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Original Article

Determination of energy resolution for a NaI(Tl) detector modeled with FLUKA code

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ABSTRACT

In this study, 3″ × 3″ NaI(Tl) detector, which is widely used in gamma spectroscopy, was modeled with FLUKA code, and calculations required to determine the detector's energy resolution were reported. Photon beams with isotropic distribution with 59, 81, 302, 356, 511, 662, 835, 1173, 1275, and 1332 keV energy were used as radiation sources. The photon pulse height distribution of the NaI(Tl) without influence of its energy resolution obtained with FLUKA code has been converted into a real NaI(Tl) response function, using the necessary conversion process. The photon pulse height distribution simulated in the conversion process was analyzed using the ROOT data analysis framework. The statistical errors of the simulated data were found in the range of 0.2–1.1%. When the results, obtained with FLUKA and ROOT, are compared with the literature data, it is seen that the results are in good agreement with them. Thus, the applicability of this procedure has been demonstrated for the other energy values mentioned.

1. Introduction

The NaI(Tl) detector, commonly used for gamma spectroscopy, takes advantage in many nuclear experiments because it has high detection efficiency even at room temperature. For this type of scintillation detector, the response function obtained is not proportional to the photon's energy and depends on the crystalline structure used. Therefore, detector's sensitivity calibration is needed. For a promising performance scintillator, energy and resolution calibration must be done precisely, along with efficiency calibration. The energy resolution for any detector is known as the ability to distinguish between two peaks. This feature depends on the FWHM (Full Width at Half Maximum) value. The lower the FWHM value, the greater the detector's sensitivity, and it will distinguish between two gamma rays with close energies coming from the source to the detector [1–3].

The calculations of resolution can also be done using simulation techniques, as can be done by establishing an experimental system. The simulation techniques are quite successful in this process, and a variety of simulation approaches are available in the literature [4–14]. For this purpose, Monte Carlo based programs such as FLUKA, MCNPX, EGS, GEANT4 are beneficial.

In this study, the resolution calculations were done with the FLUKA for 3″ × 3″ NaI(Tl) detector. The energy spectra were obtained, taking advantage of energy deposited in the NaI scintillation crystal for photons with 59, 81, 302, 356, 511, 662, 835, 1173, 1275, and 1332 keV energy. FWHM and energy resolution values were calculated from the data generated in FLUKA, based on the Poisson statistic. The results of from the present work were compared with experimental and other simulation results published found in the literature.

2. Materials and method

2.1. FLUKA simulation parameters for NaI(Tl) detector

FLUKA is a Fortran-based Monte Carlo code used to calculate particle transport and interaction with matter developed by CERN (European Organization for Nuclear Research) and INFN (Italian National Institute for Nuclear Physics). FLUKA is used in problems that include hadronic and electromagnetic interactions and can be applied in many different fields such as nuclear physics, high energy physics, and particle physics [16]. FLUKA has a FLAIR interface for editing the input file, executing the code, and visualizing the

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output files [17]. This study was done with the FLUKA version 2011.2x.8. in the Fedora 28 (Linux-based operating system), the input file was edited with the FLAIR-2.3-0 version.

In the FLUKA code, there are user default settings called "DEFAULT" cards for the specific type of problem. For this study, this card was selected as "PRECISIon". The EMF (electromagnetic interactions) is active, and the EMF cut-off energies for photons and electrons are determined as 10^{-6} GeV. The computer system for simulations is Intel Xeon 2.00 GHz CPU, 32 GB DDR3 RAM. In order to minimize the statistical errors, 10^5 particles were run ten cycles. The statistical errors of the results in all simulations were between 0.2 and 1.1%.

In this study, a detector taken from Canberra Company was modeled using the FLUKA code. This detector has been previously used in similar experimental and simulation studies [9,18]. As shown in Fig. 1, the detector is a cylindrical NaI(Tl) crystal of 7.62 cm × 7.62 cm, covered with a 0.05 cm thick Al, and the next inner layer is MgO. The SiO_2 layer is present at the end of the NaI crystal. In simulation geometry, the NaI(Tl) detector is placed inside a cylindrical 6 cm-thick Pb shield to provide precisely the experimental environment. The densities of the NaI, MgO, Al, and SiO_2 materials used in the simulation were defined as 3.67 g/cm^3, 3.58 g/cm^3, 2.70 g/cm^3, and 2.648 g/cm^3, respectively. In the simulations, the relevant energies are defined as isotropic gamma sources in the BEAM card. The gamma sources were placed 0.5 cm away from the NaI detector, and a simulation was performed for each source. The results were obtained by DETECT card, which scores energy deposition on an event by event basis. The DETECT card's output gives a signal (event) spectrum distributed over a fixed number of 1024 channels in the standard version [16].

2.2. Details of the conversion process of NaI photon pulse height distribution

The DETECT card records the amount of deposited energy per each scintillation event. The number of counts generated in the NaI crystal depending on the energy, is obtained in the FLUKA calculations; the energy deposition spectrum in these detectors behaves according to Poisson statistics. If the mean number of scintillation events generated is $\overline{N}$, the statistical fluctuation in that number is given as [2].

$$\sigma = \sqrt{\overline{N}} \tag{1}$$

The standard deviation, given in Eq. (1), can also be expressed in terms of deposited energy as follows;

$$\sigma(E) = \sqrt{E_m}.\sqrt{\overline{E}} \tag{2}$$

where $\overline{E}$ is the average deposited energy in the crystal after the scintillation events. E_m is the smallest energy value measured; it was determined to 1 keV at FLUKA calculations. If we are only concerned with fluctuations in the signal, the response function approximates the Gaussian shape because $\overline{N}$ is too large. The FWHM for a Gaussian distribution is given by;

$$\text{FWHM} = 2\sqrt{2ln2}.\ \sigma \tag{3}$$

$$R = \frac{FWHM}{E_0} \tag{4}$$

where E_0 is the central energy of the photopeak.

The single peaks obtained by FLUKA calculations were converted to real detector response through the conversion process. The Gaussian distribution fits for photopeaks in spectra were made with the ROOT analysis program (version 5.34/36) [19] using σ values calculated from Eq. (2).

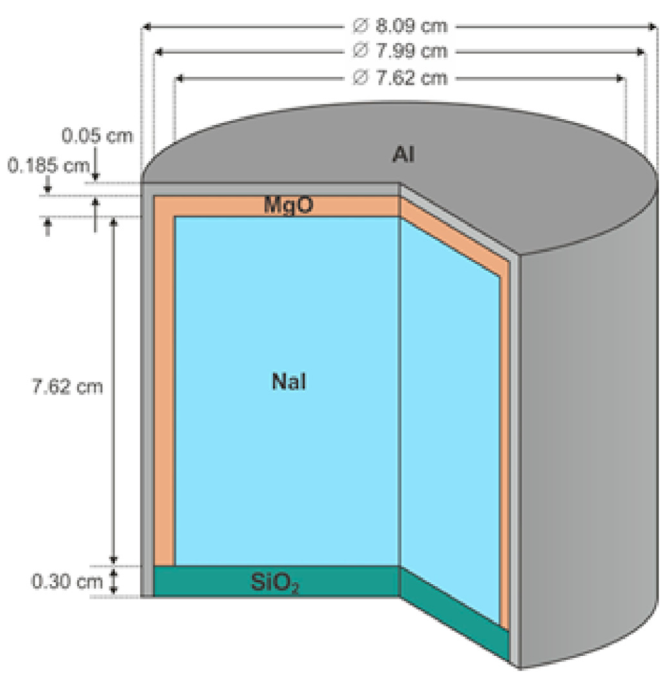

Fig. 1. Schematic representation of NaI(Tl) detector.

3. Results and discussion

3.1. Calculation the energy resolution of 3″ × 3″ NaI(Tl) detector

The energy resolution of a 3 ″ × 3 ″ cylindrical NaI(Tl) detector is usually measured using 662 keV gamma rays emitted by the ^{137}Cs source. The energy resolution at this energy is around 6–7% [2]. In this work, the energy resolution and FWHM values calculated for the 59 keV–1332 keV energy range using Eqs. (1)–(4) are given in Table 1. The calculated results were compared with the data obtained by Tam et al. [13] since the detector geometry was suitable for our study. The relative differences (RD(%) = |A − B|/Ax100) between the resolutions reported in the literature [13] (A) and the resolutions calculated in this study (B), were determined. It is observed from Table 1 that the FLUKA results are in good agreement with experimental and GEANT4 results. In the literature [15], Akkurt et al. found the energy resolution value for 662 keV and 1332 keV, respectively 7%, 4.8%. The largest difference of 4.4% was found to be for the energy of 1332 keV. As it is known, the MC uncertainties are small and only statistical. In this study, the simulation program was run with 10^6 primary particles. If the number of the particle histories is increased, these differences at high energies will decrease. Since no suitable for our geometry was found in the literature for energies lower than 511 keV, a complete comparison could not be made. However, Salgado et al. [10] found 19% resolution for 59 keV gamma energy for 1.5 ″ × 1 ″ NaI(Tl) detector and Casanovas et al. [5] 18% resolution for 2 ″ × 2 ″ NaI(Tl) detector. We calculated 22.02% resolution for 59 keV gamma energy. Depending on the obtained results and the literature, it observed that the resolution values increase rapidly at low energies. The curves of the energy resolution and FWHM are shown as a function of energy in Fig. 2(a–b). As seen in Fig. 2, as the energy increases, the FWHM increases, and the detector's energy

Table 1
Comparison of energy resolution and FWHM values of the 3″ × 3″ NaI(Tl) detector for 59 keV–1332 keV energy range.

Energy (keV)	FWHM (keV)	Energy resolution (R %)			
	Calculated (FLUKA)	Calculated (FLUKA)	Tam et al., 2017 [13] (Exp.)	Tam et al., 2017 [13] (Geant4)	Relative differences RD (%)
59	13.1	22.02	–	–	–
81	15.1	18.62	–	–	–
302	29.0	9.59	–	–	–
356	31.5	8.85	–	–	–
511	37.7	7.38	7.29	7.27	1.23 to 1.92
662	42.9	6.48	6.44	6.54	0.62 to 0.91
835	48.2	5.77	5.90	5.93	2.20 to 2.70
1173	57.1	4.87	4.98	4.96	2.21 to 1.81
1275	59.5	4.67	4.81	4.87	2.91 to 4.11
1332	60.8	4.57	4.78	4.74	4.40 to 3.58

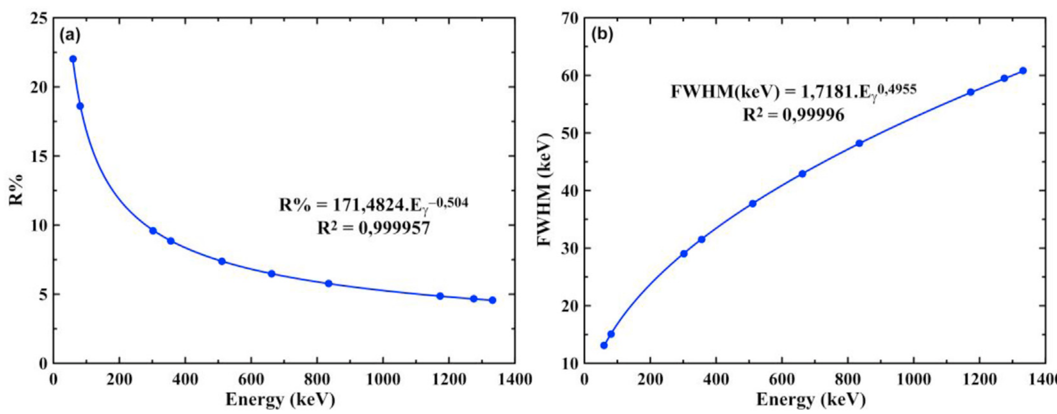

Fig. 2. The curve of (a) energy resolution and (b) FWHM as a function of gamma energy.

resolution improves. FWHM (E) function is expressed by a power law ($x.E^y$) and the value of R^2 (correlation coefficient) was found as 0.99996.

3.2. Convolution of photon pulse height simulated by FLUKA with resolution

In the model simulated energy spectrum, the energy peaks are ideally a single line. A photopeak is obtained that shows a Gaussian distribution above or below this peak, which is not a single line due to detector energy resolution in a NaI(Tl) detector. In this part of our study, the effect of energy resolution on the photon pulse height distribution obtained with the FLUKA code for a NaI(Tl) crystal with and without resolution correction was investigated.

The spectrum obtained by the FLUKA code does not include the broadening effect of the photopeak and the detector's response functions. One of the impacts that broaden photopeak is specific for the electronic circuit of the spectrometric system [10]. In other words, the photon pulse height distribution, the energy resolution, and other effects related to the photomultiplier tube, have not been taken into account in the simulation. The photon pulse height distribution consists of the bins in which each of their energy is set to 1 keV, using the DETECT card in the FLUKA code. The spectra obtained by simulation are converted to real detector response using the sigma values calculated theoretically. Fig. 3 shows the photon spectra obtained for a bare NaI(Tl) crystal with and without resolution correction for 356, 511, 662, 835, 1173, and 1332 keV, respectively. The spectra are shown only for the most commonly used energies in resolution studies to keep the figures reasonable.

Fig. 3 shows that the photopeak, photo escape peaks, Compton edge, annihilation peak, and x-ray peaks were observed at the expected energies. In addition, the main peaks in all spectra are marked on the graph. The peak observed at the lowest energy in the spectra is the characteristic X-ray that occurs in the atom's inner shells as a result of the internal conversion event. Gamma rays from the source can make Compton scattering from materials around the detector and enter the detector again. As a result, a backscatter peak may occur in the energy range of 200–250 keV in the low energy region. The electrons emitted from the Compton effect are absorbed in the detector and form the Compton area in the detector's photon energy spectrum. This area ends at a point called Compton edge. Fig. 3 shows the change of Compton edge depending on the photon energy. The equation used in determining the Compton edge is given below.

$$E_c = E\frac{2E/mc^2}{1+2E/mc^2} \quad (5)$$

Where E and E_c are the energy of the incident photon and the energy of the Compton edge, respectively. Based on Eq. (5), it is seen that the energy of the Compton edge increases as the photon energy increases. Also, the filling of the region between the Compton edge and the photopeak in the spectrum is related to more than one multiple Compton scattering of the incoming photon [2]. If the energy of the gamma rays coming out of the source is high, an annihilation peak of 511 keV is observed, as in Fig. 3 and 1332 keV, due to the possibility of pair production. Double or single escape peaks appear in the gamma spectrum if both or one of the annihilation photons of the pair production escapes from the detector volume. In the spectrum for 1332 keV gamma energy, single and double escape peaks were observed at 821 keV and 310 keV, respectively. In the energy spectrum for 1173 keV, a single escape

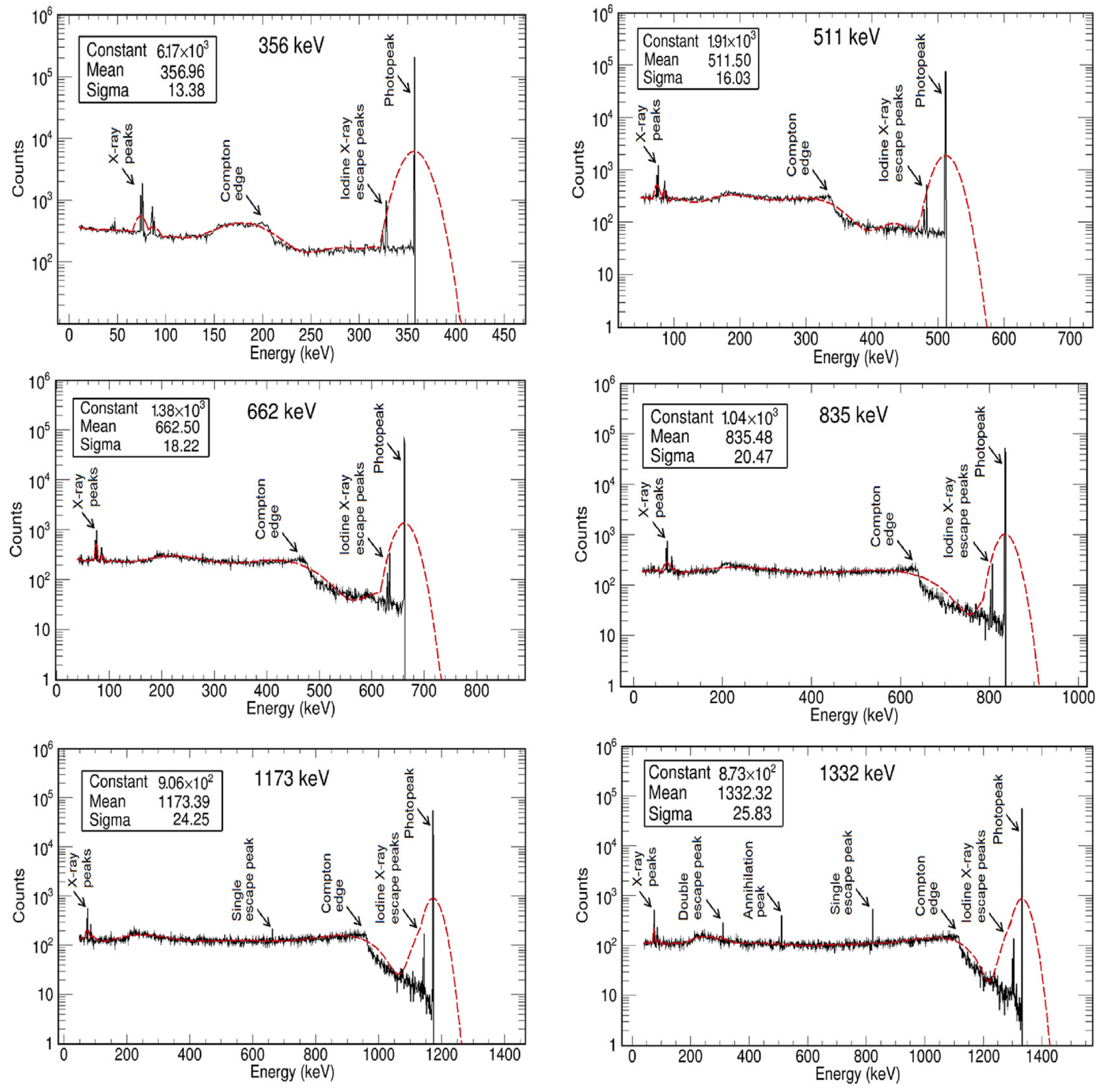

Fig. 3. The photon pulse height distribution obtained by the FLUKA code for a NaI(Tl) crystal at 356 keV–1332 keV gamma energy with and without resolution correction.

peak was observed at 662 keV, since only one of the annihilation photons escaped from the detector volume. The two consecutive peaks to the left of the photopeak in the spectra at energies ~28 keV less than the full-energy absorption peaks are attributed to Iodine X-rays escape [20].

4. Conclusion

In this study, a 7.62 cm × 7.62 cm cylindrical NaI(Tl) detector was modeled using the FLUKA code. The simulation parameters and FLUKA code information were given in detail. The pulse height distributions of a 3 ″ × 3 ″ NaI(Tl) detector were obtained for each point gamma source in the energy range 59 keV–1332 keV, and the energy resolution was calculated. It was observed that the results found were in agreement with the studies in the literature. Relative percentage differences with other results ranged from 0.62 to 4.4. In the spectra obtained, the photo peaks correspond to a Gaussian distribution with sigma values calculated from Eq. (2). Compton continuum was also fit using polynomial functions. The ROOT data analysis program performed these processes. In the literature, simulation codes such as MCNPX and GEANT4 have mainly been used to calculate the detector response function. It can be seen that there is less research on this topic using FLUKA than using other codes. This study showed that the FLUKA code can be successfully used to determine the energy resolution of a 7.62 × 7.62 cm cylindrical NaI(Tl) detector. Simulations provide accurate pre-calculations for any detector design or experiment system design. They are of great importance in terms of cost and time.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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