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Application of PHOTON simulation software on calibration of HPGe detectors

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ABSTRACT

One of the major difficulties in gamma spectrometry of voluminous environmental samples is the efficiency calibration of the detectors used for the measurement. The direct measurement of different calibration sources, containing isolated γ-ray emitters within the energy range of interest, and subsequent fitting to a parametric function, is the most accurate and at the same time most complicated and time consuming method of efficiency calibration. Many other methods are developed in time, some of them using Monte Carlo simulation. One of such methods is a dedicated and user-friendly program PHOTON, developed to simulate the passage of photons through different media with different geometries. This program was used for efficiency calibration of three HPGe detectors, readily used in Laboratory for Environment and Radiation Protection of the Institute for Nuclear Sciences Vinca, Belgrade, Serbia. The simulation produced the spectral response of the detectors for fixed energy and for different sample geometries and matrices. Thus obtained efficiencies were compared to the values obtained by the measurement of the secondary reference materials and to the results obtained by GEANT4 simulation, in order to establish whether the simulated values agree with the experimental ones. To further analyze the results, a realistic measurement of the materials provided by the IAEA within different interlaboratory proficiency tests, was performed. The activities obtained using simulated efficiencies were compared to the reference values provided by the organizer. A good agreement in the mid energy section of the spectrum was obtained, while for low energies the lack of some parameters in the simulation libraries proved to produce unacceptable discrepancies.

1. Introduction

One of the major difficulties in gamma spectrometry of voluminous environmental samples is the efficiency calibration of the detectors used for measurement. Most often the calibration by measuring standard sources is performed, a number of semi empirical methods have also been developed and, in the present time, the Monte Carlo simulations are often used to generate the spectral response of the detector [1,2]. The example of Monte Carlo simulation codes is GEANT4. It is developed to simulate the response of complex particle detectors and for variety of different high energy and nuclear interactions [3]. In case of gamma spectrometry, this code needs choosing an electromagnetic physics and corresponding database used in the development of the application for the particular detector, which may be time consuming and may require proficiency in programming language [4]. Once an application is developed, the use of GEANT4 is relatively easy.

For users that are not proficient in programming, or for any other reason need to have a readymade application, a dedicated and user-friendly program PHOTON provides a useful tool [1]. PHOTON uses a simplified input-file structure where the system and the source are described as a series of cylindrical zones. The zones that the photons traverse can be declared as active media (sources and detectors) and others as passive media (scatterers and absorbers), each with given properties [1]. After the construction of the measurement geometry, a schematic view of the system is available. It is written in Borland Delphi and contains Borland database engine and the user interface is Windows application. It also contains its own build-in cross-section libraries. However, Rayleigh scattering, fluorescence yields, form factors, and scattering factors are not included in the cross-section libraries [5]. These simplifications have proven especially useful in environmental measurements [6], where on one hand, an ultimate precision in calibration is usually not required and on the other, a variety of different sources might be measured in the laboratory. Having talked to some other gamma spectrometry practitioners, the authors of this paper found that the using of such simplified tool would be beneficial.

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The aim of this paper is to perform an efficiency calibration of three HPGe detectors, using PHOTON simulation software and to present and validate the results. The results of the calibration will be compared to the efficiencies obtained by measuring a set of secondary reference materials produced in the Laboratory for Environment and Radiation Protection of the Institute for Nuclear Sciences Vinca, Belgrade, Serbia and to the results obtained by GEANT4 simulation. The comparison should show the agreement between the results and limitations of the application of the method. The efficiencies obtained by the PHOTON simulation will then be applied on a realistic measurement of the secondary reference materials issued within the various interlaboratory proficiency tests. The measurement uncertainties for both simulated and the experimental values will also be calculated. The efficiency obtained by PHOTON and the experimental efficiency should be within the uncertainty limits in order to be declared as acceptable.

2. Materials and methods

The PHOTON simulation software defines the interaction between the γ photon and the medium through three main mechanisms: photoelectric interaction, Compton scattering and pair production. The probability of the interaction depends on the properties of the medium and on the photon energy. The cross-sections and linear absorption coefficients for the interactions are interpolated and tabulated for every defined medium at the beginning of the simulation [7]. For the actual photon energy the random interaction point for a given interaction is then found according to the following expression [1]:

$$L = -\frac{1}{\mu}\ln\eta \tag{1}$$

where L represents the path length between two subsequent interactions of the photon with the medium (or the emission of the photon and the first interaction), μ is the linear absorption coefficient for a given interaction and a given medium, while η is the pseudo-random number from the (0, 1) interval [1].

For the transport of the electrons, some simplifying algorithms exist. PHOTON code uses the Bethe–Heitler formula, with the cross-sections given by Seltzer and Berger in Ref. [8]. The interaction with the smallest distance to the interaction point (the smallest L) is chosen and the propagation of the photon through media is followed. The photon originates from and traverses through zones specified as consecutive cylinders with defined radius r and height h. If L is larger than the crossing point of the two zones, it is considered that the interaction did not occur in the first zone and the starting point is again selected, at the beginning of the next zone and so on until the interaction occurs. If L is larger than the dimension of last zone, it is considered that the interaction did not occur.

The geometrical characteristics of the measurement system are defined in the specified module of the program. The detectors considered for the simulation were the ones commonly used in our laboratory: two p-type detectors with the relative efficiency of 20% (named Detector 1) and 50% (named Detector 3) and one n-type detector with the relative efficiency 18% (named Detector 2). The characteristics of the detectors are presented in the Table 1. The geometrical parameters needed for the simulations, were defined according to the technical features obtained from the manufacturer. In case of the central void and top dead layer, which are not given in the manufacturer's certificate, the parameters were estimated based on the known dimensions of other detectors produced by the same manufacturer [9–11]. The geometry of the measured secondary reference material was also input in the program, as well as the chemical composition of the matrix. Assuming a cylindrical symmetry, geometry includes: the dimensions of the germanium crystal with the top dead layer, the aluminum end cap, the central void and the sample and its container. The geometrical description of the measurement system is simplified, since it does not take into account the buletization and the side dead layers. The chemical composition of the secondary reference material is defined by its chemical formula, mass fraction and density.

The spectra that are a result of the simulation are defined by the zone in which the deposition of energy is considered, the number of channels into which it will be simulated, the energy calibration and the peak full width at half maximum (FWHM) which is given as an empirical equation for a given type of the detector [1].

For the purpose of efficiency calibration in this paper, the simulation of the detector response on monoenergetic gamma rays was used. Namely, the response of the detector on the single energy emitted from the secondary reference material was used to calculate the efficiency on that energy and in that specific matrix. This choice excludes the need for the coincidence summing correction. The peak shape definition was performed using FWHM and FWTM (full width at tenth maximum) parameters of the detectors. Finally, the result of the simulation was a single full energy peak at each energy emitted by the radionuclide present in the secondary reference material and for all investigated secondary reference materials. The efficiency at the investigated energy was determined as the net count in the simulated peak divided by the total number of simulated events (emitted photons).

For the simulation, the equivalent of the measurement uncertainty can be estimated following the reasoning presented in Ref. [4]. For the input parameters of the simulation, the uncertainty has to be included in the uncertainty budget [4]. Since the probability of photons passing through different layers of the detector and sample is the product of individual probabilities of photon passing through an individual layer of the detector or sample, it gives the guideline for estimation of the uncertainty equivalent. Since the square of the combined relative uncertainty equals to the sum of squares of relative uncertainties, the equivalent of the relative uncertainty for the simulated efficiency, $u(\varepsilon)_{simulation}$, can be estimated according to Ref. [12]

$$u(\varepsilon)_{simulation} = \sqrt{\sum (\delta x_i)^2} \tag{2}$$

where δx_i represents the relative uncertainty of the parameter x_i (values that are input in the simulation). The geometry parameters that are defined in the simulation are 6 parameters of the detector geometry (crystal diameter and length, crystal cavity diameter and length, window thickness and window to crystal gap) and 3 parameters of sample geometry (matrix density, radius and height of the sample). Since the detector model is simplified in the simulation, we have to assume that the geometry will contribute significantly to the relative uncertainty of the results. The sum of uncertainties for crystal diameter and length and crystal cavity diameter and length can be estimated to be 5.0%, in total. The sum of uncertainties for window thickness and window to crystal gap for Detector 1 and Detector 2 is estimated at 10.0%, while it was 5.0% for Detector 3. Those contributions to the uncertainty were estimated according to the previous experience in using GEANT4 and EFFTRAN [4,11,13] for detector calibration. Relative uncertainties of height of the sample were estimated to be 0.1% in case of water samples and 1.0% in case of soil, sand, charcoal and grass samples. The density of the samples was calculated by dividing the measured mass of the sample with the volume of the sample. Since all samples were cylindrical, the volume was calculated as $r^2H\pi$ where r is measured inner radius of the container and H is the sample filling height. The uncertainty of r is estimated as the uncertainty of the measuring instrument (ruler). That leads to the conclusion that the uncertainty of the sample density is 1.0–2.0%. The equivalent of relative combined uncertainty of the simulated efficiency was estimated at 7.1–11.4%