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# Developing Software for Self-Absorption Correction for Gamma Spectrometry of Soil and Water Samples Based on MCNP5 Monte Carlo Simulations

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## ABSTRACT

*Gamma spectroscopy using high purity germanium detectors, HPGe, is one of the most effective methods in determining the concentration of gamma-emitting radionuclides in the environment. The HPGe detector was simulated using MCNP5 Monte Carlo code, whereby the detector calibration curves were obtained at various geometries and heights, and the appropriate software was designed for efficiency calibration. The results obtained in this study show that increasing the height and density of the samples can affect the detector efficiency, as the photon interactions with matter depend on the density and the thickness of the materials. Therefore self-absorption in the samples increases with the thickness and the density of the material. The results indicate there is a strong correlation, i.e., R2>0.98 between the efficiency and the height and the density of the samples. The self-absorption correction was compared using the designed software, and the results of simulations show that the developed software can predict the calibration curves for the new samples in different photon energies with error much less than 1%.*

***Keywords***: *gamma-ray spectroscopy; HPGe; self-absorption; efficiency*

## INTRODUCTION

Gamma-ray spectrometry has been widely used in the determination of radioactive nuclides in foodstuff, liquid, and solid environmental samples [1-4]. For the measurement of the activity concentration in samples, it is necessary to know the exact efficiency of the detection system. The efficiency curve of the detectors is obtained using known standard sources with known activities. The chemical composition, density, physical shapes, and sizes of the standard samples should be similar to the samples which will be analysed because the increase in height, effective atomic number, and density of the samples will increase the self-absorption and the counting efficiency. The change in the sample density will also change the solid angle subtended by the detector, and therefore the geometric efficiency and full energy peak efficiency will vary. In this way, using the samples with the same dimensions and the fill heights similar for the standard source, the sample activity can be obtained with minimised deviation. In situations that we don't have access to the standard sample with the same shape of the samples, Monte Carlo simulations have been widely used by different investigators to model the sources with different shapes and densities, obtain the calibration curves, and estimate the self-absorption of the samples [5-9]. They investigated the effect of sample shape, density, and height, on the detector calibration curve, and found the correction factors for correcting such parameters.

As the material of active volume and the window of the detector, its size, and geometry may also change the efficiency, the correction factors should be determined for each detector.

The purpose of this study is to develop software for obtaining the efficiency calibration curves for samples of different geometries and densities for the HPGe detector used in the radiation research center.

# MATERIALS AND METHODS

## Efficiency Calibration with MCNP5 Monte Carlo simulations

A coaxial HPGe detector was simulated using MCNP5 Monte Carlo Code. The efficiency calibration was performed on soil and water samples with different shapes and geometries. To do this, the soil and water samples were simulated on the detector. The samples were considered as uniform sources emitting photons of 50 keV to 2MeV with an increment of 10 keV. The probability of photons with all energies was assumed to equal. *F8 tally was used to score the pulse height distribution of the photons inside the active volume of the detector. E8 Tally Energy Card was used to score the results from 1keV to 2MeV with an increment of 1keV. The outputs of MC simulations were used for the estimation of the detector efficiency according to Equation 1:

(1)
$$\varepsilon = \frac{R^{\cdot}}{A.P_{\gamma}}$$

where the unit less $\varepsilon$ is the efficiency at specific photon energy, $R^{\cdot}$ is the net count rate of photon energy (cps), A is the activity of the desired radionuclide (in Bq, or disintegration per second), and $P_{\gamma}$ is the probability of photon emission in each energy, (in this simulations all probabilities were defined to be equal to 1).

## Simulation Geometry and Self-Absorption Correction

A coaxial HPGe detector was simulated inside a multi-layer shield, as shown in Figure 1. Soil and water samples were simulated on the detector with different geometries.

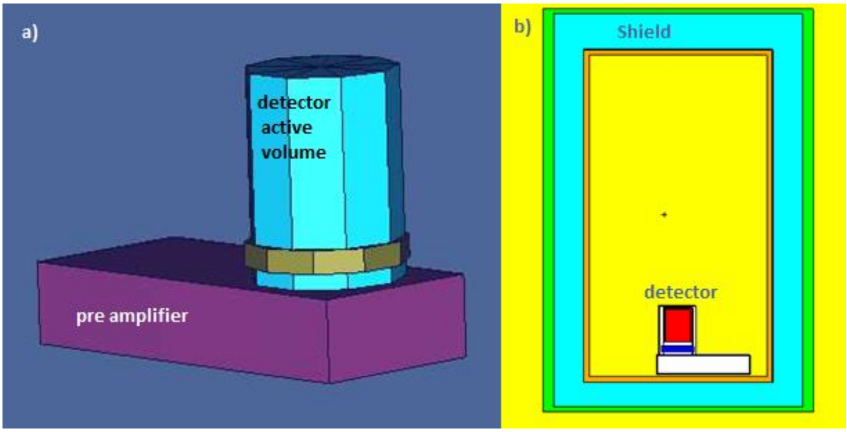


**Figure 1: The Simulation Geometry of A) Detector B) Detector Inside the Multi-Layered Shield**

To simulate the effect of soil density on the efficiency curves, samples with different densities 0.7 to 1.5 g/cm³ were simulated inside Marinelli beakers, and the efficiency curve of the detector was plotted for each density. Marinelli beakers are a particular type of sample container, with a central hollow tube, which is designed for increasing the geometric efficiency of the detectors in spectroscopy.

The effect of sample geometry on the detector was also investigated for two different geometries, i.e., Marinelli and cylindrical geometry. The efficiency curves of the detector for soil and water samples were plotted for the two geometries.

The self-absorption effects due to the samples' height were also investigated for both soil and water samples. The samples were simulated with the heights of 2 to 6cm in the Marinelli, and 1 to 11cm for the cylindrical geometry (see Figure 2).

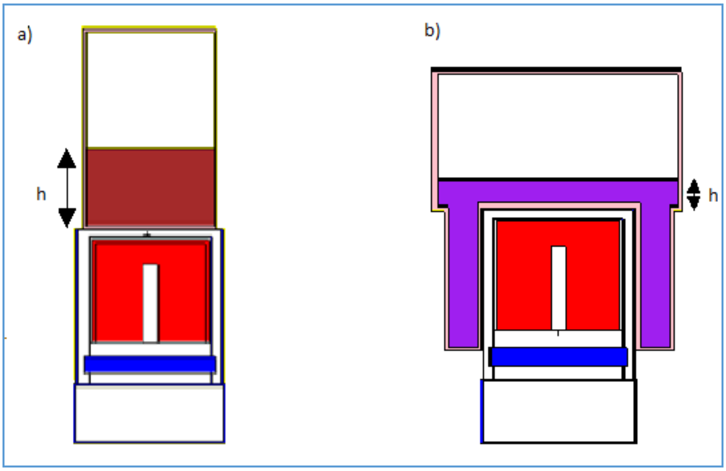


**Figure 2: Simulation of Geometry for a) Cylindrical and b) Marinelli Sample**

### Self-Absorption Correction Software

Finally, the software was developed with the GUI of Matlab for predicting the efficiency curves for different samples and geometries.

## RESULTS

The pulse height distribution of the photons was obtained inside the active volume of the detector using *F8 tally. The areas under each peak were used for obtaining the efficiency curves.

### Efficiency Calibration for Soil Samples

### The effect of density on detection efficiency

A)samples inside Marinelli containers

The efficiency curves of soil samples with a fixed height (h=1.4cm) inside the Marinelli; and with densities of 0.7, and 1.5 g/cm3 are compared in Figure 3.

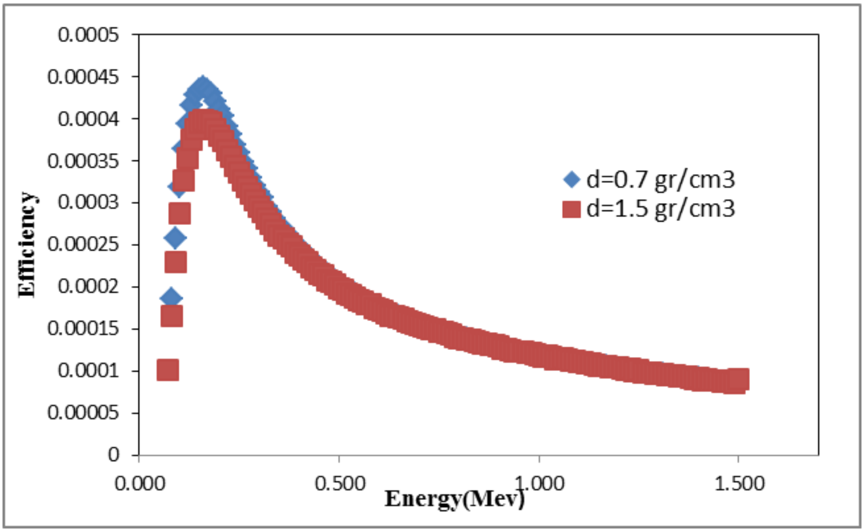


**Figure 3: Comparison of Efficiency Curves for Soil Samples with Different Densities Inside Mainelli Type Bakers**

The variations of detector efficiency with density at different photon energies are shown in Figure 4. As shown in the figure, the self-absorption effects of the soil samples increased with increasing density. Therefore, the counting efficiency of all energies decreases with increasing the density of samples.

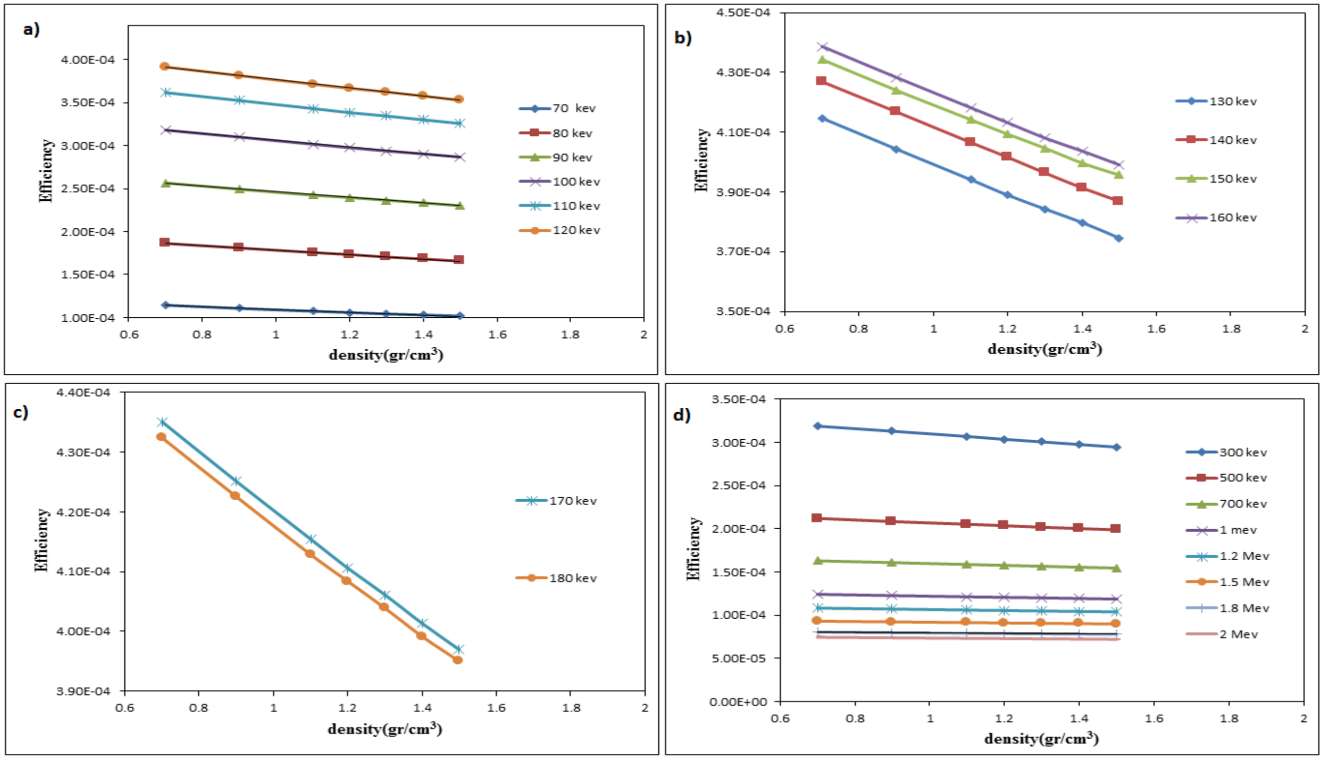


**Figure 4: Detector Efficiency at Various Density for Soil Samples with Marinelli Geometry at Different Photon Energies**

The percentage of efficiency difference between for samples with Marinelli geometry at maximum density ($\rho_{max} = 1.5\, g/cm^3$), and at minimum density ($\rho_{min} = 0.7\, g/cm^3$) were obtained at various photon energies according to Equation 2 (see Figure 5). According to Figure 5, the self-absorption was due to the density change and is more pronounced at lower energy photons.

$$\%\ Efficiency\ difference\ for\ each\ energy = \frac{Efficincy\ (\rho_{min}) - Efficincy\ (\rho_{max})}{Efficincy\ (\rho_{min})} \times 100$$

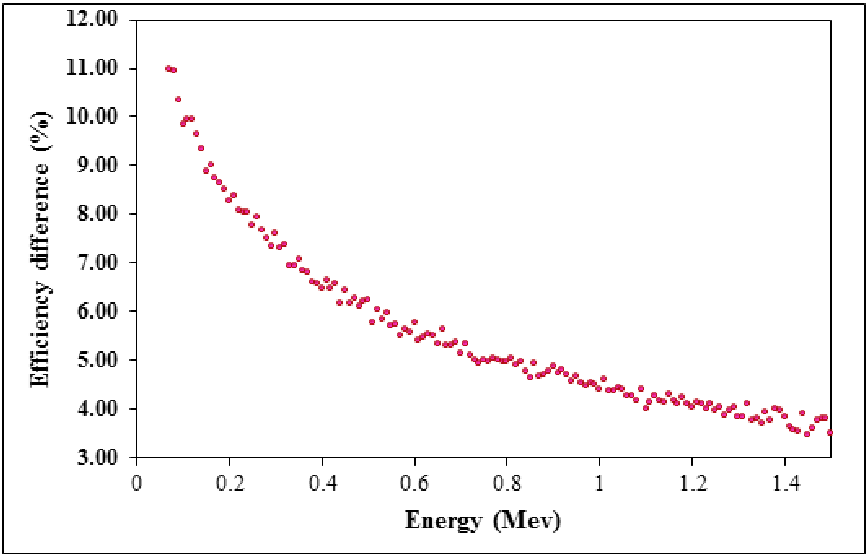


**Figure 5: The Percentage Difference between the Efficiencies for Soil Samples in Marinelli Geometry with Maximum and Minimum Densities as a Function of Photon Energy (MeV)**

## B) Samples Inside Cylindrical Containers

The efficiency curves of soil samples with a fixed height (h=1.6 cm) inside the cylindrical container; and with densities of 0.7, and 1.5 $g/cm^3$ are shown in Figure 6.

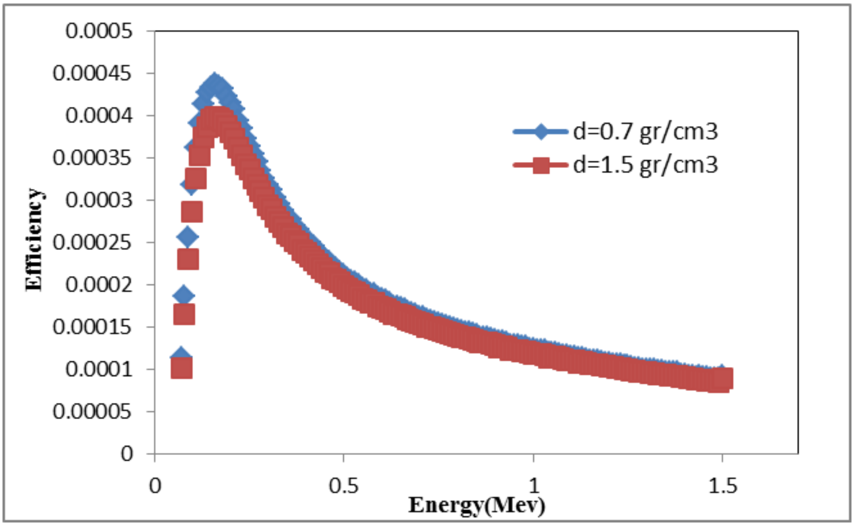


**Figure 6: Efficiency Curves for Soil Samples Different Densities inside Cylindrical Containers**

The percentage of efficiency difference between the sample with maximum density $(\rho_{max} = 1.5\, g/cm^3)$ and the one with the minimum density $(\rho_{min} = 0.7\, g/cm^3)$ were obtained for cylindrical containers, and different photon energies according to equation 2 (see Figure 7). It is evident from Figure 6 that the denser sample needs more self-absorption corrections.

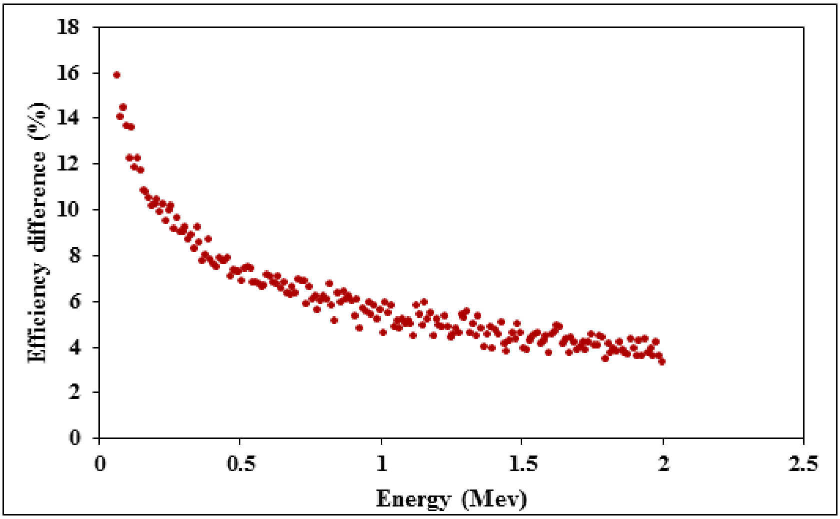


**Figure 7: The Percentage Difference between the Efficiencies for Soil Samples in Cylindrical Containers with Maximum and Minimum Densities as a Function of Photon Energy (MeV)**

## The Effect of Sample Height on Efficiency Curves for Soil Samples

### A) Soil Samples in Marinelli Geometry

The simulations were repeated for soil samples at various heights (h=1.6cm to 5.59cm) inside a container with Marinelli geometry (Figure 2). Figures 8 and 9 show the detector efficiency as a function of photon energies (MeV) at various heights.

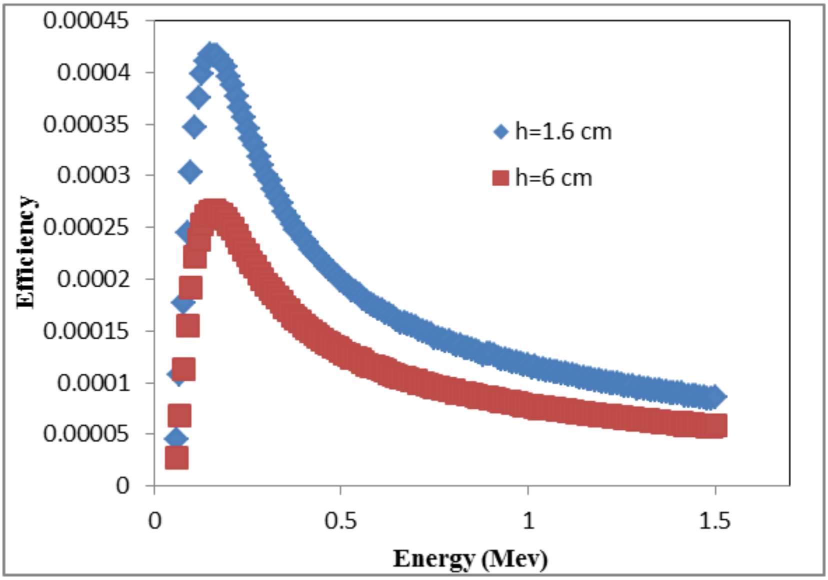


**Figure 8: Efficiency Curves for Soil Samples at Different Heights inside the Marinelli Container**

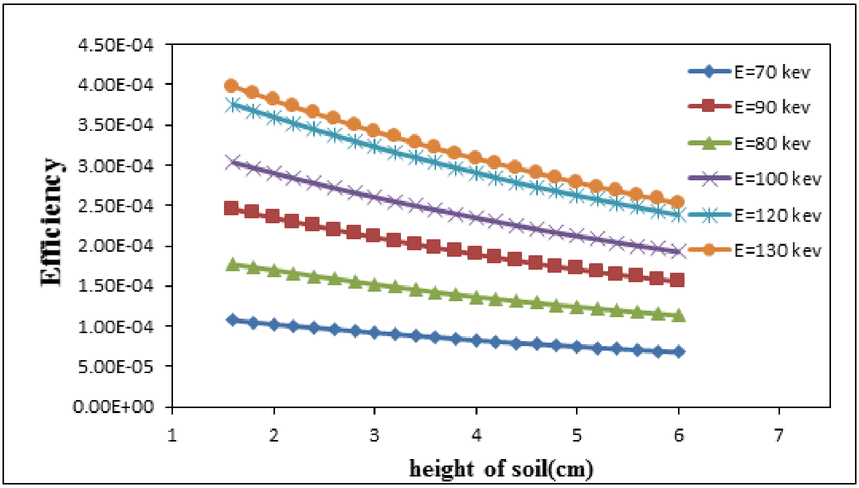


**Figure 9: Detector Efficiency as a Function Of The Height Of Soil (Cm) Inside the Marinelli Container at Various Photon Energies (70-130 Kev)**

The percentage of efficiency difference between the sample in Marinelli container at maximum height ($h_{max} = 5.59\ g/cm^3$), and minimum height ($h_{min} = 1.6\ g/cm^3$) were obtained for at various photon energies according to Equation 3 (see Figure 10). According to Figure 10, increasing the height increased self-absorption.

$$\frac{Efficincy\,(h_{min}) - Efficincy\,(h_{max})}{Efficincy\,(h_{min})} \times 100 \tag{3}$$

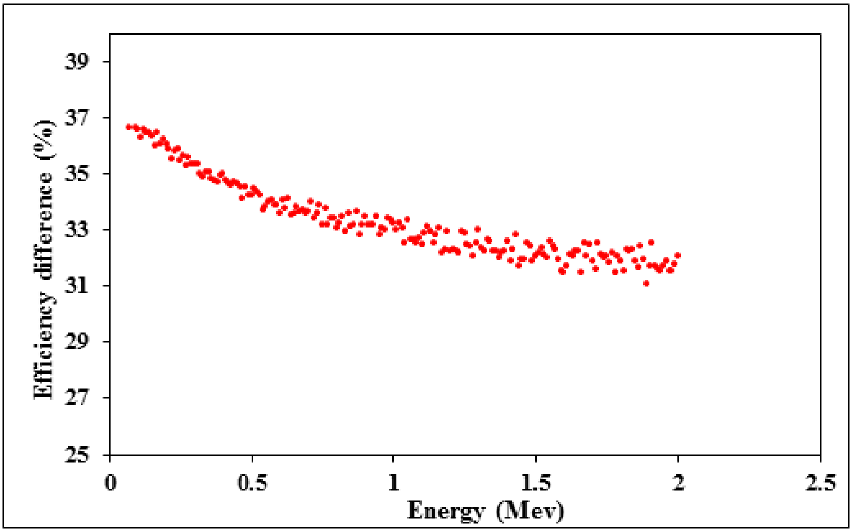


**Figure 10: The Efficiency Difference for Soil Samples in the Marinelli Container with Maximum and Minimum Heights as a Function of Photon Energy (MeV)**

## B) Soil Samples in Cylindrical Containers

The simulations were performed for soil samples at various heights (h=2cm to 11cm) inside the cylindrical container, as shown in Figure 2. Figure 11 shows the efficiency curves for h=2cm, with the curve for h=11cm. The variation of detector efficiency with height for soil samples inside cylindrical containers are compared at several photon energies in Figure 12.

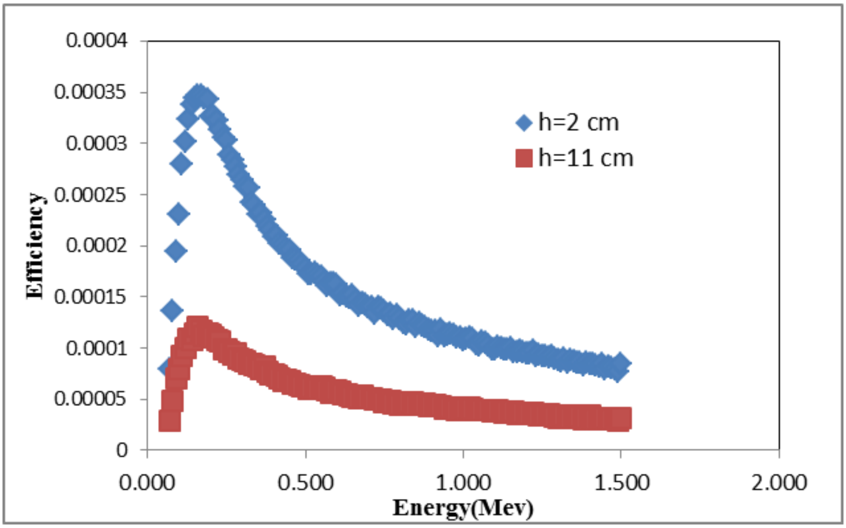


**Figure 11: Efficiency for Soil Samples inside Marinelli Container as a Function of Photon Energy (MeV) at Various Heights**

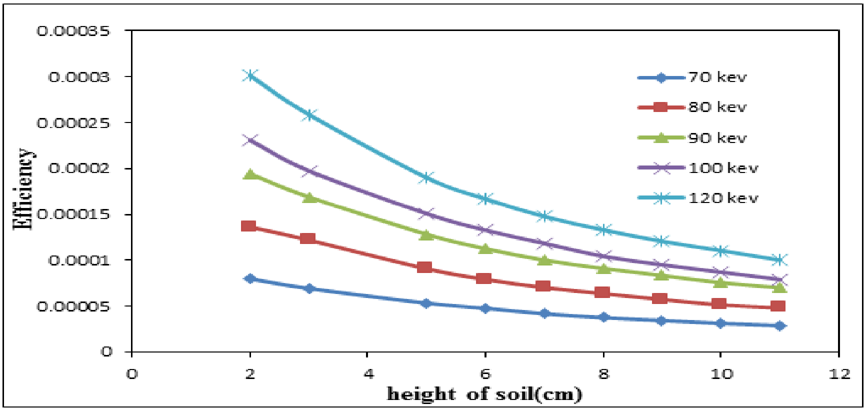


**Figure 12: Detector Efficiency as a Function of the Height of Soil Samples (Cm) inside Cylindrical Containers at Various Photon Energies (70-120 Kev)**

The efficiency differences (%), as obtained by equation 3, are compared in Figure 13.

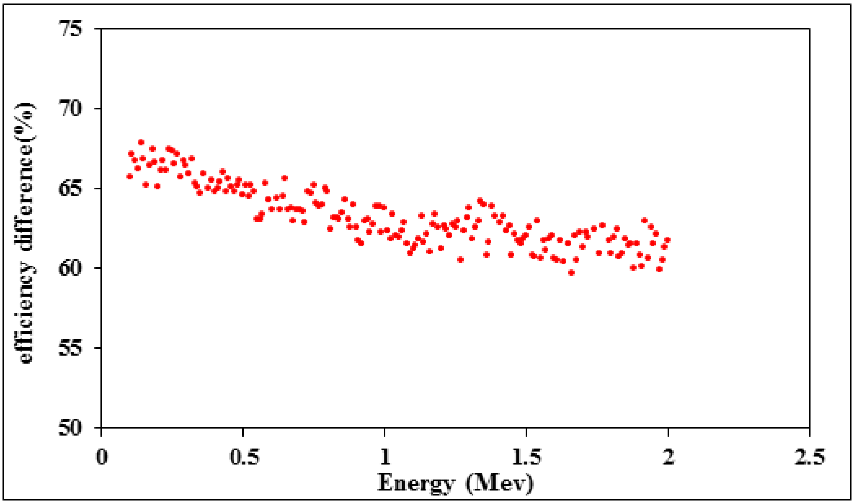


**Figure 13: The Difference between Efficiencies for Soil Samples in Cylindrical Containers at Maximum and Minimum Heights as a Function of Photon Energy (MeV)**

## Efficiency Calibration for Water Samples

### The effect of height on efficiency curves for water samples in Marinelli

Monte Carlo simulations were performed for water samples at various heights (h=1.99cm to 5.59cm) inside the Marinelli container, as shown in Figure 2. Figures 14 compares the detector efficiency for different heights and energies.

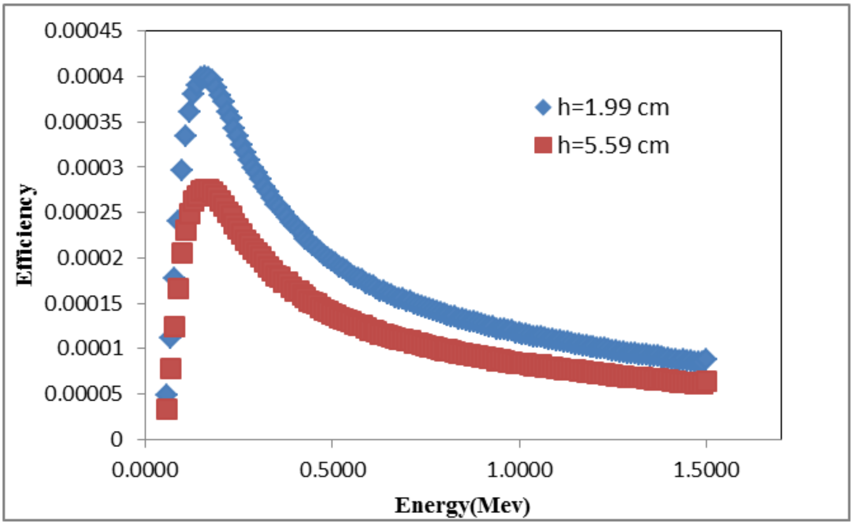


**Figure 14: Comparison of Efficiency Curves for Water Samples with Different Heights inside Marinelli**

## The effect of height on efficiency curves for water samples in cylindrical containers

The results of Monte Carlo simulations for water samples with heights of 1.8 to 10.8 inside cylindrical containers are shown in Figure 15.

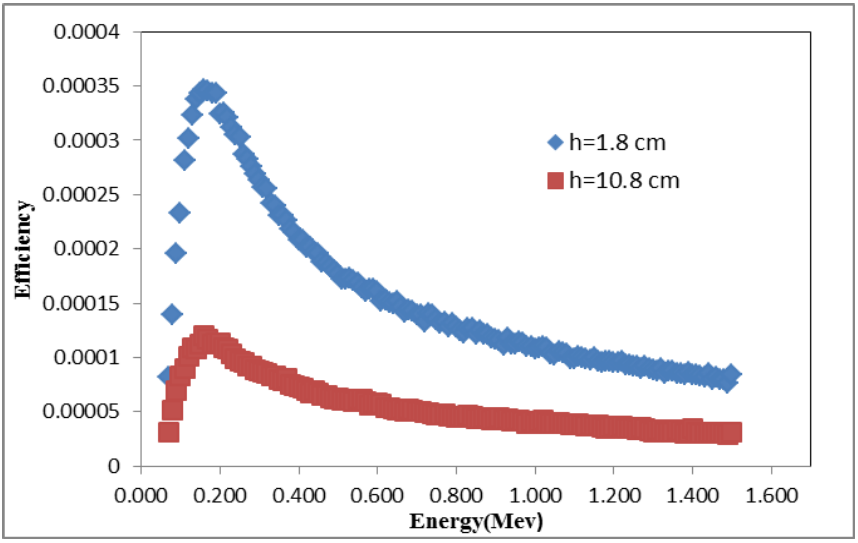


**Figure 15: Efficiency as a Function of Photon Energy (MeV) for Water Samples at Different Heights inside Cylindrical Containers**

## Developing calibration software

Figure 16 shows the software developed for self-absorption correction. The calibration curves obtained by the simulations were used as the database of the software. In this software, the sample type, i.e., water or soil, is selected from the left menu. After selecting the sample type, the geometry and sample size is selected. The software calculates the calibration curve for the chosen sample using interp2 command.

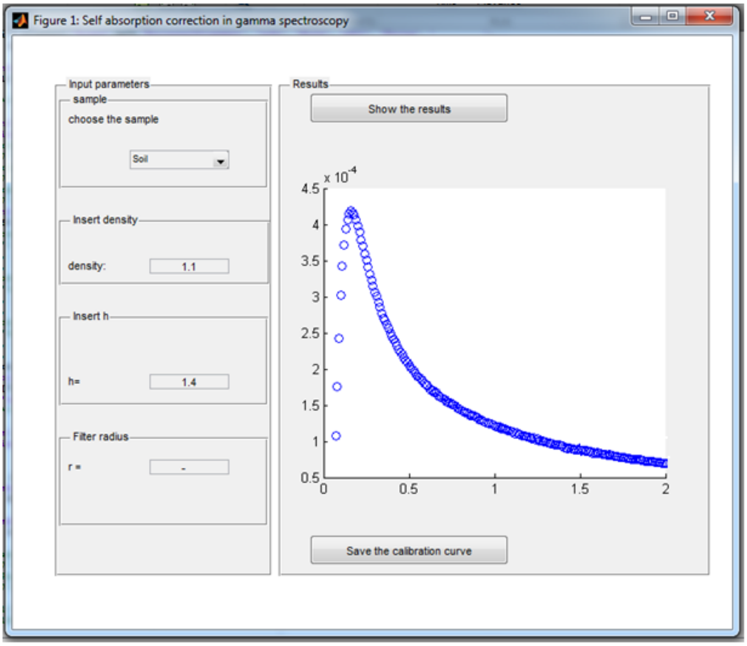


**Figure 16: The Software Developed for Self-Absorption Correction Verification of the Results**

The software uses two-dimensional interpolation command, interp2, to predict the efficiency curve for new samples with new densities and heights. To verify the results of the software, the efficiency curves for 0.7 g/cm3, 1.2 g/cm3, and 1.5 g/cm3 were inserted in the software as the database, and the efficiency curve was obtained for $\rho = 1.1g/cm^3$.

The predicted calibration curve was then compared with the MC simulation results, and the percentage difference between the predicted and the real values were obtained according to equation 4. The results indicate that the percentage differences between the predicted values and the simulation results are less than 0.2% in all energies, as shown in Table 1.

$$\%difference = abs\left(\frac{simulation - interpolation}{simulation}\right) \times 100 \quad (4)$$

| Energy (keV) | 100 | 200 | 400 | 600 | 800 | 1000 | 2000 |
|---|---|---|---|---|---|---|---|
| %difference | 0.19 | 0.14 | 0.15 | 0.08 | 0.08 | 0.06 | 0.05 |

## DISCUSSIONS AND CONCLUSIONS

Accurate quantitative gamma-ray spectroscopy is not possible without the efficiency calibration for different samples, source energies, and source or detector geometries. There are several approaches for obtaining the detector efficiencies, a) experimental method using different sample material compositions and geometries, b) semi-empirical approaches to efficiency calibration, known as efficiency transfer, and c) Monte Carlo simulations.

The experimental method is very accurate but requires standard samples with a known amount of activities, with the same geometry and material type, as the measured samples. Preparing such reference sources is not always possible. The semi-empirical approach calculates the efficiency for the measured sample, according to an experimental efficiency curve obtained for the detector, but with a reference source that is different in size, geometry, density, or composition. This method is fast but less accurate than the first one. The Monte Carlo simulation is also used widely as an accurate tool in obtaining the efficiencies for different detectors, and samples, but is a very time-consuming method. In this study, we have developed a software which uses the results of Monte Carlo simulations to obtain the efficiency calibration curves for a different type of samples. With the developed method, the efficiency calibration curve can be obtained very fast, with reasonable accuracy.

The developed software interpolates the efficiencies from the previously performed MC simulations. This method solves the difficulties of the three above- mentioned methods, and we can easily obtain the efficiency of samples whose efficiency curves were not obtained by MC simulations. The results indicate that the software can be effectively used in the efficiency calibration of HPGe detectors. In obtaining the calibration curves for HPGe detectors of different types, the simulation results of samples with several geometries, densities, and heights can be inserted in the software as the database, and the software will predict the efficiency curve for every new sample. Using this software, the efficiency calibration of the detectors can be performed without spending time and money.

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