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Technical note

Note on the comparison of experimental and simulated gamma energy spectra for NaI with ^{137}Cs, ^{60}Co, and ^{241}Am

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ABSTRACT

Experimental and simulated energy spectra of ^{137}Cs, ^{60}Co, and ^{241}Am standard gamma sources were acquired. A spectrometer consisting of a NaI(Tl) scintillation detector was used to obtain experimental spectra. The theoretical energy spectra were acquired by means of FLUKA Monte Carlo (MC) simulations, and the comparison between the experimental and simulated spectra was performed with the ROOT program. Spectral results such as energy resolution, counting efficiency, peak to total, peak to Compton and peak to valley values were compared. Good agreement between the experimental and simulated spectra was performed with the ROOT program. Good agreement between the experimental and simulated results was obtained.

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1. Introduction

The interaction of radiation with matter can be simulated using the well-known Monte Carlo (MC) method. MC simulations require relevant data such as geometry details and properties of the radiation source of interest (particle type, energy, radiation direction, etc.), description of the detector (target) of interest and its surrounding, and physics models and data libraries to be used (De Lima, 2011).

In nuclear medicine, the development of new imaging devices, reconstruction algorithms, correction and optimization techniques, acquisition protocols, and description of time variable phenomena, such as detector or source movements, are frequently based on appropriate simulations, particularly using MC techniques similar to those used in particle physics (De Lima, 2011). One of the commercially available MC programs is FLUKA (Ferrari et al., 2005; Battistoni et al., 2007). The main reason for developing FLUKA in the past was to realistically simulate radiation interactions in matter using accurate physics models (Ferrari et al., 2005; Battistoni et al., 2007).

ROOT is an object-oriented framework aimed at solving the data analysis challenges of high-energy physics. It is based on C++ language. It is additionally used for advanced data analysis such as MC simulations in the field of subjects. Further information can be found in its user guide (ROOT, 2009).

Many inorganic scintillators are crystals of the alkali metals, in particular alkali iodides, that contain a small concentration of an impurity for example NaI(Tl). The element in parentheses is the impurity or activator (Tsoulfanidis, 1995). The most notable property of NaI(Tl) is its excellent light yield. It has come to be accepted as the standard scintillation material for routine gamma-ray spectroscopy (Knoll, 2000).

In many applications of radiation detectors, the object is to measure the energy distribution of the incident radiation. These efforts are classified under the general term radiation spectroscopy (Knoll, 2000). For detectors designed to measure the energy of the incident radiation, the most important factor is the energy resolution. The energy resolution (R) is usually given in terms of the full width at half maximum (FWHM) and the energy (or channel) corresponding to the maximum of a peak (Leo, 1994).

Uncharged radiations such as gamma-rays or neutrons must first undergo a significant interaction in the detector before detection is possible. Because these radiations can travel large distances between interactions, detectors are often significantly less than 100% efficient. It then becomes necessary to have precise figure for the detector efficiency in order to relate the number of pulses counted to the number of neutrons or photons incident on the detector (Knoll, 2000). Hence, the absolute counting efficiency (ε_{abs}) is defined as

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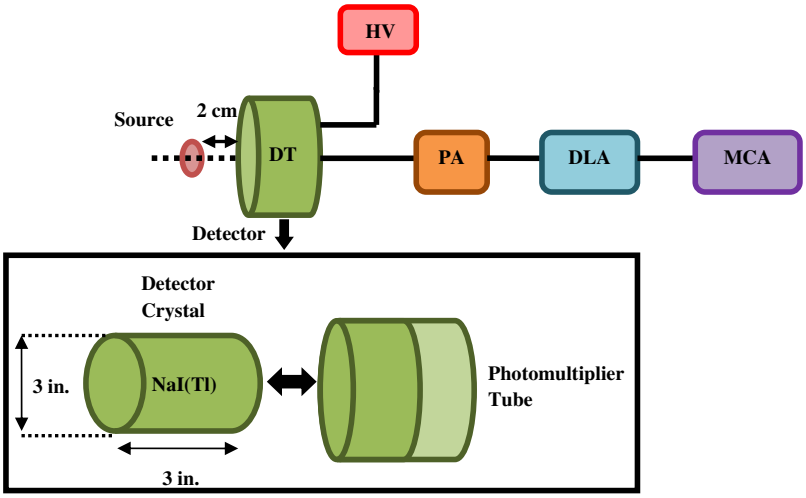


Fig. 1. Block diagram of the measurement configuration.

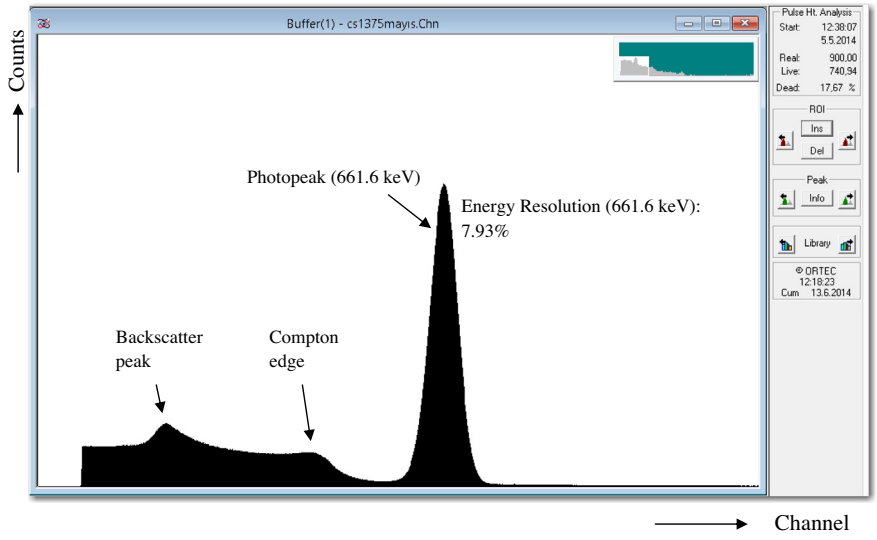


Fig. 2. Experimental energy spectrum of ^{137}Cs.

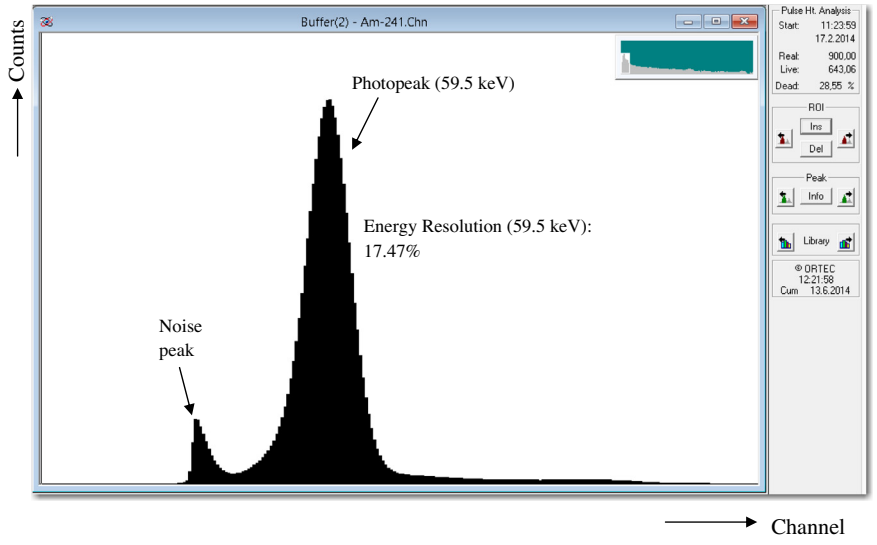


Fig. 3. Experimental energy spectrum of ^{241}Am.

$$\varepsilon_{abs} = \frac{\text{number of pulses recorded}}{\text{number of radiation quanta emitted by source}} \quad (1)$$

The peak to total ratio (PT) is determined from the number of photopeak counts divided by the total area under the photopeak (Knoll, 2000).

$$PT = \frac{\text{number of recorded photopeak counts}}{\text{total area under the photopeak}} \quad (2)$$

Peak to Compton ratio (PC) is the ratio of the counts in the highest photopeak channel to the counts in a typical channel of the Compton continuum associated with that peak (Knoll, 2000).

$$PC = \frac{\text{number of photopeak counts}}{\text{number of counts corresponding to the Compton edge}} \quad (3)$$

Peak to valley ratio (PV) is also defined as the ratio of the highest peak counts to the valley counts (Abbene et al., 2007).

$$PV = \frac{\text{number of recorded photopeak counts}}{\text{number of counts corresponding to the valley}} \quad (4)$$

Another important parameter for the measurement is the absolute photopeak counting efficiency (PCE_{abs}). This quantity is determined from Eq. (5) in parallel with Eq. (1).

$$PCE_{abs} = \frac{\text{number of recorded counts under the photopeak}}{\text{number of radiation quanta emitted by source}} \quad (5)$$

Chen and Wei (2008) studied characteristics of cadmium zinc telluride (CZT) and NaI spectrometers by using an MC code. Gamma-ray response functions of an NaI(Tl) detector were determined by means of MC simulations by Shi et al. (2002). Orion and Wielopolski (2000) carried out a simulation study of response functions of bismuth germanate (BGO) and NaI(Tl) detectors at various energies. FLUKA simulations were used to determine the response function of a neutron detector by Borio

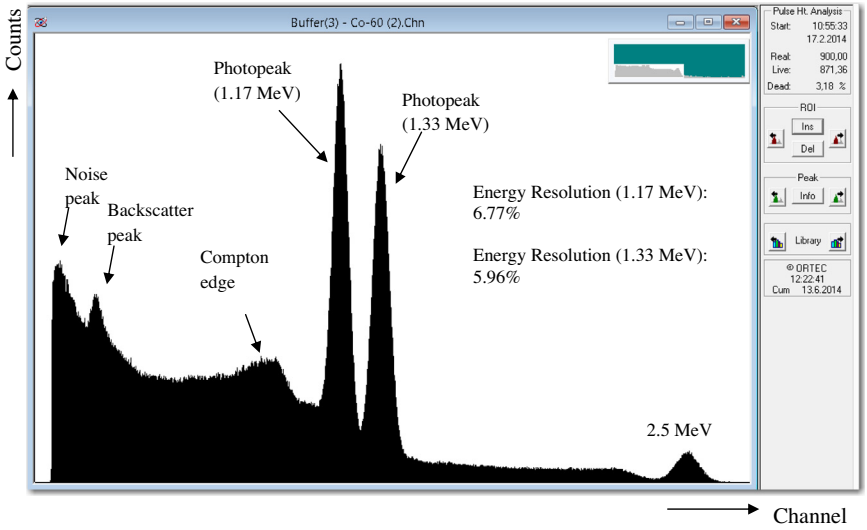


Fig. 4. Experimental energy spectrum of ^{60}Co.

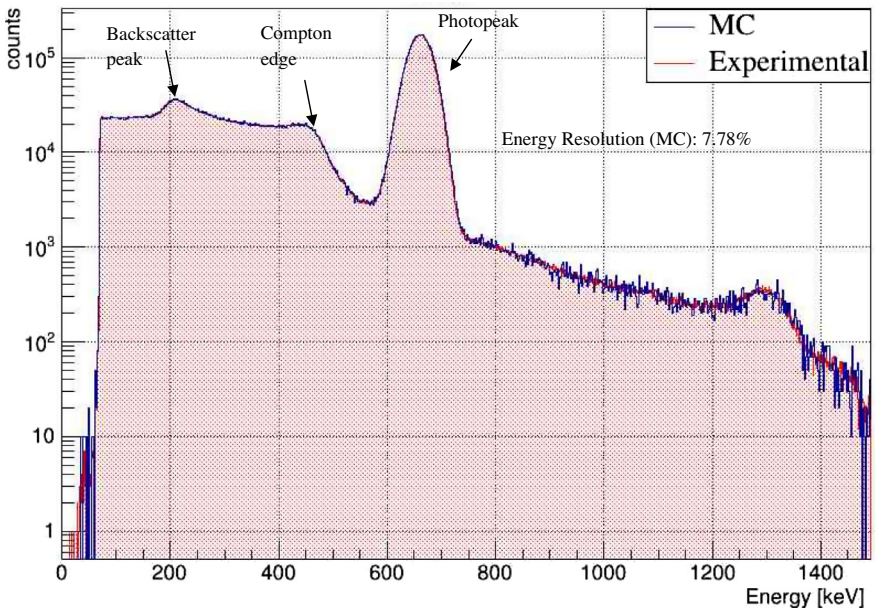


Fig. 5. Comparison of simulated and experimental gamma energy spectra for ^{137}Cs.

di Tigliole et al. (2001). Ashrafi et al. (2006) modeled an NaI(Tl) detector by using GEANT. Coincidence measurements were carried out by using a spectrometer which consisted of NaI(Tl) detectors by Britton et al. (2013), and the obtained experimental results were compared to the results acquired with GEANT4. Janus and Wojtowicz (2009) obtained ^{137}Cs energy spectrum by using BaF_2:-Ce scintillator.

The experimental and theoretical ^{137}Cs, ^{241}Am, and ^{60}Co energy spectra were obtained in this study. Their experimental energy spectra were acquired by using an NaI(Tl) detector. Energy spectra of these gamma sources, FLUKA MC simulations and ROOT program were used for direct comparison.

2. Experimental and simulation configurations

The experimental energy spectra of the aforementioned gamma sources were acquired by using an NaI(Tl) scintillation detector.

Solid ^{137}Cs, ^{241}Am, and ^{60}Co radioactive standard point sources were used in this work. The activities of the sources were 5 (±20%), 10 (±5%), and 0.1706 (±1.9%) μCi, respectively. ^{137}Cs, ^{241}Am, and ^{60}Co isotopes emit 661.60 keV, 59.50 keV, 1.17 and 1.33 MeV-energy gammas, respectively. The NaI(Tl) scintillation detector manufactured by REXON Inc. (Beachwood, OH, USA) has a diameter of 7.62 cm and a thickness of 7.62 cm. The PMT was an RCA 4879A with a diameter of 7.62 cm. It was interfaced to the crystal with an optical silicone grease 0.0762 cm thick. The unit had an aluminum housing and Teflon reflector with thicknesses of 0.07112 and 0.0508 cm have been used between the crystal and the inside. All gamma sources were placed in 2 cm away from the detector face. The data acquisition time was set to 900 s. The measurement configuration is shown in Fig. 1.

In this configuration, the detector output was sent to a preamplifier (PA, Ortec 113). Its output was connected to a delay line amplifier (DLA, Ortec 460). This amplifier was used to avoid the

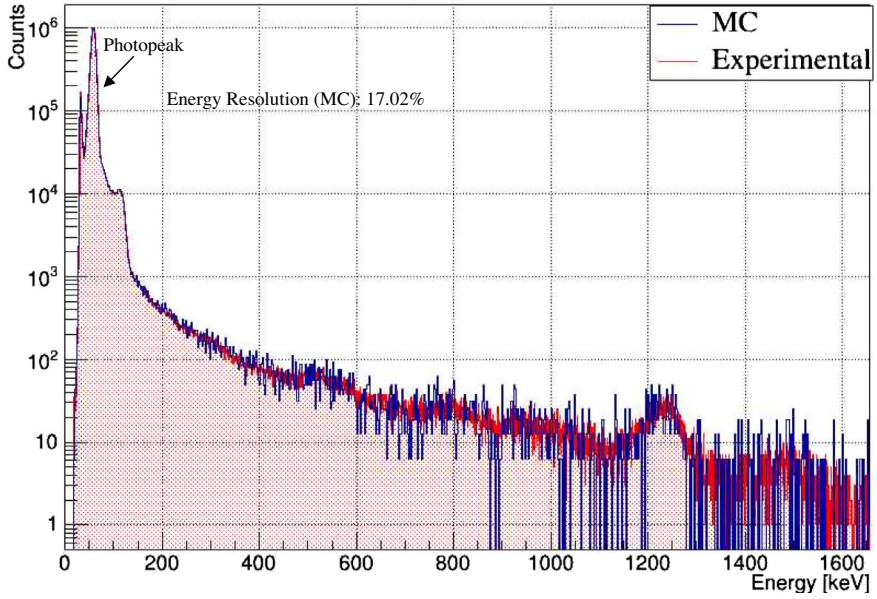


Fig. 6. Comparison of simulated and experimental gamma energy spectra for ^{241}Am.

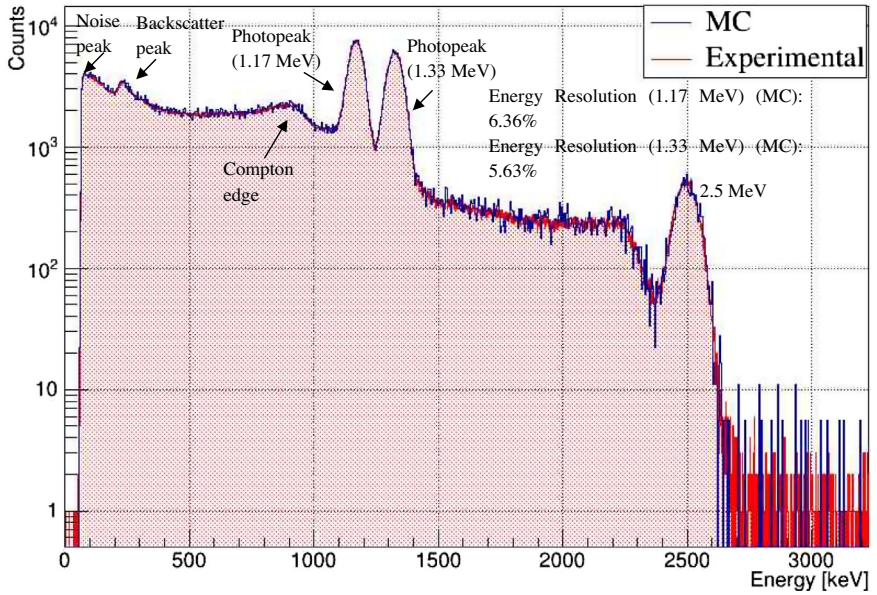


Fig. 7. Comparison of simulated and experimental gamma energy spectra for ^{60}Co.

Table 1
Obtained energy resolution (R), absolute counting efficiency (ε_{abs}), peak to total ratio (PT), peak to Compton ratio (PC), peak to valley ratio (PV) and photopeak counting efficiency (PCE_{abs}) values for ^{137}Cs.

Method	R (%)	ε_{abs} (%)	PT (%)	PC	PV	PCE_{abs} (%)
Experimental	7.93 ± 0.02	9.27 ± 0.01	2.34 ± 0.10	8.89 ± 0.03	59.06 ± 0.06	4.50 ± 0.09
Theoretical	7.78 ± 0.02	9.28 ± 0.01	2.10 ± 0.12	9.18 ± 0.03	62.89 ± 0.06	4.92 ± 0.09
Relative difference (%)	1.8915	0.1078	10.2564	3.2621	6.4849	9.3333

Table 2
Obtained energy resolution (R), absolute counting efficiency (ε_{abs}), peak to total ratio (PT), peak to Compton ratio (PC), peak to valley ratio (PV) and photopeak counting efficiency (PCE_{abs}) values for ^{241}Am.

Method	R (%)	ε_{abs} (%)	PT (%)	PC	PV	PCE_{abs} (%)
Experimental	17.47 ± 0.03	7.10 ± 0.04	4.78 ± 0.02	–	38.44 ± 0.03	7.10 ± 0.07
Theoretical	17.02 ± 0.03	7.40 ± 0.04	4.88 ± 0.02	–	37.33 ± 0.03	6.58 ± 0.08
Relative difference (%)	2.5758	4.2253	2.0920	–	2.8876	7.3239

Table 3
Obtained energy resolution (R), absolute counting efficiency (ε_{abs}), peak to total ratio (PT), peak to Compton ratio (PC), peak to valley ratio (PV) and photopeak counting efficiency (PCE_{abs}) values for ^{60}Co.

Method	R (%)	ε_{abs} (%)	PT (%)	PC	PV	PCE_{abs} (%)
Experimental (for 1.17 MeV)	6.77 ± 0.06	52.06 ± 0.03	1.51 ± 0.04	3.95 ± 0.10	5.29 ± 0.07	8.65 ± 0.01
Theoretical (for 1.17 MeV)	6.36 ± 0.06	53.82 ± 0.03	1.57 ± 0.04	4.34 ± 0.09	5.64 ± 0.06	8.67 ± 0.01
Relative difference (%) (for 1.17 MeV)	6.0561	3.3807	3.9735	9.8734	6.6162	0.2312
Experimental (for 1.33 MeV)	5.96 ± 0.06	52.06 ± 0.03	1.46 ± 0.02	4.11 ± 0.04	4.21 ± 0.04	7.12 ± 0.01
Theoretical (for 1.33 MeV)	5.63 ± 0.06	53.82 ± 0.03	1.49 ± 0.02	4.27 ± 0.04	4.39 ± 0.04	7.14 ± 0.01
Relative difference (%) (for 1.33 MeV)	5.5369	3.3807	2.0548	3.8929	4.2755	0.2809

baseline shift. The bipolar output of the DLA was then directed to a multichannel analyzer (MCA, Ortec Trump 8 K) in order to acquire the energy spectrum for each gamma source.

In order to obtain theoretical energy spectra of the gamma sources of interest, FLUKA (ver. 2011.2.15) was used. It was installed on Ubuntu (ver. 11.04) operating system. In the program, source and detector were modeled with high accuracy (the same NaI size, detector and reflector). The densities of NaI crystal and Al reflector were taken as 3.667 and 2.700 g/cm^3, respectively in FLUKA. EM-CASCA physics list was used to achieve the energy spectra of the gamma sources of interest. Electromagnetic interactions were taken into account in the physics list. Rayleigh scattering and inelastic form factor corrections to Compton scattering and Compton profiles, detailed photoelectric edge treatment and fluorescence photons were also activated. The FLUKA data were plotted with ROOT program (ver. 5.30/02). ROOT was also used to read the values such as number of recorded photopeak counts in Eqs. (1)–(5). Obtained experimental and theoretical spectra were compared through ROOT.

3. Results

The experimental energy spectra of the isotopes are shown in Figs. 2–4. These figures are the screen captured view of the MCA.

The gross count rates in the photopeaks for ^{137}Cs, ^{241}Am, and ^{60}Co (for 1.17 MeV and 1.33 MeV peaks) from the experimental results were calculated as 17,144, 26,275.541, 545.912, and 449.416 s^{-1}, respectively. The total count rates of gamma sources of interest were also determined. These values for ^{137}Cs, ^{241}Am, and ^{60}Co were calculated as 17,150, 2627, and 3286 s^{-1}, respectively.

The theoretical energy spectra obtained with FLUKA were compared with the experiments in ROOT program. Figs. 5–7 shows these comparisons.

Absolute counting efficiency (ε_{abs}), peak to valley, and peak to Compton ratios, and absolute efficiency values were calculated using Eqs. (1)–(5). The background counts were not taken into account because the background count rate was relatively low (~108 s^{-1}) when compared to the sources counts. These results, together with the calculated energy resolution values are given in Tables 1–3 with their standard deviations.

4. Conclusions and discussion

The energy spectra of standard gamma sources (^{137}Cs, ^{241}Am and ^{60}Co) were obtained by using experimental and theoretical methods. The experimental energy spectra of the isotopes were acquired with an NaI(Tl) spectrometer. FLUKA and ROOT programs were used to obtain theoretical spectra and compare them with experiments. Authors' comprehensive literature survey has indicated that no study published in the past included the simulated and measured energy spectra acquired for the aforementioned gamma sources in conjunction with an NaI(Tl) detector. In addition, the level of agreement between the spectra is excellent.

Since the dead time, which equals to real time minus live time (real time: elapsed time or clock time, live time: the time that the detector is available to accept another pulse (ORTEC MCA (Maestro For Windows) Manual, 2000), values of the MCA for each isotope were lower than 30–40% (Figs. 2–4), it can be concluded that the measurements had not included in the negative effects such as pulse pile-up, peak broadening and spectrum distortion (Knoll, 2000; Leo, 1994; Nicholson, 1974). The conclusions above can also be attributed to the theoretical results.

Obtained theoretical energy spectrum of ^{137}Cs using FLUKA and plotted via ROOT is in better agreement with the experiment (Fig. 5) than the other studies (Chen and Wei, 2008; Shi et al., 2002; Ashrafi et al., 2006; Britton et al., 2013). The ^{137}Cs simulated energy spectrum is in excellent agreement with the experiment, especially in the low energy region (Fig. 5). Such agreement was not achieved in the paper of Britton et al. (2013) since this region could not be resolved in their simulations as stated by the authors.

Unlike the study of Ashrafi et al. (2006), the simulation spectra presented in this study were acquired with FLUKA, and the experimental and theoretical spectra were compared via ROOT in the present work. While in Ashrafi et al., the authors compared their

spectra up to ~700 keV, the energy range in this study was wider (up to 1.5 MeV). Moreover, the discrepancy between the spectra is smaller in this study.

The value of energy bin, which equals number of divisions corresponding to maximum energy per energy range, was chosen as 1 keV in our study as indicated in the paper of Ashrafi et al. (2006) to compare our results with their results. Better accordance between our experimental and theoretical spectra was obtained in comparison to the work of Ashrafi et al.

The absolute counting efficiency values have increased with increasing gamma energy while the energy resolution improves as can be seen in Tables 1–3. These results were in accordance with the literature (Akkurt et al., 2014; ORTEC AN34 Application Note, 2012; Moszynski et al., 2002).

We also measured and simulated the energy spectra of ^{241}Am and ^{60}Co to verify the agreement between simulations and measurements for gamma energies different from 662 keV (^{137}Cs). The energy spectra for these gamma sources are in excellent agreement as shown in Figs. 6 and 7.

R, ε_{abs}, PT, PC, PV, and PCE_{abs} values calculated from the experimental and theoretical spectra were also in excellent agreement as shown in Tables 1–3.

In this study, for the first time NaI(Tl) simulated and measured gamma energy spectra were simultaneously compared for ^{137}Cs, ^{241}Am, and ^{60}Co. It has been concluded that the simulated and measured spectra for all three sources are in excellent agreement and that the established simulation methodology proved accurate for NaI(Tl) detectors.

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