UNCERTAINTY ANALYSIS IN THE SIMULATION OF AN HPGe DETECTOR USING THE MONTE CARLO CODE MCNP5

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ABSTRACT

A gamma spectrometer including an HPGe detector is commonly used for environmental radioactivity measurements. Many works have been focused on the simulation of the HPGe detector using Monte Carlo codes such as MCNP5. However, the simulation of this kind of detectors presents important difficulties due to the lack of information from manufacturers and due to loss of intrinsic properties in aging detectors. Some parameters such as the active volume or the Ge dead layer thickness are many times unknown and are estimated during simulations. In this work, a detailed model of an HPGe detector and a petri dish containing a certified gamma source has been done. The certified gamma source contains nuclides to cover the energy range between 50 and 1800 keV. As a result of the simulation, the Pulse Height Distribution (PHD) is obtained and the efficiency curve can be calculated from net peak areas and taking into account the certified activity of the source. In order to avoid errors due to the net area calculation, the simulated PHD is treated using the GammaVision software. On the other hand, it is proposed to use the Noether-Wilks formula to do an uncertainty analysis of model with the main goal of determining the efficiency curve of this detector and its associated uncertainty. The uncertainty analysis has been focused on dead layer thickness at different positions of the crystal. Results confirm the important role of the dead layer thickness in the low energy range of the efficiency curve. In the high energy range (from 300 to 1800 keV) the main contribution to the absolute uncertainty is due to variations in the active volume.

1. INTRODUCTION

A gamma spectrometer including an HPGe (High Purity Germanium) detector is commonly used for environmental radioactivity measurements. Monte Carlo codes are a useful tool to complement experimental measurements in the calibration procedures of the laboratory. Several MC codes have been widely used for efficiency calculations, for example, MCNP and GEANT codes offer a reliable tool for this purpose [1, 2]. Some of the data required for
the detector’s simulation are found in its certificate provided by the manufacturer, which describes its characteristics and dimensions. Nevertheless, some other data need to be determined by either direct measurement with a pachymeter, like the external diameter, or indirect measurements, such as dead layer and inner electrical contact. Dead layer strongly affects the measurements. Manufacturers do not offer clear information about this parameter: thickness or the variation along with time. An over or underestimation of the dead layer thickness produce strong effects in the simulation of the efficiency.

In this work, efficiency curves corresponding to a Petri dish using an HPGe detector and a gamma standards are obtained experimentally and by simulation with the Monte Carlo codes MCNP5 [3] and Sword-GEANT [4]. The goodness of the discrete energy efficiency is estimated by fitting these values to an energy-dependent polynomial function. It has been tested the effect of the matrix material (water and sand) on the efficiency curve of the detector. Geometrical uncertainties are mainly due to Ge dead layers thickness of the crystal. These values are not well known and it is required a deep analysis to determine its effect on the detector efficiency. The Noether-Wilks formula [5] has been used to carry out an uncertainty analysis of dead layers at different positions in the crystal.

2. MATERIALS AND METHODS

2.1. Detector features and experimental measurements

A High Purity Germanium (HPGe) coaxial detector system has been used for experimental measurements in the Laboratorio de Radiactividad Ambiental (LRA) of Universitat Politècnica de València (UPV). The detector model is an ORTECGMX40P4, with a closed–end coaxial geometry. The main performance specifications of the detector are as follows: relative efficiency at 1.33 MeV Co-60 is 40%, FWHM resolution of 2.0keV, Peak shape FWTM/FWHM 2.0 keV both at 1.33 MeV Co-60, and the peak-to-Compton ratio for Co-60 is 59:1. The crystal diameter is 60 mm and the length is 71.1 mm. The core hole diameter is 9 mm, and the core hole length is 63.1 mm. The end cap to crystal distance is 4 mm. The cup length is 105 mm. The cryostat window material is aluminum with 0.8 mm thickness. The crystal has also a layer of Mylar in front of the cryostat window (0.03 mm).

The effective thickness of the dead layer is not well known a cause of the existence of a transition zone between the inactive layer and the active germanium in the crystal whose thickness is very difficult to be accurately estimated. Anyway, manufactures provides a value of 700 µmGe/Li dead layer in the crystal.

The Petri dish is made of polyethylene and radionuclides are added into a matrix (water or sand).The source used for measurements is a calibration gamma standard solution, covering the energy range between 59 and 1800 keV. The radionuclides contained in the source solution are listed in Table 1 together with the main peak energy, the branching ratio and the certified activity. All of the measured gamma spectra were analyzed using the GammaVision acquisition and analysis software [6].
By direct measurement of calibration sources, experimental efficiencies in the energy range between 59 and 1800 keV were calculated. The experimental efficiency at energy $E_\gamma$ for a given measuring condition is:

$$\text{Eff}_{E_\gamma} = \frac{N_{E_i}}{A \cdot m \cdot t \cdot f}$$

(1)

Where $N_{E_i}$ is the net area under the full-energy peak corresponding to $E_\gamma$ energy photons emitted by a radionuclide with a known activity, $A$, $f$ is the branching ratio, $m$ is the sample mass and $t$ is the counting time [7].

### 2.2. Monte Carlo models

In this work MCNP5 [3] and Sword-Geant [4] codes have been used for simulating the experimental detection device of LRA. Both codes are based on the Monte Carlo method. MCNP5 is an advanced Monte Carlo code, which contains the necessary cross-section data for neutron, photon, and electron transport calculations. The code treats an arbitrary three-dimensional configuration of materials in geometric cells. A MCNP5 model has been developed for the system defined by the HPGe detector and the Petri dish. The Petri dish was filled with water containing the calibration gamma solution situated directly on top of the detector providing relatively high-efficiency geometry, as it can be seen in Figure 1 (obtained using the Sabrina program [8]).
Photon and electron transport (PHYS: P and PHYS: E) are considered in the MCNP5 model. The F8 tally (Pulse Height Distribution) has been used for photons and electrons. It has been used 8192 bins, corresponding to the number of channels of the actual detector device. Detailed physics has been taken into account (photoelectric effect with fluorescence production and incoherent scattering with form factors) in the energy range between 1 and 2000 keV. Electron generation and tracks have been considered in the simulation (MODE PE in MCNP). The use of the GEB (Gaussian Energy Broadening) card option provides a spectrum that can be compared with the experimental one in terms of resolution (FWHM). The GEB parameters specify the FWHM of the observed energy broadening in a physical radiation detector, according to Equation 2:

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

where $E$ is the energy of the particle. The units of $a$, $b$, and $c$ are MeV, MeV$^{1/2}$, and none, respectively. In this case $a=5.063\times10^{-4}$, $b=8.922\times10^{-4}$ and $c=8.096\times10^{-1}$.

SWORD, Software for the Optimization of Radiation Detectors is a software package designed for efficient description of $\gamma$-ray detectors. It is a fully integrated system that uses GEANT4 to conduct Monte Carlo simulations. It can analyze the resulting output in a single step. SWORD allows defining the radiation detection instruments by building them from basic geometric objects and assigning those objects materials, detection, and/or radioactive emission properties. Detector resolution (FWHM) is determined by means of Equation 3.

$$\text{FWHM (keV)} = \sqrt{c^2 + a^2 \left(\frac{E}{E_0}\right)}$$

$E_0=661.66$ keV; Constants $a$ and $c$ are obtained by fitting the function to the experimental FWHM values; in this case $a=1.232$ and $c=0.7329$. 

Figure 1: MCNP model geometry.
2.3. Uncertainty analysis

In a Monte Carlo simulation, uncertainties can be attributed to different causes. Attending these causes, simulation uncertainties can be divided in three categories:
1) Statistical: due to the stochastic nature of the MC method and the finite number of simulated events.
2) Input: due to the input parameters such as density, geometrical dimensions and material composition.
3) Physics: due to any systematic difference between the way the simulation models radiation interactions with matter and the way these interactions are observed.

The simulation uncertainty may be expressed as it is shown in Equation 4.

\[
\sigma_{\text{simulation}}^2 = (\sigma_{\text{statistics}}^2 + \sigma_{\text{inputs}}^2 + \sigma_{\text{physics}}^2)
\] (4)

Statistical uncertainties are normally given by Monte Carlo codes along with results of calculations.

In order to perform an uncertainty analysis of some variables, it is necessary to assign a Probability Density Function (PDF) to each one before the sampling process. PDFs quantify the likelihood that the variables will have specific values within the ranges of their variation. This initial phase of the analysis was the most subjective step of the entire process. One of the most frequently used PDFs is the uniform distribution, which assigns equal probability to any value in the range of variation of the variable. Normal and lognormal distributions are commonly used to describe experimental measurements and other natural variations.

The size of the sampling is determined from the characteristics of the tolerance intervals by applying the Noether–Wilks formula [5, 9], and according to the degree of precision desired for uncertainty measures. Thus, the number of required calculations does not depend on the number of input parameters or on any assumption about the probability distribution of results [10]. A tolerance defined in the interval between a lower (L) and upper (U) limit is an estimation of a random variable that contains a specified fraction of the variable probability, \( p \), with a prescribed level of confidence, \( \gamma \) [11]. Tolerance intervals are constructed from sampled data so as to enclose \( p\% \) of the population of a random variable \( X \) with a given confidence \( \gamma \).

If a random sample of output values has a normal PDF, it is possible to compute tolerance intervals from the sample mean, \( m_y \), and sample standard deviation, \( s_y \) as it is shown in Equation 5:

\[
(L, U) = (m_y - Ks_y, m_y + Ks_y)
\] (5)

where \( K \) is the tolerance factor, whose values depend on the sample size, probability coverage, \( p \), and confidence level, \( \gamma \). The values for \( K \) are tabulated for different \( p \), N and \( \gamma \) in standard statistical tables [11, 12]. To estimate the tolerance interval with a 95% of confidence level the minimum number of MCNP5 simulations required is 93.

After the PDFs and ranges of variation were assigned to the input variables and code models, the value of these random variables was sampled. The precision of the obtained results does
not depend on the number of input parameters, but it depends, among other factors, on the sample size and randomness of the sampling procedure [5].

This uncertainty methodology has been applied to determine the effect on the HPGe detector efficiency in the energy range between 59 and 1800 keV when the active volume and the different inactive Ge layers are not well known. For this purpose, and in order to obtain a tolerance interval with a confidence level of 95%, 93 different MCNP5 simulations have been run. Three variables have been taken into account in this analysis: Ge dead layer at top of the crystal, dead layer in the surrounding sides and dead layer surrounding the inner hole. In Figure 2, it is shown the geometry layout of the detector with the variables considered in the uncertainty analysis.

3. RESULTS AND DISCUSSION

In this section, it is shown the main results achieved in the simulation of the actual experimental acquisition process using the Monte Carlo codes MCNP5 and Sword. It is performed a comparison between experimental and simulated PHDs and efficiency curves. A sensitivity analysis is presented to highlight the relative importance of each inactive layer and the material matrix (water and sand). On the other hand, an uncertainty analysis using the Noether-Wilks formula [5] has been done in order to know the global effect of the different inactive (dead) Ge layers of the crystal.

Figure 3 shows a comparison between the experimental PHD (20000 seconds of acquisition live time with less than 0.1% of dead time) and PHDs obtained by simulation with MCNP5 and Sword. In both simulations, data corresponding to manufacturer’s information have been used (crystal dimensions and dead layer thickness). The PHD obtained with MCNP5 corresponds to one-photon emitted by the source. In order to compare experimental and simulated PHDs it is necessary to take into account the total number of gamma/s emitted by the source. For this purpose, the calculated PHD has been multiplied by the experimental
acquisition live time and by the total number of gamma/s emitted by the calibration gamma standard. Simulated PHDs with both codes have been adequately formatted to be imported by GammaVision software. Simulated PHDs are then treated as the experimental ones. The main differences between experimental and simulated PHDs can be observed in the Compton contribution for energies below 1000 keV. As it can be seen, in the experimental PHD Compton is slightly lower in comparison to simulated PHDs (MCNP and Sword).

Figure 3: Experimental and simulated Pulse Height Distribution.

In Table 2 is listed the efficiency curves corresponding to simulated and experimental efficiencies obtained with GammaVision. For both simulation models it has been considered the values of dead layer given by manufacturer. Water has been used as material matrix. Analyzing these results it can be said that the two codes overestimate the efficiency in the whole energy range considered (except Sword in the low energy range). Sword improves the results of MCNP5 in the whole interval. The maximum discrepancies between MCNP5 and Sword are found in the low energy range (Am-241, Co-57 and Cd-109). In the energy interval corresponding to Cs-137 and Y-88 (1898 keV), discrepancies between both codes are strongly reduced.

Y-88 and Co-60 are gamma emitters that present true coincidence phenomena due to cascade photon emission. This effect has not been considered in the models used in this work. True coincidence can partially explain the differences (up to 30%) respect to experimental efficiency in the case of Y-88 and Co-60.
Table 2. Efficiency calculations. Comparison Experimental / MCNP5 / Sword (water).

<table>
<thead>
<tr>
<th>Nuclide</th>
<th>Energy (keV)</th>
<th>gamma/s standard</th>
<th>Efficiency Exp (1sigma %)</th>
<th>Efficiency MCNP5 (1sigma %)</th>
<th>Ratio MCNP5 /Experim</th>
<th>Efficiency Sword (1sigma %)</th>
<th>Ratio Sword /Experim</th>
</tr>
</thead>
<tbody>
<tr>
<td>Am-241</td>
<td>59.54</td>
<td>25.69</td>
<td>0.090 (0.525%)</td>
<td>0.119 (0.452%)</td>
<td>1.31E+00</td>
<td>0.0831 (0.559%)</td>
<td>9.20E-01</td>
</tr>
<tr>
<td>Cd-109</td>
<td>88.03</td>
<td>13.17</td>
<td>0.097 (0.769%)</td>
<td>0.113 (0.663%)</td>
<td>1.16E+00</td>
<td>0.0922 (0.775%)</td>
<td>9.47E-01</td>
</tr>
<tr>
<td>Co-57</td>
<td>122.06</td>
<td>11.45</td>
<td>0.090 (0.935%)</td>
<td>0.105 (0.748%)</td>
<td>1.17E+00</td>
<td>0.0875 (0.863%)</td>
<td>9.75E-01</td>
</tr>
<tr>
<td>Ce-139</td>
<td>165.85</td>
<td>11.54</td>
<td>0.074 (1.094%)</td>
<td>0.091 (0.814%)</td>
<td>1.23E+00</td>
<td>0.0788 (0.920%)</td>
<td>1.06E+00</td>
</tr>
<tr>
<td>Cr-51</td>
<td>320.08</td>
<td>26.5</td>
<td>0.045 (0.905%)</td>
<td>0.055 (0.675%)</td>
<td>1.21E+00</td>
<td>0.0490 (0.730%)</td>
<td>1.08E+00</td>
</tr>
<tr>
<td>Sn-113</td>
<td>391.69</td>
<td>35.3</td>
<td>0.039 (0.716%)</td>
<td>0.047 (0.606%)</td>
<td>1.22E+00</td>
<td>0.0421 (0.650%)</td>
<td>1.09E+00</td>
</tr>
<tr>
<td>Sr-85</td>
<td>513.99</td>
<td>47.27</td>
<td>0.031 (0.799%)</td>
<td>0.038 (0.588%)</td>
<td>1.21E+00</td>
<td>0.0338 (0.626%)</td>
<td>1.09E+00</td>
</tr>
<tr>
<td>Cs-137</td>
<td>661.66</td>
<td>58.25</td>
<td>0.025 (0.899%)</td>
<td>0.031 (0.600%)</td>
<td>1.21E+00</td>
<td>0.0283 (0.632%)</td>
<td>1.12E+00</td>
</tr>
<tr>
<td>Mn-54</td>
<td>834.83</td>
<td>64.4</td>
<td>0.021 (0.698%)</td>
<td>0.026 (0.600%)</td>
<td>1.25E+00</td>
<td>0.0242 (0.624%)</td>
<td>1.17E+00</td>
</tr>
<tr>
<td>Y-88</td>
<td>898.02</td>
<td>92.36</td>
<td>0.020 (0.668%)</td>
<td>0.025 (0.511%)</td>
<td>1.26E+00</td>
<td>0.0229 (0.538%)</td>
<td>1.18E+00</td>
</tr>
<tr>
<td>Co-60</td>
<td>1173.24</td>
<td>72.57</td>
<td>0.015 (0.008%)</td>
<td>0.020 (0.613%)</td>
<td>1.32E+00</td>
<td>0.0188 (0.640%)</td>
<td>1.22E+00</td>
</tr>
<tr>
<td>Co-60</td>
<td>1332.5</td>
<td>72.66</td>
<td>0.014 (0.796%)</td>
<td>0.019 (0.637%)</td>
<td>1.35E+00</td>
<td>0.0177 (0.656%)</td>
<td>1.28E+00</td>
</tr>
<tr>
<td>Y-88</td>
<td>1836.01</td>
<td>97.6</td>
<td>0.010 (0.858%)</td>
<td>0.014 (0.600%)</td>
<td>1.39E+00</td>
<td>0.0137 (0.614%)</td>
<td>1.33E+00</td>
</tr>
</tbody>
</table>

Efficiency curves have been obtained for two different matrix materials: water and sand (density 3.2 g/cm³). In Figure 4 it is shown the efficiency curves obtained with MCNP5 and Sword. As it can be seen, the effect of the density (attenuation) is not negligible in the energy interval between 59 and 1800 keV). In the case of Am-241, Co-57 and Cd-109, efficiency is drastically reduced (up to 50%) when sand is used as matrix material (respect to water values). This effect is gradually reduced when energy increases, and finally, in energies corresponding to Y-88, Zn-65 and Co-60, differences are lower than 10%.

Regarding to the simulation results, the same behavior is observed when sand is used as support matrix. MCNP and Sword overestimates the efficiency in almost the complete energy range of interest.
Discrepancies found in these results can be also attributed to uncertainties of the actual crystal active volume. In fact, active volume of HPGe is not well known and normally manufacturers do not give exhaustive information about that. Furthermore, dead layer thickness increases in aged detectors. In order to understand the effects of the crystal inactive layer over efficiency, an uncertainty analysis of some geometrical features of the HPGe crystal has been performed using the Noether-Wilks formula. Three inactive layers has been taken into account in this study: top, lateral and inner hole. Figure 5 shows the efficiency obtained for the 93 different MCNP5 runs when dead layers thickness (top, lateral and inner hole) are independently varied according to a normal distribution ($x=0.75$ mm and $\sigma=0.25$ mm). In all cases it is assumed water as matrix material. Experimental efficiency is also shown in squared yellow markers.

Dead layer has an important effect in the whole energy range considered. In fact, the Wilks analysis shows that variations in top, lateral and inner hole dead layers with a normal distribution ($x=0.75$ mm and $\sigma=0.25$ mm) produce relative variations up to 50% in the efficiency. It can be also seen that the experimental efficiency is inside the range of variation except for the energies corresponding to Y-88 and Co-60 (due to true coincidence effects).

In order to study the effect of each dead layer, a sensitivity analysis has been done with MCNP5 varying dead layer thickness corresponding to the top position and lateral sides. Results are shown in Figure 6. Red curve considers a crystal with 0 mm of dead layer (top, lateral and inner hole); blue curve takes into account top dead layer (1.5 mm), lateral (0 mm) and inner hole dead layer (0 mm). Finally, orange curve has been obtained with 0 mm top dead layer, 1.5 mm lateral and 0 mm inner hole dead layer.
In the case of Am-241, 1.5 mm of top dead layer reduces efficiency by 90% respect to the model without dead layer. This effect is also important for energies up to 200 keV and it can be attributed to the attenuation of low energy photons. In the high energy range (200 – 1800 keV), the effect of top dead layer is reduced (20% reduction respect to non-dead layer model). Regarding to the lateral dead layer, it can be observed that efficiency is homogeneously reduced in the whole energy range (about 20% in all energies). This change is mainly due to a reduction in the active volume. Finally, increasing the dead layer of inner hole has an almost negligible effect on the simulated efficiency.

Figure 5: Efficiency values obtained using Wilks method.

Figure 6: Sensitivity analysis MCNP5 varying dead layers thickness.
In Figures 7 and 8 it is shown a comparison of efficiency curves corresponding to water and sand, respectively. Blue line represents efficiency considering 1.5 mm in all dead layers (top, lateral and inner hole). Red line represents efficiency considering 0 mm dead layers thickness. It can be seen that the effect of dead layer is quite similar when the matrix is changed (water or sand). It can be concluded that the variations in the efficiency curve when the dead layer changes, do not depend on the considered matrix material.

**Figure 7:** Efficiency calculations. Water matrix.

**Figure 8:** Efficiency calculations. Sand matrix.
4. CONCLUSIONS

MCNP and SWORD codes have been used to calculate the efficiency curve of the detectors used in LRA. It has been proved that the simulation in the low energy range presents important difficulties mainly due to the uncertainty associated to the Ge dead layer thickness. Uncertainty analysis has been performed in order to determine the effect of each operational and design parameter (dead layer thickness, gamma standard uncertainty, material matrix) on the efficiency curve. For this purpose the Noether-Wilks formula has been used.

It has been proved that Top dead layer strongly affects to low energy range (between 59 and 200 keV). Lateral dead layer homogeneously affects the whole energy interval between 59 and 1800 keV. Dead layer surrounding inner hole does not have a relevant effect on efficiency. Regarding to matrix material, it has been stated that density (or attenuation) has an important role in the efficiency curve. When sand (3.2 g/cm$^3$) is used as material matrix, efficiency in the low energy range is drastically reduced (50%) respect to the water values. In the high energy ranges, this reduction is lower than 10%.

REFERENCES