



Optimization of the Monte Carlo simulation model of NaI(Tl) detector by Geant4 code

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HIGHLIGHTS

- Effect of reflection layer on the efficiency of NaI(Tl) detector was significant.
- Effective thickness of the reflection layer was estimated by Geant4 code.
- A complete procedure for optimizing the simulation model of NaI(Tl) detector was proposed.
- A very good agreement between the simulated results and the experimental data was observed.

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ABSTRACT

This work aimed to optimize the Monte Carlo simulation model of NaI(Tl) detector by Geant4 code. For detector modeling, the geometrical parameters are usually derived from the manufacturer's specification because of availability and convenience. However, the difference between real and nominal values in geometrical parameters of the detector can considerably affect the simulation results. To overcome this problem, a complete procedure for optimizing the geometrical parameters of the detector was proposed in this study. The results showed a good agreement between the simulated and experimental values, and the maximum discrepancy between the experimental and simulated values was 3.96%, 1.69%, and 3.50% for full-energy peak efficiency, energy resolution, and peak to Compton ratio, respectively.

1. Introduction

Thallium-activated sodium iodide crystal, NaI(Tl), was invented in 1948 (Hofstadter, 1949). It has been widely used in many fields, especially in industries (Tam et al., 2015; Thanh et al., 2015) and radiological protection. This type of detector has the advantage of operating at room temperature with high detection efficiency. NaI(Tl) detector operates by collecting the visible light generated in the sensitive volume of the detector and transferring them into electric signal through a photomultiplier (PMT). Al₂O₃ or MgO powder is generally used as a reflection layer surrounding the scintillation crystal to improve the efficiency of the detector (Eissa and Arafa, 2014). The considerable effect of this reflection layer on the efficiency of the NaI(Tl) detector was reported in a previous study (Tam et al., 2016). In fact, this parameter is not always known precisely for many reasons. Therefore, to obtain more reliable data, full knowledge of the geometrical parameters is required.

Currently, the Monte Carlo method is one of the commonly used methods in nuclear physics. Geant4 code is based on this method to simulate the photon interaction within the sensitive volume of a detector. The obtained results from Geant4 code were used in such a way that the reliability of the experimental results increased. In studies that used a semi-empirical method such as the measurement of the pipe wall thickness (Nguyen et al., 2016), the simulated spectrum was used as a substitute for the measured one to save time and money. This requires a highly precise and reliable simulation model.

For studies that use the simulation spectrum as a substitute for the experimental one, the detector modeling should be evaluated in more detail, both quantitatively, the full-energy peak efficiency, and qualitatively, the response form of the spectrum, energy resolution, and peak to Compton ratio. Most studies related to Geant4 and MCNP (Monte Carlo N-Particle) simulations of NaI(Tl) detector use the geometrical parameters specified by the manufacturer. In this case, the response function is usually used to evaluate the agreement between the

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simulation model and the experimental result. This cannot be applied for all cases because Tam et al. (2016), showed that there was a big discrepancy between the simulated and experimental values of efficiency although the response forms of their spectra were similar.

In the present work, we propose a complete procedure to optimize the simulation model applied to the NaI(Tl) detector. It is to be noted that the purpose of this study is not to determine exactly the real geometrical parameters of the detector. Instead, we determine the effective geometrical parameters for the simulation model so that the features of both simulated and experimental spectra match well with each other. From the obtained results, the geometrical parameters were validated, which can be used in further practical applications. The results obtained from this work are a note for modeling the detector.

2. Methodology

Geant4 code has become a dominant and reliable toolkit. However, it can be used only if geometrical detector parameters are available. To validate the simulation modeling of NaI(Tl) detector, a three-step procedure was proposed as follows:

- First, a spectrum was simulated using the geometrical parameters specified by the manufacturer for modeling the detector.
- Second, the simulated and experimental values of full-energy peak efficiency, energy resolution, and peak to Compton ratio were compared to evaluate the accuracy of the geometrical parameters provided by the manufacturer.
- Finally, the geometrical parameters were adjusted in such a way that the response form of spectrum, energy resolution, peak to Compton ratio and especially full-energy peak efficiency are suitable with the experimental data.

In general, two indicators are used to qualitatively evaluate the response form of a spectrum: peak to Compton ratio and energy resolution. The peak to Compton ratio is defined as the ratio of the counts at the photopeak position to those at the flat portion of the Compton continuum just below the Compton edge. It was calculated using the following equation:

$$\text{Peak to Compton ratio} = \frac{C_p}{\frac{1}{m-n+1} \sum_{m-n+1}^m C_i} \quad (1)$$

where C_p is the counts in the highest photo-peak channel, C_i is the counts at the i -th channel, and m and n are the channel numbers specifying the regions of interest.

Energy resolution is defined as the ratio of full width at half maximum (FWHM) to the energy of that peak (E_0). The energy resolution was determined using the following equation:

$$\text{Energy resolution} = \frac{\text{FWHM}}{E_0} \quad (2)$$

FWHM depends on the detector type and the energy of gamma photons. The FWHM can be mathematically expressed as follows (Amgarou et al., 2009; Kovaltchouk and Machrafi, 2011; Baccouche et al., 2012):

$$\text{FWHM} = a + b\sqrt{E} + cE^2 \quad (3)$$

where a , b , and c are the parameters obtained by fitting Eq. (3) with the experimental data.

In practice, the FWHM of a spectrum is as follows (Casanovas et al., 2012):

$$\text{FWHM} = 2\sqrt{2 \ln 2} \sigma \quad (4)$$

where σ is the standard deviation.

For the quantitative evaluation of the simulation model, the full-energy peak efficiency should be used. The simulated full-energy peak

efficiency was calculated using the following equation:

$$\text{Full-energy peak efficiency} = \frac{N_{\text{FEP}}}{N} \quad (5)$$

where N_{FEP} represents the net count in the full-energy peak corresponding to energy E and N is the number of photons emitted by the source of energy E .

3. Monte Carlo simulation

3.1. Geant4 simulation code

Geant4 (G4 collaboration, 2003) is an open-source C++ toolkit for simulating the passage of particles through matter. By using the toolkit, we designed a framework for a wide-range of applications from fundamental physical phenomena to a full detector simulation. The code allowed us to control all the simulation aspects of an experimental measurement system, such as system geometry configuration, primary particle generation in the events, and types of particle and even physics processes that govern particle interactions. It can provide particle tracks and collect momentum and energy at each interaction step, and other useful information on particle interactions. In this work, we used Geant4 version 10.01 to obtain an energy spectra of gamma radiation sources deposited on the NaI(Tl) detector. The physics list used in this study is the standard provided G4EmPenelopePhysics.

3.2. NaI(Tl) detector description in Geant4 code

In this work, detector model is constructed according to 76BR76 NaI (Tl) provided by Amptek, Inc. The NaI(Tl) scintillation crystal is cylindrical in form. The cross-sectional view of the detector was described in detail in Fig. 1 with density of materials attached in Table 1.

Most geometrical parameters provided by the manufacturer, as shown in Table 1, are kept constant in the simulation, except the PMT and the Al_2O_3 reflection layer. PMT modeling is very difficult because of its complex structure. Fortunately, it can be replaced by an aluminum cylinder with dimensions of 83.2×30 mm (Shi et al., 2002). The effect of reflection layer on the full-energy peak efficiency of the detector has been already reported in the literature. In addition, the Al_2O_3 reflection material in powder form caused some difficulties in detector modeling because of its indefinite thickness. To overcome this problem, a solid

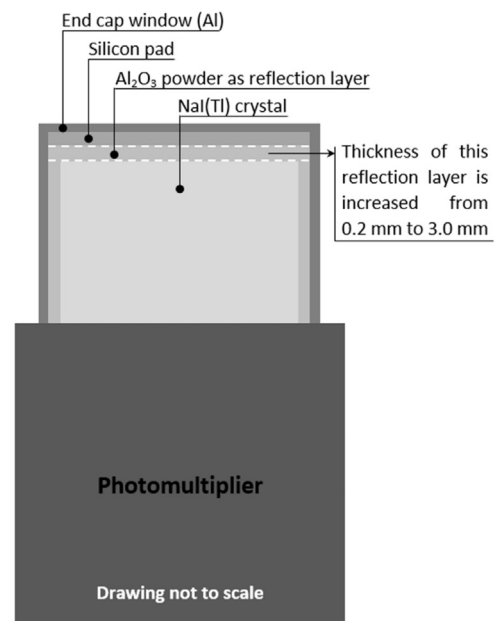


Fig. 1. Schematic diagram of the cross-sectional view of NaI(Tl) detector.

Table 1
Geometrical description of NaI(Tl) detector, as provided by the manufacturer.

Component		Value
Material	Density of Al layer	2.700 g cm ⁻³
	Density of silicon layer	2.329 g cm ⁻³
	Density of Al ₂ O ₃ layer	3.970 g cm ⁻³
	Density of NaI(Tl) crystal	3.667 g cm ⁻³
NaI(Tl) detector	NaI(Tl) crystal diameter	76 mm
	NaI(Tl) crystal length	76 mm
	End cap window thickness (Al)	1.5 mm
	Silicon pad thickness	2.0 mm
	End cap wall thickness (Al)	1.5 mm
	Al ₂ O ₃ reflection thickness at the front	3.0 mm
	Al ₂ O ₃ reflection thickness from the side	2.0 mm
	Photomultiplier tube (PMT)	To be treated as aluminum cylinder with dimensions of 83.2 × 30 mm

Al₂O₃ layer with a definite thickness was substituted for the powder Al₂O₃ in simulation. This implies the need for estimating the effective thickness of the reflection layer.

The Al₂O₃ reflection layer includes two parts: one layer is at the front of the NaI(Tl) crystal and the other surrounds the NaI(Tl) crystal. Because the source is placed at the front of the detector, the effect of the front reflection on the efficiency is much more significant than that of the side reflection layer. Therefore, in the present work, we evaluated only the effect of the front reflection layer on the efficiency.

Radioactive sources used in the simulation are gamma standards (from Eckert & Ziegler manufacturer), including the ²²Na, ¹³⁷Cs, ⁵⁴Mn, ⁶⁵Zn, and ⁶⁰Co sources. They were placed at a distance of 20 cm from the outer surface of the NaI(Tl) detector and on the symmetric axis of the detector. The source modeling in Geant4 code is identical to the real source. This implies that the geometrical specification of the source case, including the material of source, given by the manufacturer was included in modeling.

In this work, we were interested in reproducing gamma spectra using Geant4 code and determining the full-energy peak efficiency, energy resolution, and peak to Compton ratio. The spectrum was obtained from simulation by recording the deposit energy of the detector crystal. In addition, to compare with the experimental spectrum, it is necessary to apply the Gaussian distribution to the simulated data with corresponding FWHM described in Eq. (3), where a = -0.0137257 MeV, b = 0.0739501 MeV^{1/2}, and c = -0.152982 MeV⁻¹ (Tam et al., 2016), which represent the detector resolution. The spectra obtained from Geant4 code was analyzed by Colegram software (Lépy, 2004).

The relative error of simulation was calculated using the following equation:

Table 2
Full-energy peak efficiency, energy resolution, and peak to Compton ratio for different energies with geometrical parameters of the NaI(Tl) detector from the manufacturer.

Nuclides	Energy (keV)	Full-energy peak efficiency			Energy resolution			Peak to Compton ratio		
		Exp. ($\times 10^{-3}$) (Tam et al., 2016)	Geant4 ($\times 10^{-3}$)	RD (%)	Exp.	Geant4	RD (%)	Exp.	Geant4	RD (%)
²² Na	511	3.63 (11)	3.28	9.73	7.29	7.27	0.27	–	–	–
¹³⁷ Cs	661.657	2.98 (9)	2.69	9.65	6.44	6.54	1.56	9.71	9.28	4.51
⁵⁴ Mn	834.838	2.49 (7)	2.25	9.47	5.90	5.93	0.38	8.66	8.30	4.16
⁶⁵ Zn	1115.539	1.97 (6)	1.80	8.23	5.14	5.17	0.68	–	–	–
⁶⁰ Co	1173.228	1.85 (6)	1.64	11.07	4.98	4.96	0.34	3.78	3.74	1.05
²² Na	1274.537	1.75 (5)	1.63	6.95	4.81	4.87	1.28	–	–	–
⁶⁰ Co	1332.492	1.69 (5)	1.56	7.40	4.78	4.74	0.68	3.24	3.27	0.78

Table 3
Slope coefficients for different thicknesses of Al₂O₃ reflection layer.

	Thickness of reflection layer	Slope coefficient	R ²
Simulation	0.2	-0.82181	0.9943
	0.4	-0.81838	0.9949
	0.6	-0.81578	0.9954
	0.8	-0.81400	0.9943
	1.0	-0.81012	0.9951
	1.2	-0.80867	0.9956
	1.4	-0.80727	0.9949
	1.6	-0.80131	0.9947
	1.8	-0.80016	0.9951
	2.0	-0.79928	0.9948
	2.2	-0.79525	0.9954
	2.4	-0.79261	0.9949
	2.6	-0.79263	0.9945
2.8	-0.78764	0.9952	
3.0	-0.78557	0.9946	
Experiment		-0.80707	0.9989
Interpolation reflection layer (mm)	1.31		

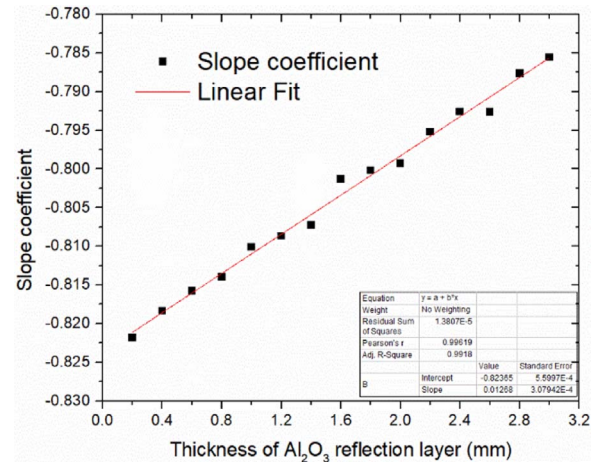


Fig. 2. Linear increase in slope coefficient with the increase in thickness of the reflection layer.

$$u_{sim} = \frac{\sqrt{N_{FEP}}}{N_{FEP}} \tag{6}$$

In the present work, the value of u_{sim} is below 0.5%.

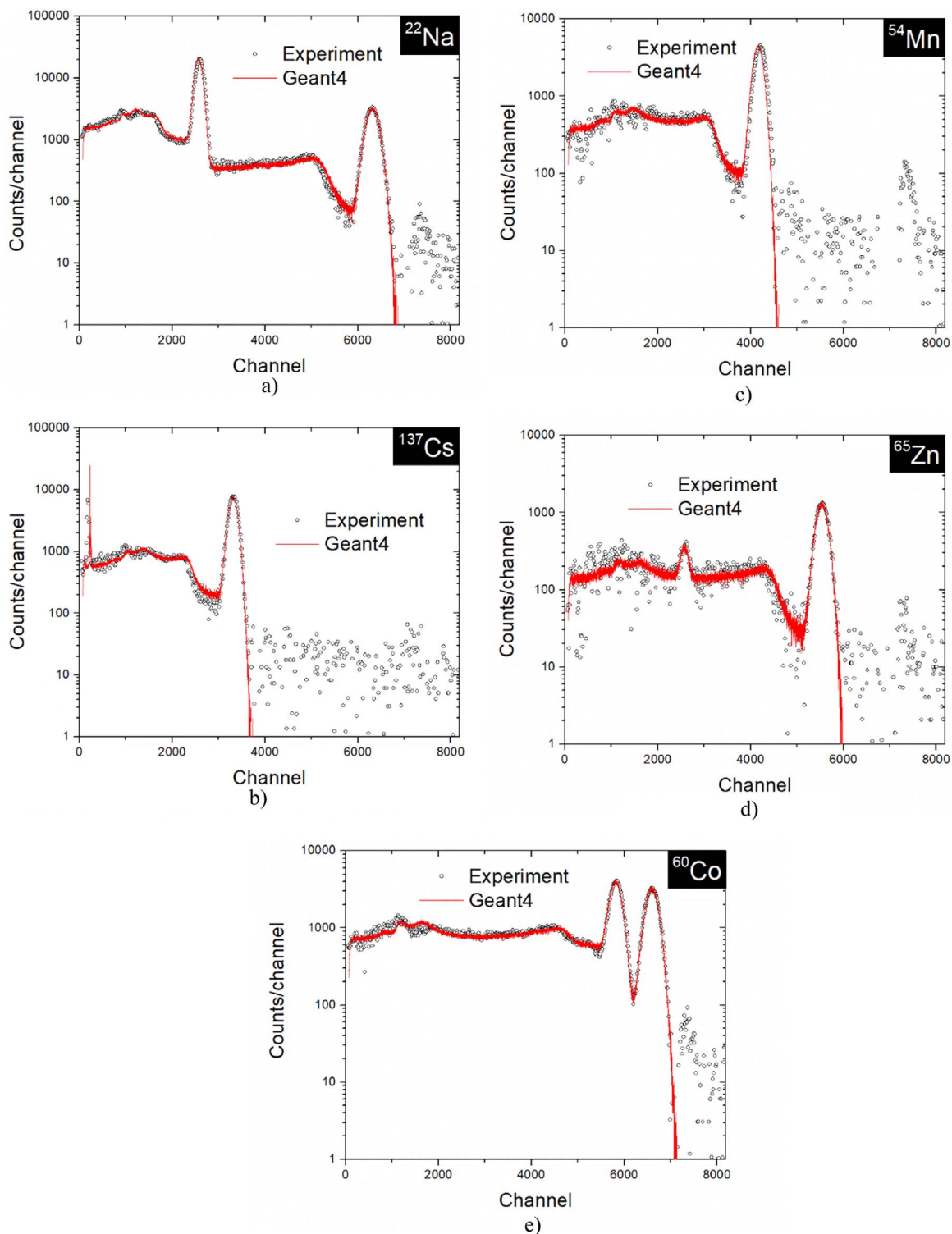


Fig. 3. Simulated and experimental spectra with the optimized thickness of reflection layer of 1.31 mm.

4. Results and discussion

4.1. Estimation of effective thickness of the reflection layer

In an attempt to evaluate the simulation model using Geant4 code, the NaI(Tl) detector was modeled using the geometrical specifications from the manufacturer, Amptek Inc. Table 2 presents the obtained results from the analysis of simulated and experimental spectra. The discrepancies between the simulated and the experimental values were

relatively small, which were below 1.6% and 4.6% for energy resolution and peak to Compton ratio, respectively. This implies that the simulated spectrum is in accordance with the experimental one in response function. However, the relative deviation values of simulated to experimental efficiencies were very significant at most energy levels and even above 11% at 1173 keV. This implies that the reliability of the simulation model is not high if the geometrical parameters from the manufacturer are used without any changes. Thus, it is necessary to optimize the geometrical parameters of the NaI(Tl) detector.

Table 4

Full-energy peak efficiency, energy resolution, and peak to Compton ratio for different energies with optimized geometrical parameters of the NaI(Tl) detector.

Nuclides	Energy (keV)	Full-energy peak efficiency		Energy resolution		Peak to Compton ratio	
		Geant4 ($\times 10^{-3}$)	RD (%)	Geant4	RD (%)	Geant4	RD (%)
^{22}Na	511	3.52	3.03	7.28	0.14	–	–
^{137}Cs	661.657	2.88	3.31	6.55	1.69	9.68	0.35
^{54}Mn	834.838	2.39	3.96	5.91	0.11	8.59	0.84
^{65}Zn	1115.539	1.90	3.30	5.19	1.12	–	–
^{60}Co	1173.228	1.80	2.37	5.04	1.30	3.91	3.50
^{22}Na	1274.537	1.71	2.10	4.88	1.37	–	–
^{60}Co	1332.492	1.67	1.17	4.78	0.13	3.35	3.32

$$\text{RD} = \frac{|\text{Exp.} - \text{Geant4}|}{\text{Exp.}} \times 100\%$$

For reducing the discrepancy between the simulated efficiency and the experimental one, we estimated the thickness of Al_2O_3 reflection layer according to the method described in a previous study (Chuong et al., 2016). The thickness of Al_2O_3 reflection layer in the simulation model was increased from 0.2 to 3.0 mm, with an increment step of 0.2 mm. For each thickness of the Al_2O_3 reflection layer, the full-energy peak efficiency, energy resolution, and peak to Compton ratio were recalculated. The dependence of efficiency ε corresponding to energy E (from 511 to 1332 keV) for each thickness can be mathematically described as follows:

$$\log_{10}\varepsilon = a \log_{10}E + b \quad (7)$$

where a is the slope coefficient and b is the intercept, which was obtained by fitting.

The obtained results of slope coefficients for different thicknesses of the Al_2O_3 reflection layer are presented in Table 3. The slope coefficients increased linearly with the increase in thickness of the reflection layer. From this, the slope data corresponding to each thickness of the reflection layer were fitted by a linear function, as represented in Fig. 2. The interpolation thickness of Al_2O_3 reflection layer was estimated to be approximately 1.31 mm. The thickness thus determined is the effective thickness.

4.2. Validation of the optimized simulation model of NaI(Tl) detector

Using the optimized model, the simulated spectra of ^{22}Na , ^{137}Cs , ^{54}Mn , ^{65}Zn , and ^{60}Co , which were generated by Geant4 code, are in good agreement with the experimental ones in response function as shown in Fig. 3. The discrepancy between the simulated and experimental energy resolutions is below 1.7%. The discrepancy in peak to Compton ratio is below 3.5%, which is slightly lower than that in the simulation model using the geometrical specification from the manufacturer.

Furthermore, Table 4 presents the calculated results of full-energy peak efficiency with the optimized thickness of Al_2O_3 reflection layer of 1.31 mm. It can be seen that the discrepancy between the simulated and experimental efficiency is below 4% for all energies. These values have decreased significantly in comparison with those obtained by the simulation model using the geometrical specification from the manufacturer. The results show that using the optimized model, a very good agreement with the experimental data is achieved not only in the simulated response function but also in the simulated efficiency.

5. Conclusions

The present work proposed a complete procedure including the

evaluation of full-energy peak efficiency, peak to Compton, and energy resolution for the optimization of the geometrical specification of the NaI(Tl) detector by Geant4 code. In particular, we studied and estimated the effective thickness of reflection layer of NaI(Tl) detector, which was found to be 1.31 mm. The obtained results imply that the assessment and optimization of technical parameters are required in modeling detection systems. In this work, we designed a precise simulation model for NaI(Tl) detector for future work using the Monte Carlo simulation.

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