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# Attenuation Effect of Sample Container in Radioactivity Measurement by Gamma-ray Spectroscopy

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**Keywords**

Gamma-Ray Spectroscopy

Efficiency

Self-Attenuation Effect

Sample Container

PHITS

GESPECOR

**Abstract**

The measurement of radioactivity in environmental samples containing natural radionuclides such as $^{238}$U, $^{232}$Th, and $^{40}$K in gamma-ray spectrometry is the most common application. One of the most widely used sample containers for environmental radioactivity measurements is volumetric sample containers of certain sizes in cylindrical geometry. These cylindrical containers can be made of materials with different densities and thicknesses. In this intention, in this study, the effect of the sample container, which is one of the many parameters affecting the detector efficiency, was investigated. For this purpose, acrylic and polypropylene materials with of different densities were examined. IAEA RGU-1, IAEA-RGTh-1 and IAEA-RGK-1 standards containing uranium, thorium and potassium environmental radionuclides analyzed in gamma-ray spectrometric measurements were used as samples for these sample containers with different densities. Additionally, since the spectra in cylindrical geometry are taken by placing them on the detector endcap, the effect of the bottom thickness was investigated by changing the bottom thickness of these materials. Different material and bottom thickness evaluations were made using PHITS and GESPECOR Monte Carlo simulation programs. Compatible results were obtained with a difference of <5% between the PHITS and GESPECOR programs. From the outcome of this study, it can be concluded that when choosing the container material, the density should be as low as possible and especially the bottom thickness should be thin.

**Cite**

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## 1. INTRODUCTION

γ-ray spectrometry is a rapid and non-destructive method used to determine the radioactivity of gamma-ray emitting radionuclides in a sample. Due to their high-energy resolution, high-purity germanium (HPGe) detectors can be used in gamma-ray spectrometry to measure the activity of natural and artificial radionuclides in environmental, geological and biological samples (Azbouche et al., 2015). There are many parameters in the calculation of activity in gamma-ray spectrometry. For an accurate calculation, we must minimize the uncertainties that may come from these parameters such as efficiency, count rate, decay, random summing and self-absorption correction, mass, sample height and homogeneity (Gilmore, 2008). This is the uncertainty that can come from the efficiency calculation, which is directly related to the sources of uncertainty. Because there are similar uncertainties when calculating the efficiency. The efficiency value, which shows the performance of HPGe detectors, must be determined accurately and precisely, no matter what the detector is used for (Modarresi et al., 2017). It has been shown by many studies in the literature that the Monte Carlo simulation method can be successfully applied in gamma-ray spectrometry, especially in the efficiency calculation (Abd El Gawad et al., 2020; Trang et al., 2021; Stríbrnský et al., 2022). Two types of Monte Carlo simulation software are used in gamma-ray spectroscopy: these are either general-purpose codes such as GEANT,

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PENELOPE, EGS4, FLUKA, PHITS, or GESPECOR, DETEFF, ETNA, EFFTRAN, etc. as dedicated-purpose codes (Lépy et al., 2019; Sima et al., 2020).

In this study, the effect of the sample container on the efficiency, which has not been examined in the literature, was investigated using PHITS and GESPECOR Monte carlo programs. The attenuation effect of the sample container material type and thickness on the radioactivity measurement of volumetric samples in cylindrical geometry was examined. For this purpose, acrylic and polypropylene, which are mostly used sample container materials in gamma-ray spectroscopy laboratories, were chosen (Knoll, 2010; Guerra et al., 2018). Such samples are usually prepared in cylindrical sample containers of different sizes according to the sample amount, and the volume source is obtained. Self-absorption and true coincidence summing corrections, which are the correction factors that need to be made in the radioactivity calculation, are also effective in the volume source geometry counted on the detector endcap. Self-absorption correction is a factor that is effective especially in high-density matrices containing elements with high atomic number, which occurs as a because of the absorption of gamma rays passing through the sample due to the sample matrix and density, causing losses in the photopeak count (Yücel et al., 2010). Therefore, this loss depends not only on the sample, but also on the sample container, as it depends on a process until it reaches the detector. The more high-density or thicker sided sample containers are used, the more absorption there will be, which will affect the count. The sample container to be used should have the appropriate size, shape and density (Knoll, 2010).

## 2. MATERIAL AND METHOD

Two Monte Carlo programs were used in this study. The first is the general-purpose Monte Carlo program, PHITS, and the other is the dedicated-purpose program, the GESPECOR Monte Carlo program. It has been shown that both programs can be used reliably in gamma-ray spectrometric studies (Sima et al., 2001; Lépy et al., 2019; Uyar & Bölükdemir, 2022). While Monte Carlo programs have similar algorithms, it is expected that there will be differences between their results because they use different cross-sections, databases and libraries. With the EGS5 (Electron Gamma Shower) library in the PHITS Monte Carlo program, the atomic interactions of electrons and photons in a wide energy range ranging from 1 keV to 1 TeV (depending on the atomic numbers of the target materials) are simulated in the desired geometry. EGS code system started with EGS1 written in FORTRAN-IV language and consists of EGS5, which is the last version developed and improved continuously as EGS2, EGS3, EGS4. The data library in EGS5 is PHOTX (Photon Interaction Cross Section Library). The PHOTX data library provides results for elements with atomic numbers between 1 and 100 and photon energies between 1 keV and 100 MeV. It provides cross sections for coherent and non-coherent scattering, photoelectric absorption and pair production (Hirayama et al., 2006). In GESPECOR, the photon interaction cross sections are evaluated for each material of interest before starting the simulations, in the step of preparing and saving the material file. The basic cross sections are computed using the XCOM program which can be dowloaded from the NIST website (Berger et al., 2010). These basic cross sections are used for evaluating the interaction coefficients in a grid of 100 energy points equally spaced in logarithmic scale between 2 keV and 4 MeV.

PHITS (version 3.28) is a multi-application, general-purpose Monte Carlo simulation program that deals with the transport of all particles from thermal energies to 1 TeV using various nuclear data libraries and nuclear reaction models (Sato et al., 2018). In PHITS, full-energy peak efficiency values are obtained using the [t-deposit] tally, a function of calculating the energy deposited in the volumes specified by the users. IAEA RGU-1, RGTh-1 and RGK-1 materials with cylindrical geometry were modeled in PHITS using s-type=1. When the s-type parameter is set to 1, the source constructs a sphere with the center coordinates (x, y, and z) and radius r in an inward direction. The HPGe detector, whose geometric parameters were given in our previous study, was modeled (Bölükdemir et al., 2021).

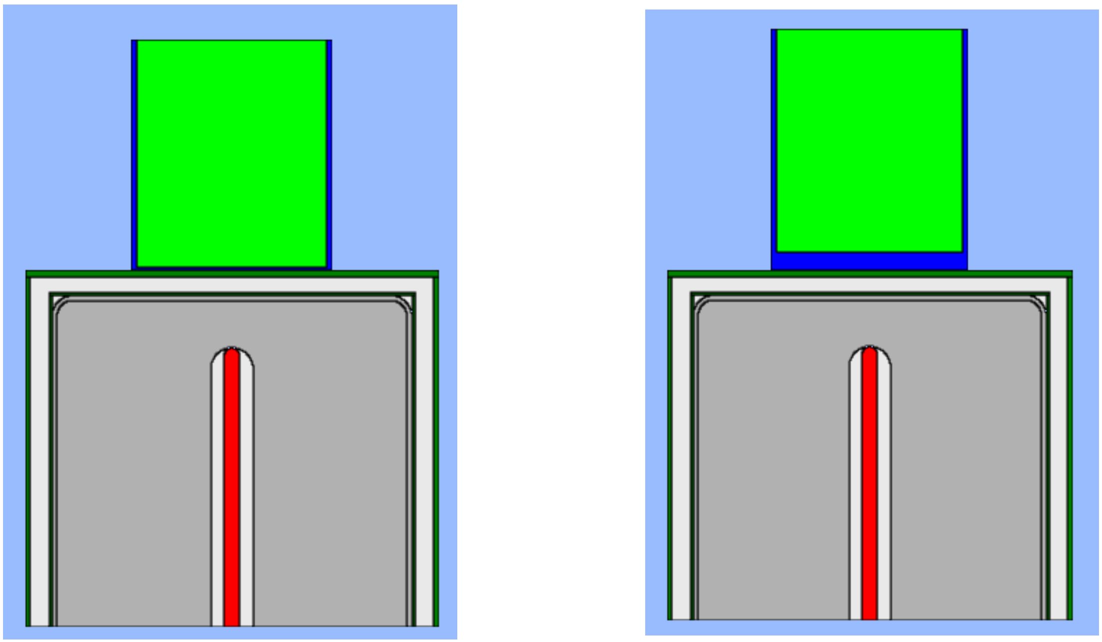
GESPECOR is a user-friendly code commonly used in gamma-ray spectrometry to obtain true coincidence summing and self-absorption correction factors and to calculate the full energy peak efficiency (Sima & Arnold, 2002). Similarly, the detector is modeled in GESPECOR by entering dimension information into the parts defined in the program. Then, the sample containers were modeled in cylindrical geometry. The geometric dimensions of the modeled cylinder are; the inner height is 6 cm, the inner radius is 2.5 cm, and the side wall thickness is 0.15 cm. These sizes are chosen because they are generally the most commonly used cylinder container sizes. Since it was aimed to examine the effect of the sample container, materials with different densities, polypropylene and polymethyl methacrylate (acrylic), which are widely preferred in gamma-ray spectroscopy laboratories, were used as container materials. Density and chemical composition data of polypropylene and acrylic from NIST are given in Table 1 (NIST, 2022).

***Table 1.*** *Densities and chemical compositions of the acrylic and polypropylene*

| | | **Chemical composition (Fraction by weight)** | | |
|---|---|---|---|---|
| | **Density (g/cm$^3$)** | **H** | **C** | **O** |
| **Acrylic** | 1.19 | 0.080538 | 0.599848 | 0.319614 |
| **Polypropylene** | 0.9 | 0.143711 | 0.856289 | - |

Additionally, the bottom thickness of the sample containers was increased from 1 mm to 5 mm at 1 mm intervals, and the effect of thickness was investigated (Figure 1). IAEA RGU-1, RGTh-1 and RGK-1 materials containing radionuclides with different energies were used as samples inside the containers. To examine the change in a wide energy range, 46.5 keV, 63.3 keV, 143.8 keV, 185.7 keV, and 1001 keV peaks in RGU-1 material, 129.1 keV, 209.2 keV, 583.2 keV, 860.5 keV, and 2614.5 keV peaks in RGTh-1 material and 1460.8 keV peak, which is the only energy found in RGK-1 material, were investigated. As can be seen, the energy range of the peaks used in the radioactive analysis results in the gamma spectrometer, in the range of 46.5 keV – 2614.5 keV, has been examined.

All simulations used 10 million particles as the number of histories. The statistical error of the simulated efficiency values obtained is less than 0.1% with this particle history number.



(a) (b)

***Figure 1.*** *Schematic representation of the sample container modeled in PHITS with* ***a)*** *bottom thickness of 1 mm,* ***b)*** *bottom thickness of 5 mm*

## 3. RESULTS AND DISCUSSION

In this study, the effect of the sample container on the efficiency was focused using IAEA-RGU-1, IAEA-RGTh-1 and IAEA-RGK-1 samples with different densities and chemical compositions. This effect was investigated in detail according to the efficiency values obtained from PHITS and GESPECOR by changing the bottom thickness of the sample container materials of different densities.

The efficiency values obtained with the PHITS Monte Carlo program are given in Table 2 and 3. Since PHITS is a general-purpose Monte Carlo program, the detector and sample container are modeled as desired. Since GESPECOR is a ready-made package program, it limits the user. For example, since there is no parameter in GESPECOR to model the front edge of the germanium crystal with rounded edges as it should be, the detector is modeled as sharp-edged and the copper contact pin in the middle of the Ge crystal cannot be included in the modeling. Therefore, there may be differences between the results obtained from the two programs due to both the modeling differences and the differences in the libraries and databases they use in the background. For this reason, the results from PHITS are given in more detail.

In Table 2, the acrylic is chosen as the container materials and the efficiency change depending on the bottom thickness of the container is seen. In Table 3, polypropylene is selected as the container materials and the efficiency change depending on the bottom thickness is given similarly. When Table 2 and 3 are examined, it is seen that the efficiency values obtained with the low density (0.9 g/cm$^3$) polypropylene container are higher than those with the acrylic material (1.19 g/cm$^3$) and the acrylic material decreases the detector efficiency.

***Table 2.*** *Effect of change in thickness of sample container material on full-energy peak efficiency (for acrylic)*

| **Reference material** | **Gamma-ray energy** | **Acrylic** | | | | | |
|---|---|---|---|---|---|---|---|
| | | **1 mm** | **2 mm** | **3 mm** | **4 mm** | **5 mm** | **% Diff.*** |
| **RGU-1** | 46.5 keV | 0.001564 | 0.001519 | 0.001474 | 0.001431 | 0.001386 | 11.4 |
| **RGU-1** | 63.3 keV | 0.015780 | 0.015241 | 0.014724 | 0.014219 | 0.013743 | 12.9 |
| **RGTh-1** | 129.1 keV | 0.062174 | 0.059630 | 0.057171 | 0.054845 | 0.052622 | 15.4 |
| **RGU-1** | 143.8 keV | 0.068012 | 0.065165 | 0.062491 | 0.059925 | 0.057507 | 15.4 |
| **RGU-1** | 185.7 keV | 0.068684 | 0.065817 | 0.063102 | 0.060509 | 0.058039 | 15.5 |
| **RGTh-1** | 209.3 keV | 0.066299 | 0.063528 | 0.060910 | 0.058425 | 0.056053 | 15.4 |
| **RGTh-1** | 583.2 keV | 0.043226 | 0.014570 | 0.039972 | 0.038483 | 0.037060 | 14.3 |
| **RGTh-1** | 860.5 keV | 0.036096 | 0.034754 | 0.033507 | 0.032299 | 0.031186 | 13.6 |
| **RGU-1** | 1001.0 keV | 0.033573 | 0.032357 | 0.031198 | 0.030087 | 0.029039 | 13.5 |
| **RGK-1** | 1460.8 keV | 0.027147 | 0.026190 | 0.025295 | 0.024444 | 0.023640 | 12.9 |
| **RGTh-1** | 2614.5 keV | 0.019522 | 0.018875 | 0.018261 | 0.017676 | 0.017109 | 12.4 |

***%** Differences between 1 mm and 5 mm thickness.

***Table 3.*** *Effect of change in thickness of sample container material on full-energy peak efficiency (for polypropylene)*

| **Reference material** | **Gamma-ray energy** | **Polypropylene** | | | | | |
|---|---|---|---|---|---|---|---|
| | | **1 mm** | **2 mm** | **3 mm** | **4 mm** | **5 mm** | **% Diff.*** |
| **RGU-1** | 46.5 keV | 0.001584 | 0.001547 | 0.001509 | 0.001473 | 0.001440 | 9.1 |
| **RGU-1** | 63.3 keV | 0.015941 | 0.015476 | 0.015013 | 0.014571 | 0.014141 | 11.3 |
| **RGTh-1** | 129.1 keV | 0.062684 | 0.060357 | 0.058120 | 0.055970 | 0.053924 | 14.0 |
| **RGU-1** | 143.8 keV | 0.068535 | 0.065953 | 0.063493 | 0.061129 | 0.058872 | 14.1 |
| **RGU-1** | 185.7 keV | 0.069155 | 0.066526 | 0.064007 | 0.061623 | 0.059326 | 14.2 |
| **RGTh-1** | 209.3 keV | 0.066733 | 0.064188 | 0.061756 | 0.059458 | 0.057249 | 14.2 |
| **RGTh-1** | 583.2 keV | 0.043405 | 0.041842 | 0.040341 | 0.038924 | 0.037576 | 13.4 |
| **RGTh-1** | 860.5 keV | 0.036223 | 0.034946 | 0.033761 | 0.032622 | 0.031539 | 12.9 |
| **RGU-1** | 1001.0 keV | 0.033682 | 0.032524 | 0.031431 | 0.030364 | 0.029355 | 12.8 |
| **RGK-1** | 1460.8 keV | 0.027225 | 0.026302 | 0.025445 | 0.024639 | 0.023859 | 12.4 |
| **RGTh-1** | 2614.5 keV | 0.019564 | 0.018931 | 0.018330 | 0.017774 | 0.017226 | 12.0 |

***%** Differences between 1 mm and 5 mm thickness.

As the bottom thickness increases, it is seen that there is a decrease of up to 15.5% in the acrylic material and 14.2% in the polypropylene material, independently of energy.

Figure 2 shows the percentage difference between acrylic and polypropylene materials at 1 mm and 5 mm bottom thickness obtained with PHITS. When polypropylene is used instead of acrylic, there is an increase of up to 0.3% - 1.2% in efficiency at 1 mm bottom thickness and up to 0.9% - 3.8% at 5 mm bottom thickness (Figure 2). While this increase is more effective, especially at low energies (46.5 keV and 63.3 keV), the material difference does not have a significant effect (<1%) on the efficiency at energies >1000 keV as the energy increases.

Similarly, in Figure 3, the percentage difference between acrylic and polypropylene materials in 1 mm and 5 mm base thicknesses obtained with GESPECOR is seen. When polypropylene is used instead of acrylic, there is an increase of up to 0.3% - 1.3% in efficiency at 1 mm bottom thickness and up to 0.8% - 4.4% at 5 mm bottom thickness (Figure 3).

It is used in some laboratories in containers made of polyethylene with a density of 1.05 g (Lépy et al., 2010). Since it has a density between the acrylic and polypropylene used in this material, it will cause a similar change. In other words, the yield values to be obtained will be between acrylic and poly, and the change depending on the thickness will be approximately 10% - 15% as in the others.

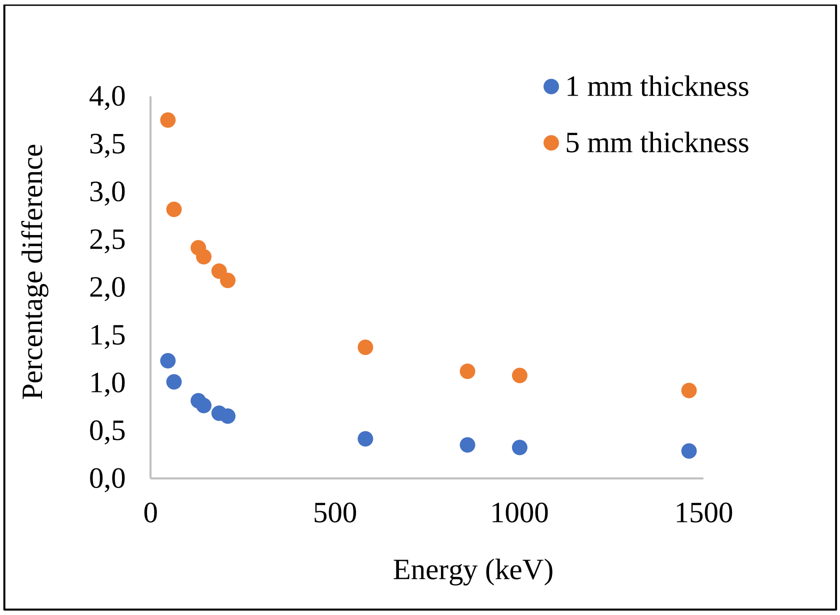


***Figure 2.*** *Percentage difference between acrylic and polypropylene materials at 1 mm and 5 mm bottom thickness (with PHITS)*

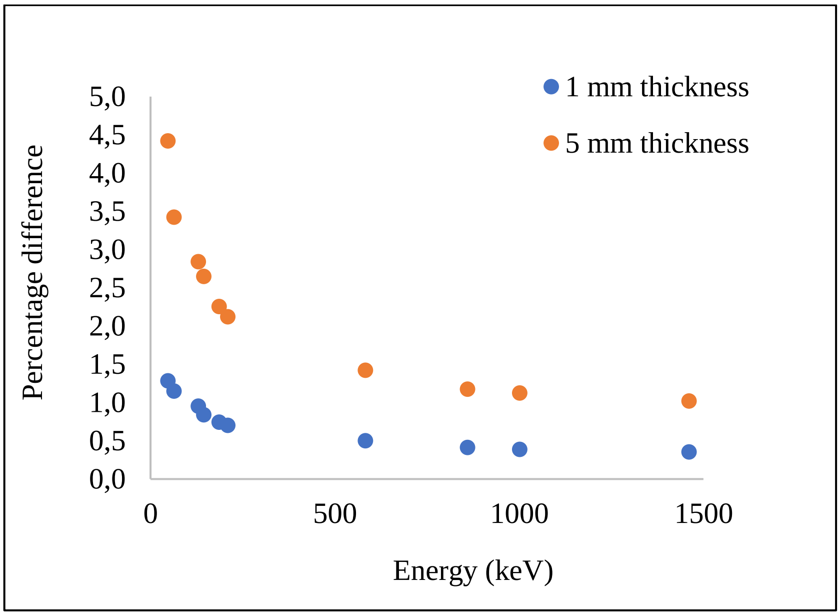


***Figure 3.*** *Percentage difference between acrylic and polypropylene materials at 1 mm and 5 mm bottom thickness (with GESPECOR)*

## 4. CONCLUSION

In this study, we examined the effect of the sample container material on the efficiency value, which is one of the most important parameters determined by the user and shows the performance of the detector. For this purpose, IAEA-RGU-1, RGTh-1 and RGK-1, which contain the most commonly used material types as container materials, acrylic and propylene, and the most radioactively analyzed uranium, thorium and potassium environmental radionuclides as samples, were modeled. The difference of <5% between the PHITS and GESPECOR programs used to obtain the efficiency values is also within acceptable limits.

According to the results obtained from both programs, it was observed that the efficiency values calculated using the sample container made of polypropylene material, which has a lower density in all energy values, increased compared with the results obtained using the acrylic sample container under the same conditions. Additionally, as the bottom thickness of the sample container increased, the efficiency decreased.

The sample container, which is easily available in the market and preferred by gamma-ray spectroscopy laboratories, is acrylic containers with a bottom thickness of 1-3 mm. Therefore, with this study, it is seen that it would be more appropriate to choose low-density materials instead of this material and the bottom should be chosen as thin as possible. In this way, while there are many parameters that reduce and affect the efficiency, there is no extra reduction from the selected sample container material provided by the user.

## CONFLICT OF INTEREST

The author declare no conflict of interest.

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