Derivation of an efficiency-calibration simulation for a well-type HPGe detector using the Monte Carlo approach and analytical techniques

E. Eren Belgin*, G.A. Aycik

Muğla Sıtkı Koçman University, Faculty of Science, Department of Chemistry, Muğla 48000, Turkey

HIGHLIGHTS

- Dependence of full-energy peak efficiency by Monte Carlo simulations was studied.
- Semi empirical model was presented (150–2000 keV) for well type detector.
- Deviations between calculated and experimental efficiencies were less than ±10%.
- Therefore, the simulation model appeared to be acceptable for 150–2000 keV.

ARTICLE INFO

Article history:
Received 21 May 2013
Received in revised form 19 September 2014
Accepted 25 October 2014
Available online 29 October 2014

Keywords:
Monte Carlo simulation
Efficiency calibration
Efficiency modeling
HPGe detector
Gamma spectrometer

ABSTRACT

Simulation is a simple method that allows for facile estimation of a detector response function when the specifications of the investigated sample and the sample-detector geometry are known. In this study, the dependence of the full-energy peak efficiency on the sample and detector specifications was studied via analytical techniques and the Monte Carlo approach in the energy range of 150–2000 keV for a well-type measuring geometry, and a semi-empirical model was developed. The modeling of the detector efficiency is described in detail. The compute results were compared with experimental data, and comparison of the calculated efficiencies with the measured values indicated that the deviations between the calculated and experimental efficiencies were mostly less than ±10%. Therefore, the simulation model appear to be suitable for routine environmental radionuclide analysis when uncertainties of up to 10% are acceptable for energies between 150 and 2000 keV.

© 2014 Elsevier Ltd. All rights reserved.

1. Introduction

Gamma-ray spectrometry with germanium detectors is one of the most widely used procedures to determine the radionuclide concentration in any type of sample by allowing a precise quantitative determination. The primary advantage of gamma-ray spectrometry is that the quantitative characterization of gamma-ray emitters can be achieved without application of tedious and skill-intensive sample preparation. To determine the activity concentration of a radionuclide Eq. (1) is used for gamma spectrometric measurements.

\[
A = \frac{N}{\epsilon \times f_e \times t}
\]  

where \(N\) is the number of net counts recorded in the full-energy peak at energy \(E\), \(t\) is the effective measuring time, \(f_e\) is the photon-emission probability, and \(\epsilon\) is the full-energy peak efficiency (FEPE) at the considered energy \(E\).

The parameters \(N\), \(t\) and \(f_e\) can be easily obtained, but the FEPE is the main concern in gamma spectrometric measurements. In practice, the FEPE represents the ratio of the number of photon counts that reach the detector to the number of photons emitted by the source. The ability to accurately obtain the FEPE is of great importance in the correct and reliable determination of the activity of each radionuclide and the quality of the results is strongly dependent on the accuracy of the efficiency calibration of the detector.

Detector efficiency (FEPE) is a complex function of the energy, spectrometer characteristics, source-to-detector geometry, sample geometry and characteristics. In the case of a well detector, the FEPE depends on factors that can be classified into two groups: The first is the intrinsic characteristics of the detector, such as the active crystal volume, detector geometry and surrounding materials. The
second is the measurement geometry, such as the detector-sample positioning, sample geometry, and physical and chemical characteristics of the sample under study, such as geometrical dimensions, particle size, density, and chemical composition.

The FEPE can be obtained experimentally by measuring large number of primary standard sources at numerous energies that have very similar geometrical dimensions, source configurations and chemical—physical specifications to those of the sample of interest. However, such primary standard sources, if available at all, are costly and would need to be periodically replaced, especially for radionuclides with short half-lives. Thus, in practice, it is not always possible to use ideally matched sets of samples and standards. In addition, calibrated gamma-ray sources can be prepared for all the geometrical arrangements used in gamma-ray spectrometry (IAEA, 1989), but this method incurs high financial cost and requires considerable, time and material for the preparation of the sources.

To properly determine the FEPE, the relevant correction factors (photon attenuations in all types of pathway materials, coincidence-summing, dead time, etc.) must also be considered for each sample matrix and geometry. When calibration standards with same geometry as the samples as well as, similar sample properties and activity concentrations are available, the comparison method is the preferred method. This method is based on comparison of the sample peak area at the energy of interest to the area of the standard source peak at the same energy. Using the comparison method, it is possible to ensure the determination of a correct and precise FEPE value.

Because of the problems encountered in experimental methods, the determination of the FEPE has been a long-standing problem, and there is no single, universal method of efficiency calculation. Several authors (Abbas et al., 2006; Arnolda and Sima, 2004; Garcia-Talavera et al., 2000; Helmer et al., 2003; Karamanis et al., 2002; Laborie et al., 2000; Lepy, 2007; Pomme, 2004; San Miguel et al., 2004; Schoenfeld et al., 2002; Vidmar et al., 2001a, 2001b) have proposed and applied various non-experimental methods of FEPE determination and have provided useful solutions for overcoming these problems.

It has become common practice to use analytical and mathematical modeling methods, mostly commercial simulation programs, as an alternative to experimental efficiency-calibration methods. In addition, various modeling methods that require an abundance of mathematics and computer-programming knowledge can offer improvements with respect to commercial efficiency-calculation programs. Simulation is the numerical modeling of a real system using its inputs and outputs and the transferral of this model to computer media for investigation in multiple situations. Properly planned simulations yield information concerning system performance much more quickly, accurately and inexpensively than do experimental methods. Thus, interactions between system variables and systems can be investigated and numerical results can be obtained without the necessity of preparing a variety of real systems.

A survey of FEPE studies has indicated that the use of computer codes based on Monte Carlo simulation is an effective approach that complements the use of experimental efficiency-calibration procedures in gamma-ray measurements (Bochud et al., 2006; Ewa et al., 2001; Helmer, 2003; Hemler et al., 2004; Hernandez ve Daoushy, 2003; Laborie et al., 2000; Nedjadi et al., 2007; Garcia-Talavera et al., 2000; Vargas et al., 2002, 2003). Monte Carlo methods are a practical tool that allows, an experiment to be reproduced numerically using statistical techniques and the efficiency values for various measurement conditions to be calculated within a short time. Nevertheless, the accuracy of such simulation techniques must be evaluated before incorporating them into the laboratory routine. Several comparisons of the responses of high-resolution gamma-ray spectrometers with the results of commercial Monte Carlo programs have been published. Most authors have reported agreement with the experimentally obtained efficiency values within 10% (Abbas, 2006 — agreement greater than 96%; Bochud et al., 2006 — agreement greater than 94%; Ewa et al., 2001 — agreement greater than 88%; Hemler, 2003 — agreement 99.8%; Helmer et al., 2003 — agreement 99.9%; Hemler et al., 2004 — agreement 99.6%; Laborie et al., 2000 — agreement greater than 85%; Garcia-Talavera et al., 2000 — agreement greater than 96.7%; Vargas et al., 2002 — agreement greater than 98%; Vargas et al., 2003 — agreement greater than 95%).

In the present work, we developed a simulation program using analytical modeling techniques and Monte Carlo principles to calculate the FEPE of a well-type HPGe detector. The proposed method combines mathematical modeling methods and certain simulation techniques.

In the simulation, the photo-electric-effect type of gamma-ray interaction was considered, and a custom simulation program for HPGe detectors was prepared instead of using commercial Monte Carlo code. The self-absorption and absorption efficiencies of the detector were calculated using Monte Carlo logic and principles. In addition, analytical models were developed for various geometric arrangements because the analyzed radioisotopes could be positioned randomly throughout the sample. Thus, many position vectors were investigated by the program for a given radioisotope, and the results were used by the efficiency-calculation program. In the developed program, the training parameters could be modified for different situations because all code was written by us using the MATLAB programming language. Our program is a novel program for the efficiency calibration of gamma detectors since there is no other study presented in the literature in which MATLAB is used as the programming language for the same purpose.

The results were compared with experimental data and literature values. The accuracy of the method is discussed at the end of this paper.

2. Experimental

2.1. Experimental set-up

Accurate data for the detector parameters and source-to-detector arrangement are important to ensure the compatibility of experimental results with simulated results. In our studies, an ORTEC HPGe well-type detector with a crystal volume of 110 cm³ was used for experimental measurement of the FEPE and modeling studies. The detector had nominal FWHM resolutions of 0.90 keV at 122.07 keV and 1.92 keV at 1332.5 keV, and the resolution of 60Co at 1.33 MeV was 3.78 keV. The detector was connected to conventional electronic components with an amplifier gain of 21.25 and a shaping time of 6 µs. The detector had a crystal height and diameter of 50 mm and 75 mm, respectively. The well depth was 54 mm, and the diameter was 33 mm. The detector was shielded with electrolytic copper of 0.5 cm and lead of 10 cm. A technical drawing of the source-detector geometrical arrangement and the physical characteristics of the detector is provided in Fig. 1.

2.2. Experimental photopeak efficiency

The photoelectric-effect interaction of gamma rays was considered for the experimental efficiency calculations, which were performed by investigating the photopeaks of the spectra. Experimental data points for the FEPE of the detector were obtained using a mixed tube standard source placed in the detector well that was emitting photons with various energies in the region between 150 and 2000 keV. The standard was obtained from Isotope Product
Laboratories (IPL) in solid form in a 9 × 7 mm tube vial, and the uncertainty on the certified IPL activity was 5% at a 99.27% confidence level (CL) for each radionuclide. Powdered sugar was used as the background matrix to avoid extraneous background counts in the spectra. It was provided in the same specifications as the calibration samples and measured in the same geometry. All measurements were conducted for a sufficiently long period of time that the statistical uncertainties in the peak areas were below. The recorded spectra of the background sources were subtracted from the corresponding standard source spectra.

The photopeaks of $^{232}$Th (583.1 keV), $^{226}$Ra (351.9, 609.3, and 1764.5 keV) and $^{40}$K (1460.8 keV) were used for calculations because the simulation was performed for a range of 150–2000 keV. The spectra were recorded, and then, a number of channels in the photopeak region and to each side of the photopeak region (5 channels to the left and 5 channels to the right) were manually selected to test for any software error. After the individual manual selection of the data points, the photopeaks of interest were processed by the ORTEC Omnigam B30 data acquisition analysis software. Only clear peaks with no pile-up events were used in the analysis to eliminate pile-up errors, and dead time was kept below 2% to eliminate dead-time errors. The FEPE calibration was obtained with a mean standard uncertainty of approximately 3% using Eq. (2).

$$\varepsilon = \frac{N}{A \times f_T}$$  \hspace{1cm} (2)

where $N$ represents the number of full-energy interactions caused by the photoelectric effect that were recorded in the spectrum; $A$ is the number of photons of energy $E$ that were emitted by the source during the measurement time, in units of Bq; and $f_T$ is the emission probability.

### 2.3. Total efficiency modeling

In this study, the efficiency of a well-type HPGe detector (Fig. 1) was modeled for the energy range of 150–2000 keV by considering the photoelectric-effect interactions of the gamma rays.

The FEPE depends on the measurement geometry and the intrinsic properties of the detector, which are characterized by the crystal diameter $d$, the crystal length $l$, the well depth $H$, the well diameter $D$, the active well depth $H_a$. All these detector parameters were assumed to be fixed in the modeling studies and were treated as the intrinsic detector geometry. On the other hand, the parameters of the measurement geometry, such as the detector-sample positioning, the sample geometry, and the physical and chemical characteristics of the sample under study (geometrical dimensions, particle size, density and chemical composition) were variables in the model.

The FEPE for a photon with energy $E_i$ was expressed as the product of five factors: the coincidence summing factor and the absorption, sample, geometric and intrinsic efficiencies; see Eq. (3) (Palacios et al., 2008).

$$\varepsilon_{\text{total}}(E_i) = f_{\text{coinc}}(E_i) \times \varepsilon_{\text{abs}}(E_i) \times \varepsilon_{\text{sample}}(E_i) \times \varepsilon_{\text{geo}}(E_i) \times \varepsilon_{\text{int}}(E_i)$$  \hspace{1cm} (3)

where $\varepsilon_{\text{total}}$ is the total efficiency of the detector, $f_{\text{coinc}}$ is the coincidence summing factor, $\varepsilon_{\text{abs}}$ is the absorption efficiency, $\varepsilon_{\text{sample}}$ is the sample efficiency, $\varepsilon_{\text{geo}}$ is the geometric efficiency and $\varepsilon_{\text{int}}$ is the intrinsic efficiency. In Eq. (3), all parameters except $\varepsilon_{\text{geo}}$ are functions of energy.

The $\varepsilon_{\text{abs}}$ and $\varepsilon_{\text{sample}}$ parameters in Eq. (3) depend on not only the gamma-ray energy and the geometric factors but also the shielding material of the detector as well as the sample type, volume and vial properties. The shielding types, the thicknesses of the shields, and the sample type, volume and vial properties were the most highly variable parameters depending on the study conditions. Thus, the Monte Carlo approach, which depends on randomly changing parameters, was used for the calculation of $\varepsilon_{\text{abs}}$ and $\varepsilon_{\text{sample}}$; whereas analytical solutions were used for the other parameters of Eq. (3).

The five functions constituting $\varepsilon_{\text{total}}$ were studied individually, and the results were used in the modeling of $\varepsilon_{\text{total}}$. The $\varepsilon_{\text{total}}$ model (Eq. (3)) and the necessary parameters were introduced into code written for the calculation of $\varepsilon_{\text{total}}$ using the MATLAB programming language, and the $\varepsilon_{\text{total}}$ values were calculated by the program. Then, the $\varepsilon_{\text{total}}$ and energy values were used to plot the $\varepsilon_{\text{total}}$ curve. The models for the parameters that constitute $\varepsilon_{\text{total}}$ are explained in detail in the following sections.

#### 2.3.1. Coincidence summing factor

The first term of Eq. (3), $f_{\text{coinc}}$, arises from the phenomenon that occurs when the time required for the system to recover sufficiently after an interaction to produce a new, separate signal is longer than the time between the interactions with the detector crystal of two or more photons formed in the same decay. As a result, only one signal is produced instead of several different signals. In this situation, there will be either a decrease or increase in the signals at the corresponding energies.

---

**Fig. 1.** Geometrical arrangement and source-detector geometrical parameters of the detector used.
If the sample that is analyzed using a gamma spectrometer has a low activity, then the electronic system has sufficient time to produce a signal for each count because the number of gamma rays per unit time is low. If the detector efficiency is low or the detector solid angle is small, then the electronic system also has sufficient time to produce separate signals because the number of counts per unit time is low. Thus, in either situation, the likelihood that the coincidence summing effect will come into play decreases. In the case of a summing correction factor below 5%, the correction factor can be assumed to be unity (Alfassi, 2000; El-Daoushy and García-Tenorio, 1995; Pérez-Moreno et al., 2002). In this study, the investigated samples were generally environmental samples with low activities, leading to dead times below 2%; thus, it was assumed that coincidence summing had no effect on \( t_{\text{total}} \), and this factor was taken to be unity in Eq. (3).

### 2.3.2. Geometric efficiency

\( \epsilon_{\text{geo}} \) is independent of photon energy because it is the fraction of emitted photons that are intercepted by the detector because of the sample-detector geometry and the source-to-detector positioning. The simplest approach to \( \epsilon_{\text{geo}} \) modeling is to use an axial point source located on the detector end cap on its symmetry axis. In the case that the sample consists of an extended volume, it is necessary to know the spatial dependence of the detector efficiencies within the detector volume. The volumes of samples used in well-type detector generally lie within the range of 0.5–3.0 cm³. For point sources, the geometric efficiency can be measured without any difficulty, but for extended sources, even a small tube volume, it is necessary to calculate geometric correction factors.

The geometric factor depends on the position of the point source (radionuclide) within the well of the detector. Although any displacement in a plane perpendicular to the axis of the well induces very little change in \( t_{\text{total}} \), the displacement along the axis has a more important effect (Sima, 2000).

The dependence of the geometric factor on the spatial extension model based on this approach is given by Eqs. (4) and (5).

\[
\epsilon_{\text{geo}} = \frac{1}{Z_m-Z_i} \int_{Z_i}^{Z_m} \frac{\Omega(z)}{4\pi} dz = \frac{1}{2} \left[ 1 + g(Z_i) - g(Z_m) \right]
\]

(4)

\[
g(z) = \sqrt{\left(Z_i-Z\right)^2 + v^2 - v}
\]

(5)

In Eq. (5), the parameter \( v \) is the \( y \)-axis position of the source in the tube, and it is assumed that the maximum \( v \) value is equal to \( R_i \) because the height of the sample in the tube does not exceed the well depth. The parameter values and the limiting values in Eqs. (4) and (5) were introduced individually into the MATLAB program written for the determination of \( \epsilon_{\text{geo}} \). Then, Eqs. (4) and (5) were introduced into the program as the \( \epsilon_{\text{geo}} \) model, and the values for various sample heights (0.5–2.5 cm) were calculated by the program.

### 2.3.3. Absorption efficiency

The effects of materials between the sample and detector that absorb some of the incoming radiation before it interacts with the detector are accounted for by \( \epsilon_{\text{abs}} \). A photon released from the sample first passes through the sample itself, which is accounted for by the \( \epsilon_{\text{sample}} \) term; then the PVC sample tube, of 0.1 cm in thickness; and finally the detector shielding materials — aluminum coating (0.5 mm thick) and inactive germanium coating (0.3 \( \mu \)m thick) — before it reaches the detector crystal. Thus, \( \epsilon_{\text{abs}} \) depends on the various materials used as coatings, the sample container and the characteristics of the sample itself in addition to the energy of the photon.

The most convenient analytical model for \( \epsilon_{\text{abs}} \) calculations is given by Eq. (6) (Palacios et al., 2008).

\[
\epsilon_{\text{abs}} \left( E_i \right) = e^{- \left\{ \mu(E_i) \rho \left[ \sigma_{\text{Al}} + \sigma_{\text{Ge}} \right] \right\} t_{\text{tube}}}
\]

(6)

Here, the values represented by \( \mu(E_i) \) are the mass-absorption coefficients of the absorber materials, and those represented by \( \rho \) and \( x \) are the density and thickness, respectively, of the detector housing (aluminum and inactive germanium) or the container (PVC tube vial) (Palacios et al., 2008).

The \( \mu(E_i) \) values used in Eq. (6) were modeled using the Monte Carlo approach for each of three coating materials because the only energy-dependent variables in this model are the \( \mu(E_i) \) values. Before the Monte Carlo calculations were begun, mass-absorption data from the literature (NIST, 2011) were fitted to the basic mathematical model that demonstrated the best agreement, Eq. (7).

\[
\mu \left( E_i \right) = e^{a + b Z_i + c \ln E_i}
\]

(7)

where \( a \), \( b \) and \( c \) are model coefficients. After the selection of the model, the model coefficients were calculated via the Monte Carlo approach.

The objective of the Monte Carlo program was to introduce many random values into the proposed model (Eq. (7)) as model coefficients and to identify the coefficient values that minimized the difference between the model results and the literature data for the \( \mu(E_i) \) values. The requirement imposed on this method was that the random numbers used for the solution have a Gaussian distribution because the number of random events was very large. A Gaussian distribution is a convenient model because it is a continuous function that is a good approximation of the exact binomial distribution of events. The least-squares best-fit technique for non-linear systems was used to implement the method. The model (Eq. (7)) was introduced into the program written using the Monte Carlo method via the MATLAB program for optimization. In the program, the objective was to identify the values produced by the least-squares method that were closest to the literature values for the coefficients \( a \), \( b \), and \( c \). The program was run for up to 500,000 coefficients, which were created in 10 loops with 50,000 random coefficient combinations in each loop. The most suitable values, which were found by assigning random numbers to coefficients \( a \), \( b \), and \( c \) individually, were assumed to be the model coefficients, compatible with the Monte Carlo approach.

After the determination of the model (Eq. (7)) coefficients, then Eqs. (6) and (7) and their coefficients as well as the absorber material densities and thickness limits were introduced into the program for the calculation of \( \epsilon_{\text{abs}} \) as a function of energy.

### 2.3.4. Sample efficiency

\( \epsilon_{\text{sample}} \) primarily represents the self-absorption effect of the sample, and like \( \epsilon_{\text{abs}} \), it is a function of energy; see Eq. (8) (Palacios et al., 2008). The atomic number of the sample matrix becomes a predominant factor in determining the self-absorption correction factor, especially for low-energy photons, and \( \epsilon_{\text{sample}} \) is the reciprocal of the sample self-absorption correction.

\[
\epsilon_{\text{sample}} \left( E_i \right) = 1 - e^{- \left\{ \mu(E_i) \rho \left[ \sigma_{\text{sample}} \right] \right\} t_{\text{sample}}}
\]

(8)

Bakelite was chosen as the sample matrix for the model because of its similarity to the epoxy matrix of the standards used in the
study. The Monte Carlo approach was used to calculate the $\mu(E_i)$ values of Bakelite as explained in Section 2.3.3, using Eq. (7). After the determination of the model (Eq. (7)) coefficients, again using 500,000 random numbers, $\varepsilon_{\text{sample}}$ was determined as a function of energy by introducing the mass–absorption coefficient model (Eq. (7)), the model coefficients determined using the Monte Carlo approach, model (8) and the sample specifications (density and thickness limits) into the program.

2.3.5. Intrinsic efficiency

$\varepsilon_{\text{intrinsic}}$ is the probability that a gamma ray that enters the detector will interact with the detector crystal and produce a pulse in the full-energy peak. Thus, it depends on the electrical instrumentation of the detector and the properties of the detector crystal. Therefore, this quantity should have a unique and constant value for the detector that can be determined based on the manufacturer’s specifications of the technical parameters of the detector, although these specifications are not always sufficiently accurate. In our simulation, the dimensions provided by the manufacturer were used to calculate the intrinsic efficiency of the modeled detector. To obtain the most accurate results, better geometrical and/or physical knowledge of the detector would be required.

In this study, the intrinsic efficiency data provided by the manufacturer were first fitted to the mathematical model that yielded the results that exhibited the best agreement with the manufacturer data. The best-fit model for 150–2000 keV was a polynomial function of the third order, Eq. (9).

$$
\varepsilon_{\text{intrinsic}}(E_i) = a + bE_i + cE_i^2
$$

After the selection of the model, the model coefficients $a$, $b$, and $c$ were calculated using a curve-fitting program. $\varepsilon_{\text{intrinsic}}$ was modeled as a function of energy by introducing Eq. (9) and the coefficients into the MATLAB program.

3. Results and discussion

3.1. Experimental results

The experimental efficiency ($\varepsilon_{\text{exp}}$) values for the well-type HPGe detector were obtained using radionuclide sources placed in the well hole, as explained in Section 2.2, and the efficiency calibration curve (Fig. 2) was plotted using the obtained $\varepsilon_{\text{exp}}$ data (Table 1).

The experimental efficiency curve of an HPGe detector can be divided into two regions. The first is the region in which the efficiency values increase with increasing energy up to a knee gamma energy of nearly 130 keV. The efficiency values then begin to decrease with increasing energy. In our study, energies in the second region were studied because the first region is also the X-ray region, where the photopeaks are generally not clear. In this study, the experimental efficiency results obtained in this second region for the studied detector exhibited the expected decreasing behavior, as observed in Fig. 2.

3.2. Simulation results

3.2.1. Geometric efficiency ($\varepsilon_{\text{geo}}$)

In this study, $\varepsilon_{\text{geo}}$ was modeled for the geometry of a sample tube in a well-type HPGe gamma detector, as described in Section 2.3.2. Model calculations were performed for sample heights of 0.5, 1.0, 1.5, 2.0 and 2.5 cm, and the dependence of $\varepsilon_{\text{geo}}$ on the sample height is presented in Fig. 3.

According to the results, $\varepsilon_{\text{geo}}$ decreases with increasing sample height. This decrease in efficiency is expected based on geometrical laws because of the decreasing counting angle.

If $A$ is the angle that represents the non-countable region of the geometric arrangement, then when the sample height increases, the counting angle ($360^\circ - A$) decreases; see Fig. 4. Thus, the number of gamma rays that do not interact with the detector crystal increases. Because the efficiency is the ratio of the number of gamma rays that reach the detector crystal to the number of emitted gamma rays, $\varepsilon_{\text{geo}}$ decreases with decreasing counting angle. In this study, $\varepsilon_{\text{geo}}$ was found to be 0.9869 for a sample height of 0.5 cm and 0.9707 for a sample height of 2.5 cm.

3.2.2. Absorption efficiency ($\varepsilon_{\text{abs}}$)

The $\mu(E_i)$ values of the gamma-ray pathway materials — aluminum, germanium and the material of the sample container (PVC) — were modeled using the Monte Carlo approach, as described in Section 2.3.3. The first parameter to be determined for the use of the modeling program was how many random numbers and loops would be used to create random numbers in the program. These quantities were determined via trial and error.

![Fig. 2](image-url)
values. The agreement between the literature data (NIST, 2011) and the model results obtained after the selection of the loop and trial numbers is presented in Fig. 6 for aluminum, germanium and PVC. The simulated and literature values for aluminum, germanium and PVC were found to exhibit good agreement of 98.50%, 89.31% and 98.92%, respectively. According to these results, the lowest agreement that was achieved was for the Ge absorber coating of the detector (not the detector crystal itself), which was 0.3 μm thick. This Ge coating was the thinnest of the absorber layers, causing the associated error percentage to be the highest. The agreement value for the Ge coating could have been increased by increasing the numbers of loops and trials used in the program, but such optimization was unnecessary because the very low thickness of the layer meant that it did not significantly affect the final results. The overall percentage error for the attenuation coefficients was less than 3%. Thus, the coefficients determined using 10 loops and 50,000 random numbers per loop that exhibited the best agreement with the literature data (NIST, 2011) were accepted as the model (Eq. (7)) coefficients.

Comparison with the literature indicates that this error percentage was acceptable, as Monte Carlo simulations presented in the literature typically exhibit 0.1−15% errors (Abbas, 2006 — agreement greater than 96%; Bochud et al., 2006 — agreement greater than 96%; Ewa et al., 2001 — agreement greater than 88%; Hemler, 2003 — agreement of 99.9%; Helmer et al., 2003 — agreement of 99.8%; Hemler et al., 2004 — agreement of 99.6%; Laborie et al., 2000 — agreement greater than 85%; Garcia-Talavera et al., 2000 — agreement greater than 96.7%; Vargas et al., 2002 — agreement greater than 99.8%; Vargas et al., 2003 — agreement greater than 95%).

The determined Monte Carlo model coefficients, mass-absorption model (Eq. (7)) and absorption-efficiency model (Eq. (6)) were introduced into the MATLAB f_abs Calculation program, and the f_abs curve was obtained; see Fig. 7. f_abs was found to be 0.98353 at 150 keV and 0.98759 at 2000 keV. Thus, as the energy increased, f_abs increased, and at higher energies, it became close to unity. This was an expected result because low-energy gamma rays are absorbed proportionally much more often by absorbing layers than are high-energy gamma rays. Photons that do not have sufficient energy will be totally absorbed by the absorbing layers before they reach the detector crystal. The probability of reaching the crystal

![Fig. 3. Simulated results for geometric efficiency vs. sample height for a tube geometry.](image)

![Fig. 4. Schematic representation of the effect of the sample height on the counting angle for 1) a low sample height and 2) a high sample height.](image)

In Fig. 5, several trials with different numbers of random numbers and loops used for the calculation of the mass−absorption coefficient of aluminum are presented. As the loop and trial numbers increased, the agreement between the Monte Carlo results and the literature data (NIST, 2011) increased. The agreement for 2 loops and 5000 trials was 93.8%, whereas it was 98.2% for 8 loops and 35000 trials. For more than 8 loops, the increase in agreement was not significant. Thus, 500,000 coefficients created by 10 loops and 50,000 random coefficient combinations in each loop were used in the final program for the calculation of $\mu(E)$.
increases with increasing photon energy. Thus, as the gamma energy increases, the effect of absorption on the total efficiency will decrease. For gamma rays of sufficiently high energy, absorption by gamma-ray pathway materials has no effect on the total efficiency, and the $\varepsilon_{\text{abs}}$ term in Eq. (3) must be closer to unity. This trend is evident in Fig. 7.

### 3.2.3. Sample efficiency ($\varepsilon_{\text{sample}}$)

First, the $\mu(E_i)$ values of the sample (Bakelite) were determined using the Monte Carlo method (Section 2.3.3) for the calculation of $\varepsilon_{\text{sample}}$. The coefficient combinations that exhibited the best agreement with the literature data (NIST, 2011) after 10 loops and 50,000 random-number trials per loop were taken to be the $\mu(E_i)$ model (Eq. (7)) coefficients. The agreement between the model results and the literature data (NIST, 2011) was found to be 97.72% for Bakelite; see Fig. 8. Thus, the error in the results was less than 3%.

Afterward, Eq. (7), the coefficients determined using the Monte Carlo method, the $\varepsilon_{\text{sample}}$ model (Eq. (8)) and the density and thickness limits of the sample were introduced into the $\varepsilon_{\text{sample}}$.
calculation program, and the \( \epsilon_{\text{sample}} \) values were determined as discussed in Section 2.3.4. Then, the curve of \( \epsilon_{\text{sample}} \) vs. energy was plotted (Fig. 9).

\( \epsilon_{\text{sample}} \) was found to be 0.9559 at 150 keV and 0.9843 at 2000 keV. The effect of \( \epsilon_{\text{sample}} \) on the total efficiency became insignificant as the gamma-ray energy increased, as seen in Fig. 9. Because the absorption efficiency and the sample efficiency exhibit the same behavior in this respect, this was an expected result.

### 3.2.4. Intrinsic efficiency (\( \epsilon_{\text{int}} \))

\( \epsilon_{\text{int}} \) values with respect to energy were determined by introducing the model represented by Eq. (9) and the model coefficients \( a, b, \) and \( c \) that were determined via curve fitting into the MATLAB program, as described in Section 2.3.5. Thus, the \( \epsilon_{\text{int}} \) vs. energy curve was obtained; see Fig. 10.

\( \epsilon_{\text{int}} \), the last term of \( \epsilon_{\text{total}} \), is a function only of energy for any given detector. \( \epsilon_{\text{int}} \) was found to be 0.0351 at 150 keV and 0.0036 at 2000 keV for the simulated detector. The results demonstrated agreement with the typical second-region behavior of an efficiency calibration curve: \( \epsilon_{\text{int}} \) was found to decrease with increasing energy. The investigated range of the simulation lay within this second region, between energies of 150 and 2000 keV.

### 3.2.5. Total efficiency (\( \epsilon_{\text{total}} \))

The \( \epsilon_{\text{total}} \) of the detector was the product of the \( \epsilon_{\text{geo}}, \epsilon_{\text{abs}}, \epsilon_{\text{sample}} \) and \( \epsilon_{\text{int}} \) parameters, as indicated by Eq. (3). Thus, all models (Eqs. (4)–(9)) that were used for the calculation of these factors and the model coefficients that were determined via Monte Carlo or analytical techniques were introduced into the final MATLAB program for calculating \( \epsilon_{\text{total}} \). Then, the \( \epsilon_{\text{total}} \) model (Eq. (3)) was also introduced into the final program, and the \( \epsilon_{\text{total}} \) values were calculated by the program (Table 2).

The \( \epsilon_{\text{total}} \) values for the modeled detector with respect to gamma energy (the efficiency curve) were obtained from the output of the program. The agreement between the experimental (Table 1) and simulated results (Table 2) for \( \epsilon_{\text{total}} \) was found to be 91.84%; see Fig. 11.

\( \epsilon_{\text{total}} \) was found to be 0.0305 at 150 keV and 0.0033 at 2000 keV, according to the simulation results. The efficiency curves of gamma spectrometers tend to initially increase with increasing energy, and then, after a knee value, generally at approximately 130 keV, they begin to decrease, as noted above. In this study, the 150–2000 keV range

<table>
<thead>
<tr>
<th>Energy (keV)</th>
<th>( \epsilon_{\text{total}} )</th>
<th>Energy (keV)</th>
<th>( \epsilon_{\text{total}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>150</td>
<td>0.0305</td>
<td>1100</td>
<td>0.0056</td>
</tr>
<tr>
<td>200</td>
<td>0.0239</td>
<td>1150</td>
<td>0.0054</td>
</tr>
<tr>
<td>250</td>
<td>0.0198</td>
<td>1200</td>
<td>0.0052</td>
</tr>
<tr>
<td>300</td>
<td>0.0170</td>
<td>1250</td>
<td>0.0050</td>
</tr>
<tr>
<td>350</td>
<td>0.0149</td>
<td>1300</td>
<td>0.0048</td>
</tr>
<tr>
<td>400</td>
<td>0.0133</td>
<td>1350</td>
<td>0.0047</td>
</tr>
<tr>
<td>450</td>
<td>0.0120</td>
<td>1400</td>
<td>0.0045</td>
</tr>
<tr>
<td>500</td>
<td>0.0110</td>
<td>1450</td>
<td>0.0044</td>
</tr>
<tr>
<td>550</td>
<td>0.0101</td>
<td>1500</td>
<td>0.0043</td>
</tr>
<tr>
<td>600</td>
<td>0.0094</td>
<td>1550</td>
<td>0.0042</td>
</tr>
<tr>
<td>650</td>
<td>0.0088</td>
<td>1600</td>
<td>0.0040</td>
</tr>
<tr>
<td>700</td>
<td>0.0082</td>
<td>1650</td>
<td>0.0039</td>
</tr>
<tr>
<td>750</td>
<td>0.0078</td>
<td>1700</td>
<td>0.0038</td>
</tr>
<tr>
<td>800</td>
<td>0.0073</td>
<td>1750</td>
<td>0.0037</td>
</tr>
<tr>
<td>850</td>
<td>0.0070</td>
<td>1800</td>
<td>0.0037</td>
</tr>
<tr>
<td>900</td>
<td>0.0066</td>
<td>1850</td>
<td>0.0036</td>
</tr>
<tr>
<td>950</td>
<td>0.0063</td>
<td>1900</td>
<td>0.0035</td>
</tr>
<tr>
<td>1000</td>
<td>0.0061</td>
<td>1950</td>
<td>0.0034</td>
</tr>
<tr>
<td>1050</td>
<td>0.0058</td>
<td>2000</td>
<td>0.0033</td>
</tr>
</tbody>
</table>
energy range was studied, and this range lies in the second region, where the efficiency value decreases with increasing energy. The reason for selecting this energy range for investigation was that the gamma spectrum below the knee energy of approximately 130 keV includes X-rays. Moreover, there are few peaks above 2000 keV. By comparing the simulated results with the experimental data, it can be seen that the modeled efficiencies agreed quite well with the experimental efficiencies, as shown in Fig. 11. This result confirms the validity of peak-efficiency calibration using the proposed method.

4. Conclusion
In this study, the dependence of the full-energy peak efficiency on the sample and detector specifications was studied using analytical techniques and the Monte Carlo approach in the energy range of 150–2000 keV for a well-type measuring geometry. The computed results were compared with experimental data, and good agreement was obtained for a well-type HPGe detector for a sample-height range of 0.5–2.5 cm. The agreement value calculated by the program was 91.84%. Thus, the developed simulation program yielded only an 8.16% error. In general, it can be concluded that the computed results and the measured efficiency values should agree within 10%. This result confirms the validity of the present model in computing well-type detector efficiencies.

The program developed in this study was written in accordance with the specifications of the selected sample and detector using the MATLAB programming language. Thus, the model is capable of handling abrupt changes in the efficiency curve caused by the parameters of the sample material, the geometry and the detector itself. For instance, the efficiency curves for various sample heights or densities can be obtained by changing only these parameters in the program code. The proposed method does not require the use of reference materials or point sources to obtain FEPE curves. Thus, the difficulties of preparing a series of standard sources such as those required in typical efficiency-calibration procedures are avoided.

This computational method for detector efficiency calibration was found to be sufficiently accurate to be routinely applied in gamma-ray measurement systems for environmental samples. Some advantages of the proposed method include its relative simplicity of implementation and the relatively short time required to obtain reliable and repeatable results for well-type HPGe detectors.

The results reported here demonstrate that it would be highly advantageous to utilize this method for the efficiency calibration of HPGe detectors, as the experimental approach is often difficult to execute. Instead, the detector efficiency can be determined via mathematical modeling with an uncertainty of less than 10%.

Acknowledgments
We are especially grateful to Dr. O. Akpolat for his invaluable assistance with MATLAB programming. We are also grateful to Mугла Ситки Кочман University Scientific Research Projects Department for their sponsorship (Project no. 10/01).

References
NIST, 2011. NIST Physical Measurement Laboratory. The National Institute of Standards and Technology. US Department of Commerce. US.


