DETERMINATION OF TRUE COINCIDENCE CORRECTION FACTORS USING MONTE-CARLO SIMULATION TECHNIQUES

by

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Aim of this work is the numerical calculation of the true coincidence correction factors by means of Monte-Carlo simulation techniques. For this purpose, the Monte Carlo computer code PENELOPE was used and the main program PENMAIN was properly modified in order to include the effect of the true coincidence phenomenon. The modified main program that takes into consideration the true coincidence phenomenon was used for the full energy peak efficiency determination of an XtRa Ge detector with relative efficiency 104% and the results obtained for the 1173 keV and 1332 keV photons of ^{60}Co were found consistent with respective experimental ones. The true coincidence correction factors were calculated as the ratio of the full energy peak efficiencies was determined from the original main program PENMAIN and the modified main program PENMAIN. The developed technique was applied for ^{57}Co, ^{88}Y, and ^{134}Cs and for two source-to-detector geometries. The results obtained were compared with true coincidence correction factors calculated from the "TrueCoinc" program and the relative bias was found to be less than 2%, 4%, and 8% for ^{57}Co, ^{88}Y, and ^{134}Cs, respectively.

Key words: true coincidence, Monte Carlo, PENELOPE, correction factor

INTRODUCTION

The true coincidence phenomenon is defined as the cascade emission of two or more photons from the same decay branch of a radionuclide and the simultaneous detection of these photons as one with energy equal to the sum of the photon energies deposited on the detector. Many factors affect this phenomenon that depend on source parameters, such as the type of the radioactive source [1, 2], the type of the decay, the cascade decay scheme, its complexity and the angular correlation between the emitted photons [3-5]; and on geometrical parameters, such as the geometry of the radioactive source and the detector characteristics [5-7]. The True Coincidence phenomenon may significantly affect the photopeak area of the corresponding photopeaks in the spectrum, resulting to the miscalculation of either the full energy peak efficiency or the activity concentration of an analyzed radioactive source [8].

Since the early 1970's, many methods have been developed for the confrontation of the True Coincidence phenomenon in gamma spectroscopic analysis. Theoretical [9, 10], empirical [11] and semi-empirical models have been established, as well as numerical codes using Monte Carlo simulation techniques [12-16]. In all cases, the main goal was the determination of the correction factor that should be applied to the photopeak area of the photon energy under investigation, to take into consideration of the True Coincidence effect.

The determination of the true coincidence correction (TCC) factors at the Nuclear Engineering Department of the National Technical University of Athens (NED-NTUA) is based on the use of the "TrueCoinc" program [17], which was developed at the Institute of Experimental Physics, Kossuth University, Hungary and is supported by the International Atomic Energy Agency (IAEA). The program requires as input the full-energy peak efficiency and the total-to-peak efficiency curves, which should be provided by the user and gives as output the TCC factors. The cascade decay scheme needed for this calculation is incorporated within the program libraries, which are based on the ENSDF database.

METHODOLOGY

Aim of this work is the appropriate modification of the Monte Carlo simulation code PENELOPE (version 2005), in order to take into consideration the ef-

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fect of True Coincidence. The modified code may then be used for determination of the detector efficiency and provide output results, which can be used for the calculation of the respective TCC factors for specific radionuclides. PENELOPE is a FORTRAN code consisting of a set of subroutines, which are called by a user developed main program to tackle with the specific simulation problem [18]. A small set of user main programs is available together with the PENELOPE Code package. One of these is the generic main program PENMAIN that was properly modified during this work. One of PENMAIN main features is the simulation of a photon history, which means that in every simulation loop – called "shower" – the interactions of a single photon and its secondary radiation are taken into consideration. At the end of each shower all information for the simulated photon are recorded and stacks and counters are reset. As a result, the full energy peak efficiency that may be determined using this code completely neglects any summation effect involving more than one photon, such as true coincidence summing, pile-up, *etc*. This work is focused on the modification of the main program PENMAIN to simulate a nucleus decay, which means that every simulation loop may involve more than one photon, or other particle, interacting with the detector. As a result, the program output results may be used for the determination of the full energy peak efficiency, taking into consideration the detection of more than one photon from the same decay, which results to true summation.

True coincidence correction (tcc) factors may then be calculated as the ratio of the full energy peak efficiency values determined using the modified (eff_{mod}) and the original (eff_{ori}) main program PENMAIN

$$\text{tcc} \quad \frac{eff_{mod}}{eff_{ori}} \qquad (1)$$

It must be noted that using formula (1) for the calculation of the tcc factor, type B uncertainties introduced due to detector incomplete geometry description are significantly reduced.

Several modifications had to be made so that the main program PENMAIN would simulate the nucleus decay. Firstly, for each source to be simulated, a subroutine describing the decay scheme of the radionuclide had to be developed. For complicated decay schemes, some simplifications may be necessary. Using a random number generator within the subroutine, the decay path is randomly selected, taking into consideration the emission probabilities. The subroutine output, which is the photon or photons emitted for the specific decay, is then fed to PENMAIN to be simulated. Therefore, one simulation loop corresponds to one subroutine call and one or more photons emitted by the source. In the course of this work, subroutines were developed for ^{60}Co, ^{88}Y, ^{57}Co, and ^{134}Cs decay. A suitable variable incorporated into the main program input file is used for the radionuclide selection. The major modifications within the main program PENMAIN include a new loop to simulate all photons emitted from the same decay event within the same shower. Stacks and counters, originally reset upon the conclusion of a photon simulation history, are now reset after a decay loop is concluded.

Qualitative evaluation of the modified code

In order to qualitatively evaluate the results of the modified main program PENMAIN, several scenarios were simulated, for:

- an Extended Range Ge (XtRa) detector of 104% rel.eff. and FWHM = 2.04 keV @ 1332.5 keV, and
- four point sources (^{60}Co, ^{88}Y, ^{57}Co, and ^{134}Cs) positioned on the detector endcap.

Figure 1 presents the simulation spectrum of the ^{60}Co point source positioned on the XtRa detector endcap. The photopeaks of the two photons emitted in cascade are observed at the energies of 1173 keV and 1332 keV, respectively, as well as the summing photopeak at 2505 keV. Furthermore, the backscatter peak at ~210 keV, the single escape peak of the 1173 keV photon at 821 keV and the two Compton edges at ~960 keV and ~1120 keV are also observed. The small peak observed at the energy of 1994 keV is due to the summation of one of the two photons emitted by the source with the escape peak of the other (1173 keV + 1332 keV – 511 keV). Finally, the Compton edge observed at ~2300 keV is due to the summation of one of the photons emitted by the source with the other photon scattered at the detector.

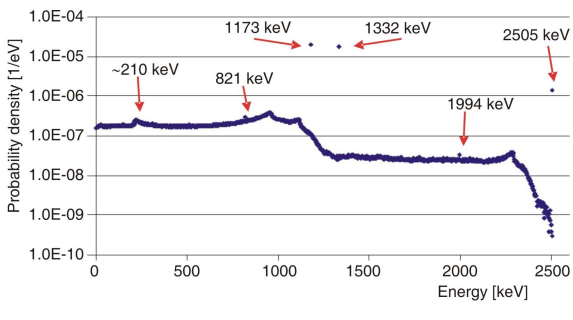

Figure 1. Simulation spectrum of a ^{60}Co point source on the XtRa detector endcap

In a similar way, the simulated spectrum of ^{134}Cs source is presented in fig. 2. In this spectrum, the nine photopeaks due to its most significant photons are observed at the energies of 475 keV, 563 keV, 569 keV, 604 keV, 795 keV, 801 keV, 1038 keV, 1167 keV, and 1365 keV, respectively. Furthermore, summation peaks at 1079 keV, 1173 keV, 1399 keV, 1407 keV, and 1642 keV and Compton edges at ~425 keV and ~600 keV are also observed.

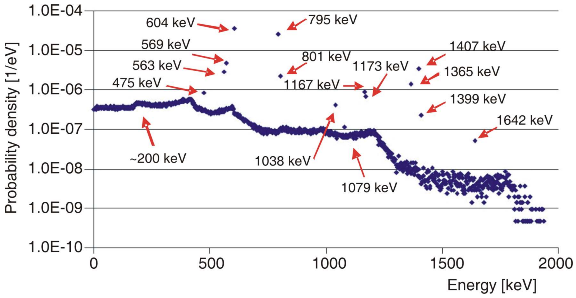

Figure 2. Simulation spectrum of a ^{134}Cs point source on the XtRa detector endcap

From the simulation results presented in figs. 1 and 2, it can be concluded that the modified PENMAIN may reproduce with a single run the full spectrum of a simulated radioactive source, including True Coincidence photopeaks.

Quantitative evaluation of the modified code

For the quantitative evaluation of the modified code results, comparison of the full energy peak efficiency calculated using the modified code, with the experimentally determined peak efficiency was made. The XtRa detector geometric characteristics used for this simulation have been previously determined using an iterative procedure [19]. Efficiency was determined for 1173 keV and 1332 keV photon energies (^{60}Co) and for a point and a volume source geometry. For the experimental determination of the detector efficiency two certified ^{60}Co experimental sources were used: a point source and a cylindrical source (Ø72 mm, height: 69 mm), both positioned on the detector endcap.

The comparison of the modified code results with the respective experimental ones is presented in tabs. 1 and 2 for the XtRa detector and for the two geometries. This comparison was based on the relative bias and a *U*-test calculated as [20]

$$U \quad \frac{|Value_2 \quad Value_1|}{\sqrt{unc_1^2 \quad unc_2^2}} \qquad (2)$$

where $Value_1$ and $Value_2$ are the individual results under comparison and unc_1 and unc_2 the corresponding uncertainties at 1σ level. The results are considered as statistically different at a 95% confidence level for $U < 1.96$. From the results presented in tabs. 1 and 2, it can be concluded that the full energy peak efficiency values obtained experimentally and via simulation are not statistically different. Overall, the relative bias for all source geometries was lower than 4%. It should be noted that the uncertainties of the simulated results given in tabs. 1 and 2 are underestimated, since they do not include type B uncertainty due to detector geometrical characteristics, which is estimated to ~3%. However, if this uncertainty is also taken into consideration, the *U*-values will be even lower.

RESULTS AND DISCUSSION

For the calculation of the tcc factors using the simulation results, the following procedure was followed for each radioactive source:
- the original main program PENMAIN was used for the determination of the full energy peak efficiency for all photons emitted by the sources under investigation. It is implied that the code should run separately for each photon energy,
- the modified main program PENMAIN was used for the simulation of the decay of each source under investigation. From the simulation results the full energy peak efficiency was calculated for all photons emitted by the source, and
- true coincidence correction factors were calculated using formula 1.

The tcc factors were determined for two source geometries: (1) point source at the detector endcap, and (2) volume source Ø72 mm, height 69 mm on the detector endcap, and four radionuclides (^{60}Co, ^{88}Y, ^{57}Co, and ^{134}Cs).

For each source-to-detector geometry and photon energy, tcc factors were also determined using the TrueCoinc program. The full-energy peak efficiency and the total-to-peak efficiency curves needed as input for TrueCoinc program were determined experimentally or via simulation.

Table 1. Cobalt-60 point source positioned on the XtRa detector endcap

Energy [keV]	Experiment		Simulation		Comparison	
	Efficiency	unc. (1σ)	Efficiency	unc. (1σ)	Relative bias	*U*-test
1173	0.051	4.05%	0.0513	0.51%	–0.49%	0.121
1332	0.046	4.05%	0.0465	0.54%	–2.74%	0.670

Table 2. Cobalt-60 volume source (72 mm, height: 69 mm) positioned on the XtRa detector endcap

Energy [keV]	Experiment		Simulation		Comparison	
	Efficiency	unc. (1σ)	Efficiency	unc. (1σ)	Relative bias	*U*-test
1173	0.0159	3.02%	0.0165	1.44%	–3.71%	1.099
1332	0.0148	3.02%	0.0151	1.50%	–2.31%	0.683

Table 3. Cobalt-60 point source on the XtRa detector endcap

Energy [keV)]	Efficiency ratio (PENELOPE)		TrueCoinc program results		Comparison	
	Ratio	unc. (1σ)	tcc	unc. (1σ)	Relative bias	*U*-test
1173	0.8025	1.00%	0.785	2.00%	–2.23%	0.992
1332	0.7904	1.04%	0.784	2.00%	–0.81%	0.359

Table 4. Yttrium-88 point source on the XtRa detector endcap

Energy [keV)]	Efficiency ratio (PENELOPE)		TrueCoinc program results		Comparison	
	Ratio	unc. (1σ)	tcc	unc. (1σ)	Relative bias	*U*-test
898	0.732	0.74%	0.709	2.00%	–3.20%	1.497
1836	0.725	1.19%	0.715	2.00%	–1.29%	0.554

Table 5. Cobalt-57 point source on the XtRa detector endcap

Energy [keV)]	Efficiency ratio (PENELOPE)		TrueCoinc program results		Comparison	
	Ratio	unc. (1σ)	tcc	unc. (1σ)	Relative bias	*U*-test
14.4	0.685	0.15%	0.669	2.00%	–2.40%	1.195
122	1.009	0.22%	0.982	2.00%	–2.72%	1.352
136	1.115	0.24%	1.139	2.00%	–2.08%	1.031

Table 6. Ceasium-134 point source on the XtRa detector endcap

Energy [keV)]	Efficiency ratio (PENELOPE)		TrueCoinc program results		Comparison	
	Ratio	unc. (1σ)	tcc	unc. (1σ)	Relative bias	*U*-test
604	0.734	0.86%	0.733	2.00%	–0.11%	0.049
795	0.734	1.01%	0.734	2.00%	0.05%	0.021
801	0.64	1.69%	0.621	2.00%	–3.41%	1.285
1038	0.87	3.17%	0.936	2.00%	6.74%	1.890
1167	1.29	2.47%	1.375	2.00%	6.07%	1.984
1365	1.65	2.13%	1.610	2.00%	–2.62%	0.885

Table 7. Cobalt-60 volume source (72 mm, height: 69 mm) on the XtRa detector endcap

Energy [keV)]	Efficiency ratio (PENELOPE)		TrueCoinc program results		Comparison	
	Ratio	unc. (1σ)	tcc	unc. (1σ)	Relative bias	*U*-test
1173	0.929	1.72%	0.930	2.00%	0.14%	0.054
1332	0.900	1.82%	0.928	2.00%	–3.06%	1.147

Table 8. Yttrium-88 volume source (72 mm, height: 69 mm) on the XtRa detector endcap

Energy [keV)]	Efficiency ratio (PENELOPE)		TrueCoinc program results		Comparison	
	Ratio	unc. (1σ)	tcc	unc. (1σ)	Relative bias	*U*-test
898	0.97	1.59%	0.933	2.00%	–3.64%	1.407
1836	0.89	1.56%	0.928	2.00%	3.96%	1.583

Table 9. Cobalt-57 volume source (72 mm, height: 69 mm) on the XtRa detector endcap

Energy [keV)]	Efficiency ratio (PENELOPE)		TrueCoinc program results		Comparison	
	Ratio	unc. (1σ)	tcc	unc. (1σ)	Relative bias	*U*-test
14.4	0.87	1.46%	0.902	2.00%	3.72%	1.522
122	0.959	0.40%	1.000	2.00%	4.09%	2.099
136	1.043	0.41%	1.000	2.00%	–4.32%	2.111

Table 10. Ceasium-134 volume source (72 mm, height: 69 mm) on the XtRa detector endcap

Energy [keV)]	Efficiency ratio (PENELOPE)		TrueCoinc program results		Comparison	
	Ratio	unc. (1σ)	tcc	unc. (1σ)	Relative bias	*U*-test
604	0.94	1.62%	0.905	2.00%	–3.98%	1.521
795	0.95	1.69%	0.905	2.00%	–4.56%	1.711
801	0.88	2.30%	0.858	2.00%	–2.60%	0.842
1038	0.89	4.73%	0.967	2.00%	8.02%	1.674
1167	1.03	3.57%	1.095	2.00%	6.33%	1.625
1365	1.10	3.11%	1.166	2.00%	5.40%	1.519

The TCC factors obtained via Monte-Carlo simulation and the TrueCoinc program are presented in tabs. 3-6, for the case of the point source positioned on the detector endcap and in tabs. 7-10 for the case of the volume source (Ø72 mm, height: 69 mm).

In almost all cases, the experimental and the simulation results are statistically in agreement, with the relative bias lower than 3% for ^{60}Co, 4% for ^{88}Y, 5% for ^{57}Co, and 8% for ^{134}Cs, indicating that the proposed procedure can be used for the accurate determination of tcc factors. It is interesting to notice that, in the case of ^{57}Co volume source (tab. 9) although the relative biases are lower than ~5%, the values of the *U*-test are within the uncertainty region. This could be attributed to the very low energy of the 14.4 keV photons involved, for which, the full energy peak efficiency and total-to-peak efficiency curves that were fed to TrueCoinc program, were experimentally determined, with relatively high uncertainty.

CONCLUSION

During this work the simulation code PENELOPE (version 2005) was appropriately modified in order to simulate the decay of a series of radionuclides. For this purpose, a simulation loop includes all photons emitted from a single nucleus decay. The modified code is therefore capable of simulating the effect of the True Coincidence phenomenon. For the determination of tcc factors a procedure based on the use of the modified PENELOPE code was proposed and applied for several scenarios of real sources for which True Coincidence may be a significant problem. The obtained tcc results were compared to the respective experimental results, showing that deviations were, in most cases, very low and statistically insignificant.

AUTHOR CONTRIBUTIONS

The modifications of the Monte Carlo code PENELOPE were carried out by D. A. Chionis and M. I. Savva under the supervision of M. J. Anagnostakis. The evaluation of the modified code using the True Coinc program was carried out by D. A. Chionis and K. L. Karfopoulos under the supervision of M. J. Anangostakis. All authors analysed and discussed the results. The manuscript was written by M. I. Savva and reviewed by all other authors.

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ОДРЕЂИВАЊЕ КОРЕКЦИОНИХ ФАКТОРА ЗА ДЕТЕКТОВАЊЕ СТВАРНЕ КОИНЦИДЕНЦИЈЕ УПОТРЕБОМ МОНТЕ КАРЛО СИМУЛАЦИЈА

Циљ овог рада је нумерички прорачун корекције детекције стварне коинциденције употребом Монте Карло симулација. За ово је коришћен Монте Карло програмски пакет PENELOPE тако што је главни програм PENMAIN прилагођен како би се испитао феномен детекције стварне коинциденције. Овако прилагођен главни програм коришћен је за утврђивање ефикасности детекције максималног пика енергије код XtRa Ge детектора са релативном ефикасношћу од 104% уз добро слагање добијених и експерименталних резултата за фотоне ^{60}Co енергија од 1173 keV и 1332 keV. Корекциони фактори за детекцију стварне коинциденције одређени су као однос ефикасности детекције максималног пика енергије добијене оригиналним и модификованим програмом PENMAIN. Развијена метода примењена је на ^{57}Co, ^{88}Y и ^{134}Cs, као и на две геометрије извор-детектор. Добијени резултати упоређени су са оним добијеним кодом TrueCoinc и релативно одступање било је мање од 2%, 4% и 8% за ^{57}Co, ^{88}Y и ^{134}Cs, респективно.

Кључне речи: стварна коинциденција, Монте Карло, PENELOPE, корекциони фактор