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A simple methodology for characterization of germanium coaxial detectors by using Monte Carlo simulation and evolutionary algorithms

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ABSTRACT

The determination in a sample of the activity concentration of a specific radionuclide by gamma spectrometry needs to know the full energy peak efficiency (FEPE) for the energy of interest. The difficulties related to the experimental calibration make it advisable to have alternative methods for FEPE determination, such as the simulation of the transport of photons in the crystal by the Monte Carlo method, which requires an accurate knowledge of the characteristics and geometry of the detector. The characterization process is mainly carried out by Canberra Industries Inc. using proprietary techniques and methodologies developed by that company. It is a costly procedure (due to shipping and to the cost of the process itself) and for some research laboratories an alternative in situ procedure can be very useful. The main goal of this paper is to find an alternative to this costly characterization process, by establishing a method for optimizing the parameters of characterizing the detector, through a computational procedure which could be reproduced at a standard research lab. This method consists in the determination of the detector geometric parameters by using Monte Carlo simulation in parallel with an optimization process, based on evolutionary algorithms, starting from a set of reference FEPEs determined experimentally or computationally. The proposed method has proven to be effective and simple to implement. It provides a set of characterization parameters which it has been successfully validated for different source-detector geometries, and also for a wide range of environmental samples and certified materials.

1. Introduction

Gamma spectrometry with HPGe detectors is a common technique to identify and quantify a wide range of gamma emitting radionuclides due to its high energy resolution. In particular, these detectors are commonly used for the analysis of low-level activity environmental samples. In the estimations of activity concentration of a sample by gamma-ray spectrometry is needed to know the full energy peak efficiency (FEPE) of the system for the photopeak of interest, which depends on the photon energy, density and composition of the sample, and source-detector geometries. The calibration of the measuring system can be performed experimentally by using certified reference sources whose activities are well known. Nevertheless, it demands the creation of standards, for each geometry, composition and density of the sample to analyse, using known quantities of radionuclides. In many situations, such as in the analysis of soil, the preparation of standard samples that are identical to the sample matrices can be a very complex process. For the aforementioned reasons, empirical method for efficiency calibration may become a costly process in term of time and budget. Additionally, the analysis of important effects such as the coincidence summing on the detector efficiency or the optimisation of sample geometry on the detector sensitivity not be able addressed by experimental calibration procedures (McNamara et al., 2012; Britton et al., 2014).

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Monte Carlo simulations have been widely used as a computational alternative to empirical calibration to avoid these problems. The Monte Carlo methods are numerical techniques based on the creation of a stochastic model of the system under study, so that the desired values of the physical quantities characterizing the system are derived from the expected values of certain random variables (Abbas et al., 2002). These variables are obtained in turn as combinations of other random variables describing the different processes occurring in the system. In the case of gamma spectrometry, physical processes to be considered are the transport and interaction of gamma rays into the sample itself and detector. For this, it is needed to know the physical characteristics of the source and detector, and to implement a physical model for the interaction of photons into the detector based on atomic processes involved (photoelectric absorption, Compton scattering and pair creation), and the coefficients of absorption and attenuation of the different media involved. Calibration methods based on Monte Carlo have been applied to a wide variety of source distributions and measurement conditions (Ewa et al., 2001; Helmer et al., 2004; Hurtado et al., 2004; Kamboj and Kahn, 2003; McNamara et al., 2012; Nikolic et al., 2014; Salgado et al., 2006; Sima and Arnold, 2009; van der Graaf et al., 2011), even to calibrate portable HPGe detectors for environmental monitoring (Boson et al., 2009; Gutiérrez-Villanueva et al., 2008; Hurtado and Villa, 2010; Rostron et al., 2014; Zhang et al., 2013). These simulation techniques allow to establish a summing free efficiency or to correct for self-absorption effects (Dababneh et al., 2014; Dziri et al., 2012; Laborie et al., 2000; Vargas et al., 2002), also accurate efficiencies have been obtained by optimizing of several sample factors, as density, matrix composition or geometrical configuration (Huy et al., 2012; Kaminski et al., 2014; Yang et al., 2013). The unknowing of detector geometry parameters has been reported as one of main causes of discrepancies in the efficiency determination (Nikolic et al., 2014), then several Mote Carlo model have been focused in characterizing the detector geometry (Boson et al., 2008; Budjas et al., 2009; Courtine et al., 2008; Hardy et al., 2002; Huy et al., 2007; Maleka and Maucec, 2005; Rodenas et al., 2003; Szentmiklósi et al., 2014).

Thus a key element for calibration by Monte Carlo simulation is the accurate knowledge of the physical and geometrical characteristics of the detector such as length and diameter of the Ge crystal, thickness of the dead layers, dimensions of the package and window, etc. The process to determine these parameters is usually known as characterization of the detector. This characterization procedure increases the cost of the equipment but it has the advantage that, once characterized the detector, it can be used to generate calibration by software for a wide range of geometries and compositions of the samples and containers without the need for reference sources (Bronson, 2003; Cornejo Díaz and Jurado Vargas, 2008; Venkataraman et al., 2005).

The characterization of the detector is usually performed before the acquisition of the system and combines the use of experimental measurements of FEPEs and Monte Carlo Simulation. An initial model of the specific detector to be characterized is created by using the nominal dimensions provided by the manufacturer and it is used as input of a Monte Carlo code. This detector model is then validated by comparing the FEPEs provided by the Monte Carlo code with experimental efficiencies obtained for several source-detector geometries and samples material in a wide range of energies. If needed, changes are made in the dimensions of the detector, and new computational FEPEs are generated by the Monte Carlo code. The detector model is considered valid if the computational efficiencies are in agreement with the experimental ones within a level of acceptable uncertainty. This characterization procedure requires several weeks of work by the manufacturer and increases the cost of the equipment, but it has the advantage that, once characterized the detector, it can be used to generate calibration by software for a wide range of geometries and compositions of the samples and containers.

Due to its high cost and time consumed in the process, it is not a common practice to characterize detector once installed in the laboratory. Furthermore the characterization processes is based on the properties and dimensions of the HPGe detector at the time of the characterization. Therefore, any changes in crystal properties (e.g. it is known that the thickness of the dead layer increases over a period of years if the detector is not kept refrigerated at the proper temperature) could induce an error in the efficiency calculations. This implies that the detector must be characterized again over time, with the disadvantages that this entails. Another drawback of the characterization process is that no commercial procedure has been developed to characterize some types of detectors, such as the well detectors. Therefore a methodology to characterize a detector in the laboratory, using efficiency data provided by another procedure (theoretical or experimental) can be a useful tool.

This paper shows a new methodology developed for computational characterization of an Extended Range Germanium Hyperpure detector (HPGe XtRa) by obtaining the geometrical characteristics of an equivalent model of the detector, which can be used in Monte Carlo calculations of efficiency calibration curves. This methodology only requires knowing an accurate set of experimental or theoretical FEPEs for a given spectrometer and one or several source-detector geometries and sample's material. These FEPEs can be obtained at the laboratory through a standard calibration procedure.

2. Material and methods

2.1. Instrumentation, computational codes to FEPE calculation and certified reference sources

The gamma-ray spectrometry equipment used in this study is a Canberra XtRa HPGe detector, model GX3518. The detector has 38% of relative efficiency in relation to an NaI(Tl) detector with an active area of $3 \times 3''$ and nominal FWHM of 0.875 keV at 122 keV and 1.8 keV at 1.33 MeV and it works coupled to a DSA-1000 Canberra multichannel analyzer. The detector is shielded with Fe 15 cm thick and located in a room with walls and ceiling made of concrete in the ground of a three plants building. The spectral analysis is performed using the Canberra Genie 2000 software package (Canberra, 2002). The detector has been characterized to permit the efficiency calibration by the Canberra's LabSOCS (Laboratory SOurceless Calibration Software) code (Canberra, 2013) that performs mathematical efficiency calibrations of Ge detectors, without any use of radioactive sources by the laboratory user. The Canberra's characterization methodology uses an experimental procedure to analyse the response of the detector to sources in the vicinity thereof over a range of photon energy of 10 keV to 7 MeV, combined with a computational process to determine the detector parameters using the MCNP Monte Carlo Code (Briesmesiter, 1992; X5 Monte Carlo Team, 2008). As result, a characterization file with a comprehensive array of point-source efficiencies in different locations around detector is obtained. This information is exclusive for a given detector and it has to be introduced as a LabSOCS input file. In this work the LabSOCS code was used to generate the FEPEs used as reference values, but any other method could be used to determine them such as experimental procedures based on the use of Certified Reference Material (CRM).

To develop the computational characterization methodology proposed in this work we have used the PENELOPE code (Salvat et al., 2001, 2011; Sempau et al., 1997; Sempau et al., 2003), a