (1st series) & MCNP (2nd series) codes*

Calculation of TCC factors

For the determination of true coincidence correction factors (TCC), the Full Energy Peak Efficiency (FEPE) value for the energy of interest taking into consideration the true coincidence effect (FEPE$_{coinc}$) and the FEPE value without consideration of the effect (FEPE$_{no-coinc}$) are calculated in two separate simulations. Then, the simulated correction factor is derived as their ratio:

$$TCC = \frac{FEPE_{coinc}}{FEPE_{(no-coinc)}} \qquad (1)$$

In order to account for the true coincidence phenomenon, the modification of the appropriate parameters in the input files of the codes is needed. In PENELOPE code, "DRTIME" parameter, which is included in "penmain" program, needs to be set to its default value, while in MCNP–CP the "CPS" card can be omitted. In order for the codes to ignore the effect, "DRTIME" parameter needs to get a negative value, while in MCNP input file "CPS" card has to be equal to –1.

Due to the fact that comparable results were needed, all other user defined parameters were same in the inputs of the codes. It is stressed, that in the case of the mixed nuclide source, since PENELOPE code cannot handle multiple nuclides in a single simulation the definition of separate input files for each radionuclide examined was required. On the other side, MCNP–CP allows the simulation of a mixed nuclide source in a single run, leading to more complex simulated spectra in this case.

RESULTS AND DISCUSSION

MCNP and Penelope calculated TCC factors

In Tables 1 & 2, the TCC factors calculated using MCNP–CP (f$_{TCC(MCNP)}$) and PENELOPE (f$_{TCC(Pen)}$) codes as well as their ratios (Ratio$_{M/P}$) are shown, along with their uncertainties (1σ), for the Ge33 and LEGe detector, respectively, for the cascade emitting isotopes studied. It is noted that in the case of ^{22}Na and ^{65}Zn isotopes, the 511 keV peak is not shown, however it was taken into account in simulations since it contributes to the coincidence effect.

Moreover, in Tables 3 & 4, the FEPE ratios calculated using MCNP–CP (Eff$_{ratio(MCNP)}$) & PENELOPE (Eff$_{ratio(Pen)}$) codes, as well as their ratio (Ratio$_{M/P}$), are shown for two isotopes that are non–cascade emitters, namely the ^{137}Cs and ^{54}Mn isotopes that emit a single γ–ray, for the Ge33 and LEGe detector, respectively. The efficiency ratios shown in Tables 3 & 4 have been calculated as the ratio of the FEPE value for the energy of interest taking into consideration the true coincidence effect and the FEPE value without consideration of the effect, modifying the respective parameters in the input files of the two codes. Nevertheless, since the studied isotopes (^{137}Cs and ^{54}Mn) are non–cascade emitters, it was chosen to designate the corresponding calculated ratios as FEPE ratios (Eff$_{ratio}$) and not as TCC factors (f$_{TCC}$).

To further compare the results, U–test value was calculated for each of the cases studied as the difference between PENELOPE and the MCNP–CP results, divided by the combined uncertainties of the two. U–test values are then compared to determined classification being |U|<1.95 considered satisfactory, 1.95<|U|<2.58 considered of questionable quality and |U|>2.58 considered unsatisfactory.

It is stressed that the uncertainties presented in Tables 1–4 represent the 1σ statistical uncertainties of the simulations and do not take into account errors related to the representation of the studied geometry, namely discrepancies that may exist among the developed models and the actual detector configuration.

As it can be observed from Table 1, a satisfactory agreement (U–test≤1.95) is observed between the two codes for the ^{60}Co and ^{22}Na point sources studied in the Ge33 detector. However, in the case of the mixed nuclide source larger discrepancies are observed. In particular, the largest difference

observed is 18% for the energy of 223.4 keV of ^{133}Ba radionuclide. Moreover, for the ^{57}Co & ^{65}Zn isotopes, U–test values greater than 2.58 occur, indicating unsatisfactory agreement among the results.

Larger discrepancies are observed for the isotopes studied in the LEGe detector (Table 2), where an unsatisfactory agreement (U–test>2.58) occurs for three peaks of the ^{133}Ba radionuclide and the two energies of the ^{57}Co isotope.

These differences could be attributed to the different way in which the mixed nuclide source is handled by each code, namely the fact that MCNP–CP allows the simulation of a mixed nuclide source in a single run leading to more complex simulated spectra, while PENELOPE cannot handle multiple nuclides in a single simulation, thus requiring a separate input file to be defined for each radionuclide of the mixed source. In addition, deviations could be related to the differences among the nuclear data libraries used by the two codes.

Regarding the non–cascade emitters, as it can be seen from Tables 3 & 4, the calculated FEPE ratios (FEPE$_{coinc}$/FEPE$_{no-coinc}$) are statistically equal to 1 in the case of ^{137}Cs, nevertheless, for ^{54}Mn discrepancies are observed. In particular, FEPE ratios of ~1.05 are derived from PENELOPE simulations for the ^{54}Mn isotope, for both detector configurations studied. This result could indicate inadequacy in the way the specific isotope was simulated and needs to be further investigated, since it deviates from the anticipated ratio of 1.

Table 1. *Ge33 detector–TCC factors*

Isotope (source)	Sdd (cm)	Shielding	Energy (keV)	$f_{TCC(Pen)}$		$f_{TCC(MCNP)}$		Ratio$_{M/P}$		U–test
				Value	Error(1σ)	Value	Error(1σ)	Value	Error(1σ)	
^{60}Co (point)	1.2	open	1173.228	0.904	0.003	0.902	0.004	0.998	0.005	0.41
			1332.492	0.904	0.003	0.894	0.005	0.989	0.006	1.76
		closed	1173.228	0.908	0.003	0.901	0.004	0.993	0.005	1.45
			1332.492	0.904	0.003	0.893	0.005	0.988	0.006	1.93
	9.5	open	1173.228	0.968	0.010	0.991	0.014	1.024	0.017	1.35
			1332.492	0.993	0.011	0.979	0.015	0.986	0.018	0.75
		closed	1173.228	0.970	0.010	0.995	0.014	1.026	0.017	1.47
			1332.492	0.979	0.011	0.977	0.015	0.998	0.018	0.11
^{22}Na (point)	1.2	open	1274.537	0.891	0.003	0.888	0.005	0.997	0.006	0.53
		closed	1274.537	0.884	0.003	0.888	0.005	0.999	0.006	0.71
	9.5	open	1274.537	0.989	0.010	0.981	0.014	0.992	0.018	0.47
		closed	1274.537	0.977	0.010	0.970	0.014	0.993	0.018	0.41
^{133}Ba (mixed)	0	closed	53.1622	0.750	0.019	0.682	0.098	0.910	0.100	0.69
			160.6121	0.980	0.004	1.010	0.070	1.032	0.073	0.43
			223.2368	0.925	0.005	0.759	0.123	0.820	0.124	1.35
			276.3989	0.885	0.014	0.890	0.018	1.006	0.023	0.23
			302.8508	0.951	0.027	0.931	0.011	0.979	0.029	0.72
			356.0129	0.952	0.043	0.943	0.006	0.990	0.043	0.22
			383.8485	1.174	0.020	1.144	0.017	0.974	0.027	1.03
^{57}Co (mixed)	0	closed	122.0606	1.040	0.001	1.005	0.004	0.966	0.004	8.47
			136.4735	1.042	0.028	1.005	0.011	0.964	0.030	1.19
^{65}Zn (mixed)	0	closed	1115.539	1.026	0.007	0.987	0.011	0.963	0.013	2.97

Table 2. *LEGe detector–TCC factors*

Isotope (source)	Sdd (cm)	Shielding	Energy (keV)	$f_{TCC(Pen)}$		$f_{TCC(MCNP)}$		$Ratio_{M/P}$		U–test
				Value	Error(1σ)	Value	Error(1σ)	Value	Error(1σ)	
^{57}Co (point)	0	closed	122.0606	1.038	0.001	1.018	0.001	0.981	0.001	13.88
			136.4735	1.052	0.03	1.076	0.003	1.023	0.026	0.76
^{133}Ba (mixed)	0	closed	53.1622	0.775	0.008	0.788	0.018	1.017	0.021	0.68
			160.6121	1.035	0.012	1.026	0.027	0.991	0.037	0.30
			223.2368	1.028	0.019	0.970	0.036	0.944	0.036	1.42
			276.3989	0.530	0.009	0.634	0.025	1.196	0.025	4.09
			302.8508	0.564	0.006	0.635	0.018	1.126	0.019	3.88
			356.0129	0.650	0.003	0.695	0.011	1.069	0.012	4.03
			383.8485	1.006	0.009	0.989	0.025	0.983	0.032	0.64
^{57}Co (mixed)	0	closed	122.0606	1.021	0.001	1.018	0.001	0.997	0.002	2.10
			136.4735	1.079	0.004	0.931	0.003	0.863	0.005	28.16
^{65}Zn (mixed)	0	closed	1115.539	1.001	0.007	0.971	0.027	0.970	0.028	1.08

Table 3. *Ge33 detector–FEPE ratios*

Isotope (source)	Sdd (cm)	Shielding	Energy (keV)	$Eff_{ratio(Pen)}$		$Eff_{ratio(MCNP)}$		$Ratio_{M/P}$		U–test
				Value	Error(1σ)	Value	Error(1σ)	Value	Error(1σ)	
^{137}Cs (mixed)	0	closed	661.657	1.000	0.002	0.998	0.007	0.999	0.007	0.27
^{54}Mn (mixed)	0	closed	834.848	1.048	0.002	1.00	0.007	0.955	0.007	6.57

Table 4. *LEGe detector–FEPE ratios*

Isotope (source)	Sdd (cm)	Shielding	Energy (keV)	$Eff_{ratio(Pen)}$		$Eff_{ratio(MCNP)}$		$Ratio_{M/P}$		U–test
				Value	Error(1σ)	Value	Error(1σ)	Value	Error(1σ)	
^{137}Cs (mixed)	0	Κλειστή	661.657	1.000	0.004	0.991	0.014	0.991	0.015	0.62
^{54}Mn (mixed)	0	Κλειστή	834.848	1.051	0.004	0.993	0.015	0.945	0.016	3.72

Comparison against TrueCoinc

The TrueCoinc software is based on a combinatorial method for deriving coincidence correction factors. It is dependent on the knowledge of FEPE and the Total Efficiency (TE) curve, which are provided as input data. In this study, the FEPE and TE curves fed into TrueCoinc were derived via MCNP code simulations. It is noted, that TrueCoinc correction factors were calculated for the energies of interest, namely the ones provided with satisfactory counting statistics during experiments. Subsequently, these factors were applied to the measured net area of each peak to obtain a "true" value (FEPE$_{exp\_corr}$), unaffected by true coincidence effects, which was then compared against the ones calculated from simulations (for the non–coincidence case). Indicative results for the case of point sources (^{60}Co and ^{22}Na) examined in Ge33 detector, in sdd of ~1cm and 10cm, with open or closed shielding, are presented in Table 5. The uncertainties presented along with the calculated values are,

as in the previous tables, the ones related to the PENELOPE and MCNP simulations. The experimental uncertainties accompanying the corrected efficiency values (FEPE$_{exp\_corr}$) were determined by combining all identified sources of error, including the counting statistics, activity of reference sources and nuclear data (uncertainties related to isotope half-lives and gamma-ray emission probabilities) as well as the uncertainties of TrueCoinc correction factors.

Table 5. *Simulated and experimentally determined FEPE values corrected for the coincidence effect for point sources studied in the Ge33 detector*

Isotope (source)	Sdd (cm)	Shielding	Energy (keV)	FEPE$_{Pen}$		FEPE$_{MCNP}$		FEPE$_{exper\_corr}$	
				Value	Error(1σ)	Value	Error(1σ)	Value	Error(1σ)
^{60}Co (point)	1.2	open	1173.228	0.0218	0.002	0.0222	0.002	0.0230	0.04
			1332.492	0.0189	0.002	0.0200	0.002	0.0209	0.04
		closed	1173.228	0.0211	0.002	0.0222	0.002	0.0234	0.07
			1332.492	0.0190	0.002	0.0200	0.002	0.0208	0.04
	9.5	open	1173.228	0.0020	0.007	0.0021	0.007	0.0020	0.05
			1332.492	0.0018	0.007	0.0019	0.007	0.0018	0.05
		closed	1173.228	0.0020	0.007	0.0021	0.007	0.0020	0.05
			1332.492	0.0018	0.007	0.0019	0.007	0.0018	0.05
^{22}Na (point)	1.2	open	1274.537	0.0195	0.002	0.0208	0.002	0.0234	0.05
		closed	1274.537	0.0195	0.002	0.0208	0.002	0.0234	0.05
	9.5	open	1274.537	0.0019	0.007	0.0020	0.007	0.0019	0.05
		closed	1274.537	0.0018	0.007	0.0020	0.007	0.0019	0.05

As shown in Table 5, a satisfactory agreement is observed among the simulated FEPE values and the experimental efficiencies corrected using the TrueCoinc factors. For the sdd of ~10 cm, an excellent agreement within 2.5% occurs for all isotopes and shielding configurations studied. For the sdd of ~1cm, larger discrepancies are observed (differences up to 16%), with the simulated FEPE values underestimating the corrected experimental efficiencies. The discrepancies among the simulated and the corrected experimental values could be attributed to uncertainties related to the description of the actual detector geometry in the developed model, which also affect the TrueCoinc derived factors, since the FEPE and TE curves used in the software were in the present study derived using MCNP code.

CONCLUSIONS

In the present work, the true coincidence effect was studied for a variety of isotopes and Germanium detector configurations using Monte–Carlo simulations. In particular, MCNP–CP and PENELOPE 2018 codes were used, in order to derive correction factors for this effect. It was shown, that these tools could lead to reliable results provided that the studied geometry is described in detail for avoiding systematic errors. Additionally, TCC factors were produced via the TrueCoinc program for the same cases, and they were applied on the experimental FEPE values, in order to account for the true coincidence effect. A satisfactory agreement was observed among the simulated and the corrected experimentally determined FEPE values. To conclude, the utilization of simulation codes offers great flexibility for TCC factor calculations, especially when the modification of parameters and the study of different measurement configurations is required. Computational tools, like TrueCoinc software, could additionally contribute to the verification of the factors of interest.

Acknowledgments

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