Equivalent detector models for the simulation of efficiency response of an HPGe detector with PENELOPE code

Abstract

In this work some "equivalent" models for the simulation of efficiency response of an High-Purity Germanium (HPGe) detector, installed inside a "low-background" bunker in the Engineering Department of the University of Palermo, were developed. The main feature was to attribute the uncertainties of the model to only one of the parameters, the dead layer of the detector, keeping unchanged the other data provided by the manufacturer. With this technique, using the Monte Carlo PENELOPE code in the 2011 version, the efficiency response was evaluated and compared with previous one performed with MCNP5 code.

The validation of equivalent models is performed by comparing the simulation results with the ones of experimental spectrometric measurements of calibrated point sources and characterized volumetric sources such as a Marinelli beaker and an air filter reduced to a "packet-sample".

The use of equivalent models makes easier and faster the evaluation of efficiency curves with a Monte Carlo code and requires only a few experimental values for validation.

Keywords: Gamma-ray spectrometry, Monte Carlo, HPGe detectors, efficiency, modeling.

1. Introduction

Gamma-ray spectrometry with High-Purity Germanium detectors (HPGe) is the most widespread analysis technique to identify and determine activities of gamma-emitting radionuclides present in a sample. For this task, a standard with certified activity and same geometry and matrix of the sample is needed to evaluate the detection efficiency response of the spectrometric system. Since it is often difficult to have such a standard, especially in the environmental monitoring of radioactivity, Monte Carlo (MC) simulation of response of a HPGe detector is increasingly used to evaluate counting efficiencies *(1-5)*.

The results of the simulation depend on detailed knowledge of the characteristics of the detector, able to define a model that better corresponds to detector performances. Since some data on detector are missing and a X-ray graph is unworkable, in this work some "equivalent" models have been studied and adopted. The main feature was to attribute the uncertainties of the model to only one of the parameters, the dead layer (DL) of the detector, keeping unchanged the other data provided by the manufacturer.

Adopting this model and using the Monte Carlo PENELOPE (PENetration and Energy LOss of Positons and Electrons in Matter) code, simulation of the response of an HPGe detector to determine the detection efficiency for different types of gamma sources was carried out. A similar activity had already been performed with the use of the MCNP (MC N-particle Transport) code, version 5 *(6),* with appreciable results both from the operational and numerical evaluations point of view, that can be considered a reference for evaluating the data obtained with the PENELOPE code *(7)*.

To compare the results obtained with the two codes, the same HPGe detector of the analysis with MCNP5 code was taken into consideration, i.e. an ORTEC GEM-50195S, already arranged with its shielding and the measurement spectrometric instrumentation inside a “Low Background” bunker in the Engineering Department of the University of Palermo *(8)*. The comparison was performed in terms of Full-Energy-Peak Efficiency (FEPE), defined as the ratio of the number of counts in the full-energy peak to the total number of gamma rays emitted from the source. FEPE value is proportional to the solid angle subtended by the detector, and then, to source-to-detector distance. Furthermore, it is a function of energy and strongly depends on the thickness of the dead layer and other detector geometrical characteristics *(9)*.

Since the results obtained with PENELOPE code are comparable with the ones related to MCNP5 code, it can be considered that the models developed and the simulation procedures constitute a quick analysis tool for the evaluation of efficiencies and the determination of radionuclide activities in a sample.

2. Materials and Methods

2.1 The HPGe Detector

The HPGe detector used in this study is a p-type HPGe coaxial detector, with a cryostat in HV (Low Background) configuration, manufactured by ORTEC model GEM-50195S. Germanium crystal has a straight cylinder shape with a diameter of 69.4 mm and a height of 69.3 mm, with a dead layer of about 700 µm and a 1.5 mm thick magnesium cap. Its efficiency, compared to the one of a NaI (Tl) 3"x3" crystal at 1.33 MeV for a ^{60}Co source measured at a distance of 25 cm, was 60.8%. The FWHM (Full Width at Half Maximum) at 1.33 MeV results to be 1.75 keV.

The detector is put in a composite shielding which attenuates the natural background to very low levels. A first shielding, the innermost one, consists of a rectangular parallelepiped made of OFHC (Oxygen Free High Conductivity) copper, 30 mm thick, followed by a second layer of 120 mm thick lead bricks. A third solid HBO_3 shielding with a thickness of 30 mm, contained in large Plexiglas boxes, have the function of absorbing the thermal neutrons, and finally a covering in Polyethylene bricks of 150 mm of thickness have also the function of thermalizing the fast neutrons associated with the radiation of natural background. In order to further attenuate the environmental radiation of cosmic origin and limit as much as possible the temperature changes, the complex is located inside a concrete bunker with walls no less than 70 cm thick, including the roof, with a labyrinth entrance *(8)*.

Fig.1 shows a photograph of the detector-shielding complex and the associated spectrometric system units, as well as a photograph of the measurement cavity with the detector and the OFHC copper coating that acts as attenuation of the fluorescence radiation of lead.

The spectrometer system is remotely controlled via Ethernet connection with IPX protocol for managing all the operating modes, while the ORTEC GAMMAVISION code, version 7 *(10)* was used for the acquisition and analysis of the spectrometric data.

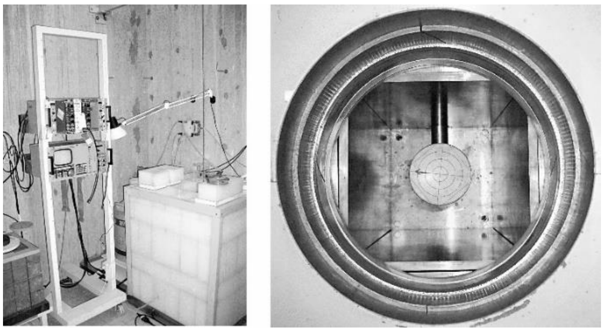

Figure 1. Photographs of the detector-dewar-shielding complex with associated spectrometric measurement instrumentation and measurement cavity with detector capsule and OFHC copper chamber coating. The concrete walls of the bunker in which the complex is located are visible.

2.2 The PENELOPE Code

The Monte Carlo code used, PENELOPE in the 2011 version, was developed entirely in Fortran 77 by Salvat et al. (*11*) in order to have a simple, fast and relatively easy to manage tool for the simulation of the interactions of photons in material systems constituted by a number of homogeneous regions delimited by interfaces. The interaction models adopted by the program and the associated databases allow the simulation of photon transport in coaxial germanium detectors *(12)* for energies in the range 1 keV ÷ 1 GeV. The program can also be implemented in Windows environment and therefore the most common personal computers can be used, even if the running speed of the various routines and associated programs is significantly reduced with simulation times, according to cases, even rather prohibitive. As regards simulations described in this work, the code was implemented in a Windows environment in a suitable portable PC with a parallel CPU architecture.

For the realization of the simulation procedure, it was decided to use the main program of the code, PENMAIN, which allows to simulate not only the detector, but also volumetric sources that do not have a well defined cylindrical geometry, such as the "packet sample" geometry introduced in the following. Furthermore, after correctly compiling the input file, a number of strictly formatted text lines which define the different elements of the geometry, PENMAIN is able to directly output the quantity of our interest, namely the FEPE values. The modeling of the detector can be easily carried out with the geometry viewer GVIEW3D, an executable binary program written to help the user to debug the geometry definition file, whose results can be appreciated in fig. 2 where a 3D section of the simulated detector is given.

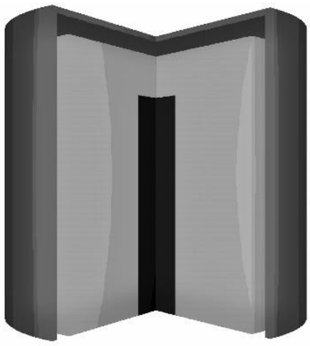

Figure 2. GVIEW3D representation of ORTEC GEM50195S detector model in a 3D projection section. The thickness of the magnesium cap, the cold finger and the germanium crystal are highlighted.

2.3 Equivalent Models and Simulation

In order to elaborate a detector model it is necessary to provide characteristic data of the detector with a good precision. Sometimes, despite having the manufacturer's certification, a radiograph of the detector is used to accurately determine the size of the various components and their mutual position.

Since some geometrical characteristics of the detector are not provided with required precision and it is not possible, due to the structure of the shielding described above, to carry out an X-ray analysis of the detector, it was decided to adopt a model of the detector defined by incorporating all uncertainties within the dead layer (DL), assuming for the remaining parameters the values supplied by the manufacturer *(9,13-15)*.

In this way the definition of a detector model able to guarantee minimum deviations between the simulation results and the experimental data is simplified and rapid.

The resulting model can therefore be defined as "equivalent", since it takes into account the interaction properties of the radiations in the same detector, even though the DL parameter is substantially different from the value furnished by the manufacturer. The verify of the effectiveness of the use of this modeling is one of the aims of the present work.

For validation of equivalent models, it is needed to have reliable experimental data in order of efficiencies for given gamma-ray energies obtained from spectrometric measurements of calibrated sources. For this study FEPE data have been obtained a few years ago for point-type gamma-ray sources and for two volumetric sources, 1L Marinelli container filled with powder of calcium carbonate ($CaCO_3$) and the “packet-sample” geometry used for the measurement of atmospheric particulate filters in the framework of environmental monitoring *(16-20)*.

2.4 Calibrated gamma-ray emitting point sources

The experimental measurements used to define the models refer to point sources whose activity is certified by the "Commissariat à l'Énergie Atomique" (CEA) with an uncertainty of less than 2% (1σ). These were part of a kit of single-line sources - that is, with a single gamma emission – reliable for determining efficiencies. The sources consist of radionuclides ^{241}Am, ^{109}Cd, ^{57}Co, ^{139}Ce, ^{51}Cr, ^{113}Sn, ^{85}Sr, ^{137}Cs, ^{54}Mn, ^{65}Zn and a source of ^{88}Y, not included in the kit, but acquired to extend the energy range up to 1836 keV.

These sources were measured at different distances in axis from the detector cap up to 30 cm to have a FEPE data set. It should be noted, however, that some measurements were realized at different times, even after some years, so that - as shown below - a variation over time of the characteristics of the detector may be occurred and a modification of the corresponding "equivalent" model may be required.

2.5 The packet-sample measurement geometry

This measurement geometry has been adopted for several years *(16-20)* for the spectrometric measurement of atmospheric particulate filters collected during the night-time suctions with the “Sampling Station” located on the roof of the Department. At the end of filtration, the filter, supplied by Sofiltra-Poelman, size 45x45 cm, treated with a suitable fixative, is reduced to 16 strips, stacked and pressed to obtain a "package" of 6cm×6cm×0.7cm dimensions, named "Packet-sample". Since a standard with the same geometry and composition is not commercially available, a secondary standard has been studied and implemented using a blank filter and a small amount (1-2 g, usually equal to the amount of particulate collected) of a powder mixture consisting of calcium carbonate

($CaCO_3$) and thorium oxide (ThO_2) with known activity This standard allowed us to determine the trend of efficiencies, with the results reported in *(21)*.

Fig.3 shows a section and a top view of the simulation model representing the measurement geometry, obtained with the GVIEW3D program where 1 mm Plexiglas plate, over which the packet sample is placed, is highlighted.

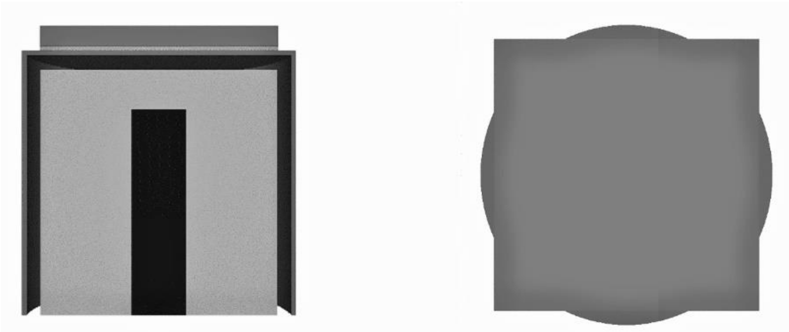

Figure 3. GVIEW3D representation of «packet-sample» model, including 1 mm of a Plexiglas plate where the filter is placed for the measurement.

2.6 The Marinelli Beaker (1 L)

Other experimental efficiency data were obtained using the known Marinelli geometry (volume 1 L) filled with a pure inert, calcium carbonate, $CaCO_3$, supplied to Merck with 99% purity, and a small amount of ThO_2. Fig. 4 shows a 3D section of the configuration of the detector model and the Marinelli container. Details on the preparation of the standard and the results obtained can be found in *(22,23)*.

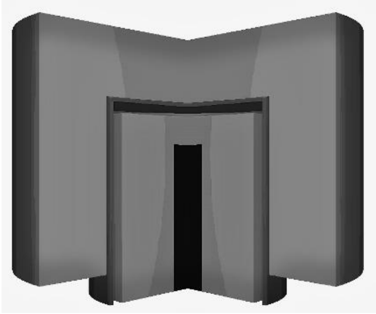

Figure 4. Section of simulation model: detector and Marinelli beaker.

3. Results and discussion

Simulation results were verified in comparison with the previous ones obtained with MCNP5 modeling *(7)*. Fig. 5 shows the experimental trends of point source FEPEs for some measurement geometries. It can be noted that the efficiency values measured at a distance of 0 cm (on the magnesium cap), 10 cm and 30 cm from the cap were obtained from measurements carried out a few years earlier than measurements carried out at a distance of 1 cm, 2.5 cm and 6 cm from the cap.

For each gamma energy, simulations were carried out with different DL values. Figs. 6-11 reports, for clarity, only some trends of simulated FEPEs and relative differences with respect to the experimental values. From the comparison of all the results obtained with the experimental data for the distances 0 cm (on top), 10 cm and 30 cm, as shown in Figs. 6-8, an optimal DL value was identified for the equivalent model with DL=0.23 cm. This determination was in line with the conclusions reported in *(7)* in which the DL value was assumed equal to 0.21-0.22 cm. The greatest differences occur with low-energy gamma radiations, as already noted in the analyses with the MCNP5 code *(7)*.

The same value of DL cannot be adopted for the other geometries, with distance 1 cm, 2.5 cm and 6 cm from the cap, whose experimental measurements were carried out in a different period of time. The results shown in Figs. 9-11, only for some values of DL, lead to identify a value DL = 0.30 cm as more appropriate, with a significant difference compared to the previous one. This difference can be ascribed to a variation of the characteristics of the spectrometric system whose parameters are modified, both as regards the detector performances and the operating conditions of the whole measurement system. For this reason, it can be deduced that a calibration cannot be assumed in absolute terms but must be - as usual - periodically repeated and checked again. Similarly, the simulation models studied, even “equivalent”, must be periodically updated in relation to new measurement conditions and significant variations in operating parameters.

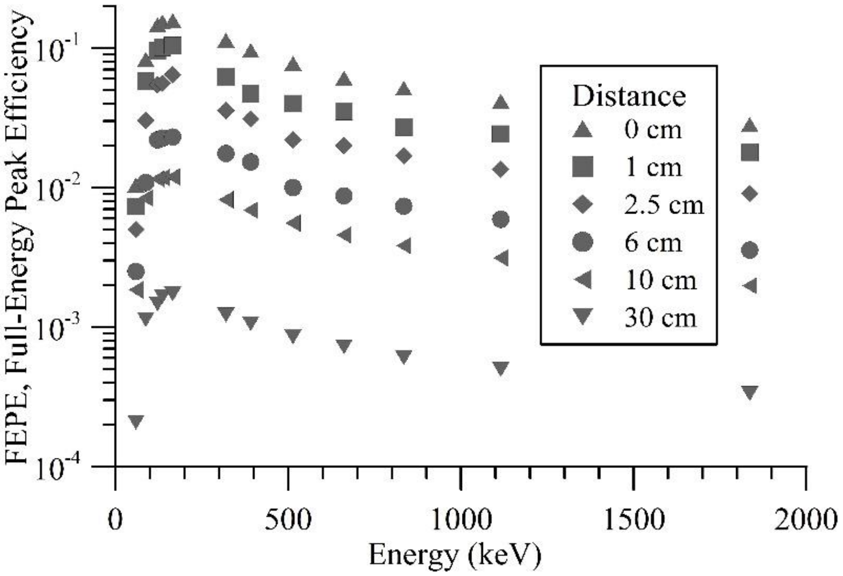

Figure 5. Experimental FEPE trends for gamma-ray point source geometries. Detector: HPGe ORTEC GEM50195S.

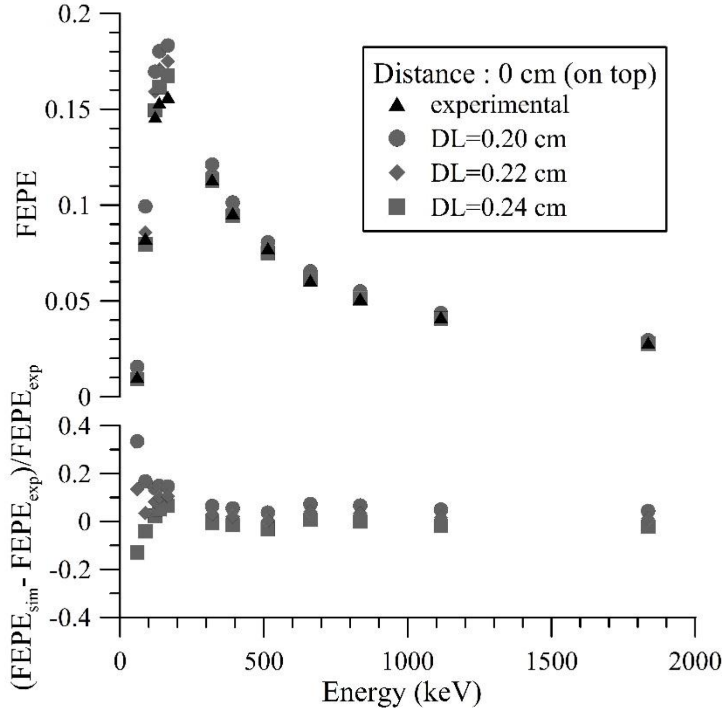

Figure 6. Simulated FEPE values and differences with respect to experimental values for point sources measured at a distance of 0 cm (on the magnesium cap) from the HPGe detector ORTEC GEM 50195S.

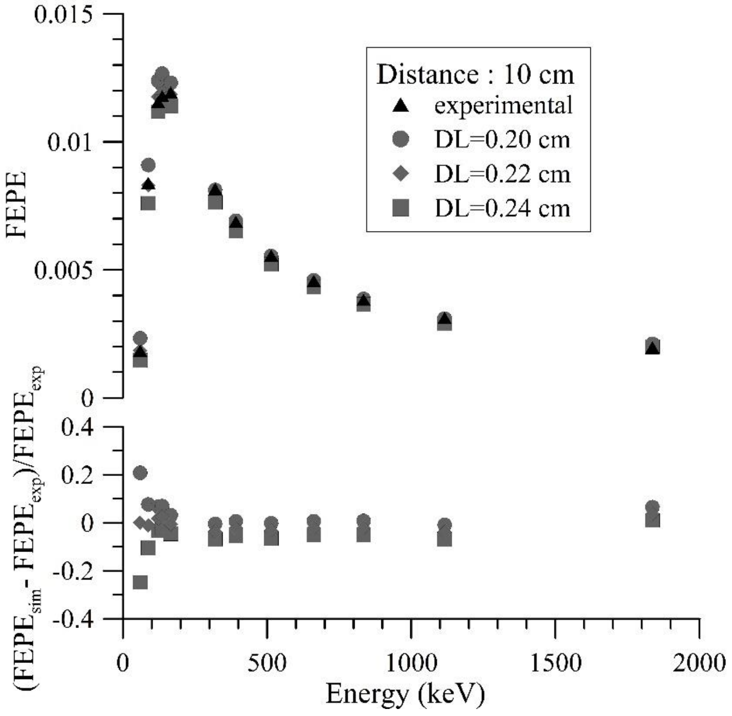

Figure 7. Simulated FEPE values and differences with respect to experimental values for point sources measured at a distance of 10 cm from the HPGe detector ORTEC GEM 50195S.

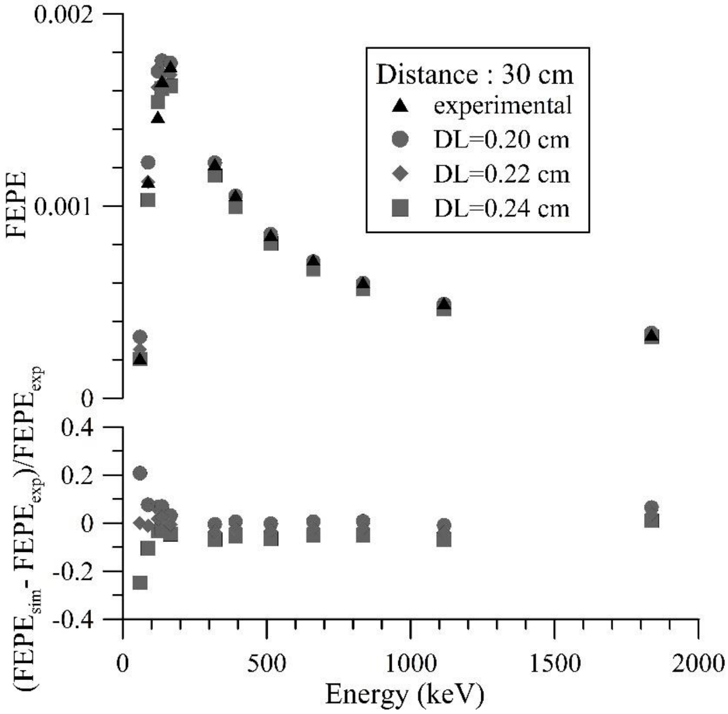

Figure 8. Simulated FEPE values and differences with respect to experimental values for point sources measured at a distance of 30 cm from the HPGe detector ORTEC GEM 50195S.

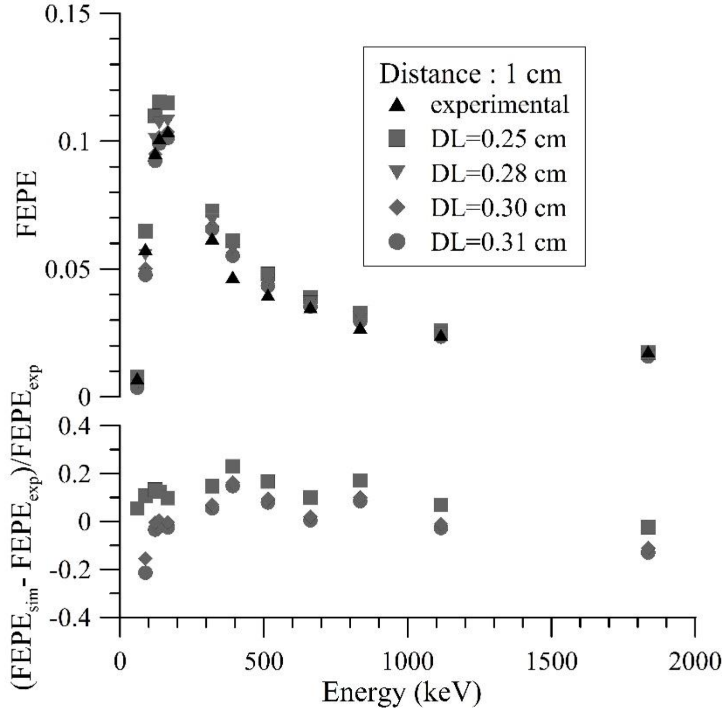

Figure 9. Simulated FEPE values and differences with respect to experimental values for point sources measured at a distance of 1 cm from the HPGe detector ORTEC GEM 50195S.

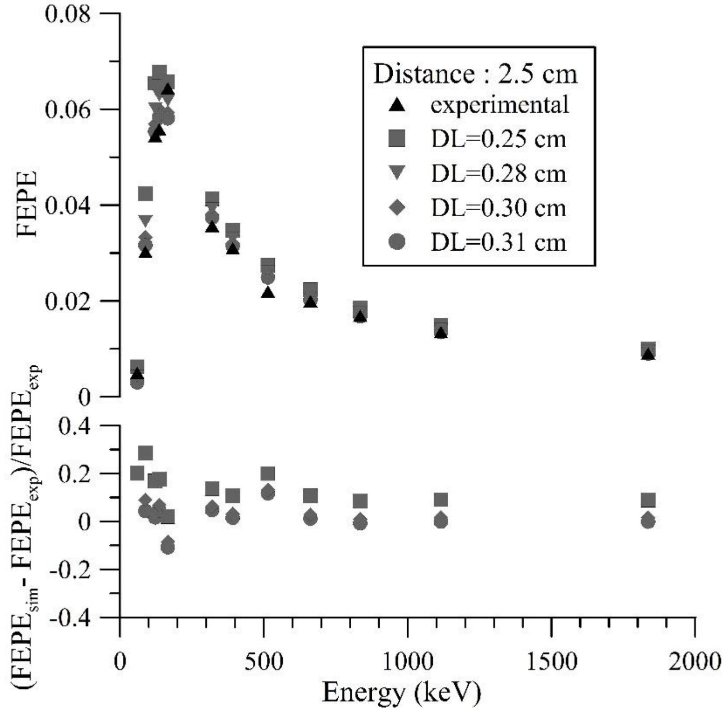

Figure 10. Simulated FEPE values and differences with respect to experimental values for point sources measured at a distance of 2.5 cm from the HPGe detector ORTEC GEM 50195S.

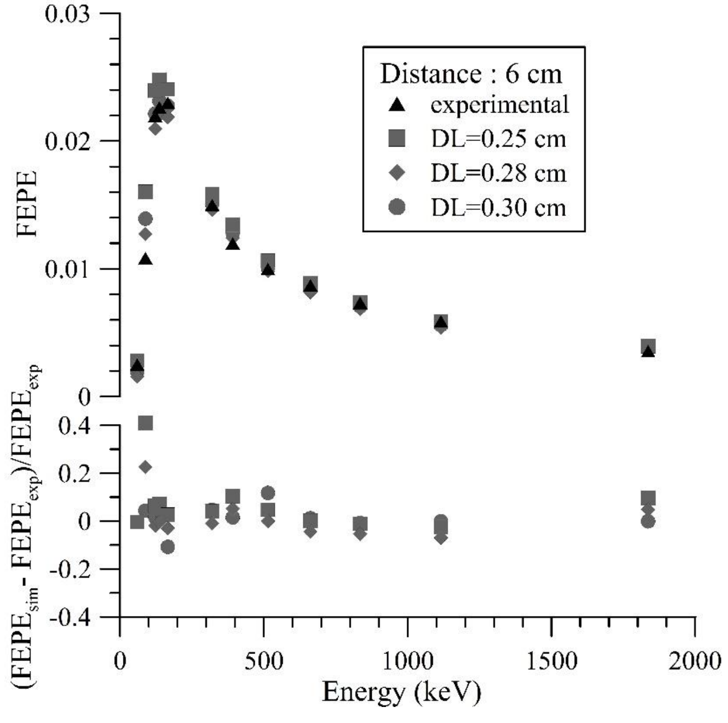

Figure 11. Simulated FEPE values and differences with respect to experimental values for point sources measured at a distance of 6 cm from the HPGe detector ORTEC GEM 50195S.

After the validation of simulation model for point sources, models to evaluate the detection efficiency for two volumetric sources, a "packet-sample" (air filter) and a 1 L "Marinelli " beaker filled with $CaCO_3$, were considered. The simulation results are shown in Figs. 12 and 13. Even in this case, although it has reported only three values of DL, it seems that the value of DL = 0.40 cm evaluated for the "packet-sample" can also be adopted in Marinelli geometry with an error of about 10% compared to the experimental values *(22,23).*

As can be seen from the examination of the curves shown in Figs. 6-11, and in particular in Figs. 12-13, the simulations carried out with the previously defined models lead, in the worst cases, to deviations of the order of 20%. Probably, assuming an intermediate DL value for an equivalent model for “packet sample” or for Marinelli beaker, lower differences can be achieved. The difference is anyway justifiable, for example for "packet-sample" geometry, taking into account that cellulose was used as the material of the filter, since the paper, whose chemical composition is rather complex, does not appear among the materials envisaged in the code.

It can be observed that the use of the code and the respective models allow to evaluate FEPE values in absence of calibrated standards. This consideration is important in environmental radioactivity measurements in which it is often essential to have rapid assessments of activities with acceptable measurement errors in samples not well characterized.

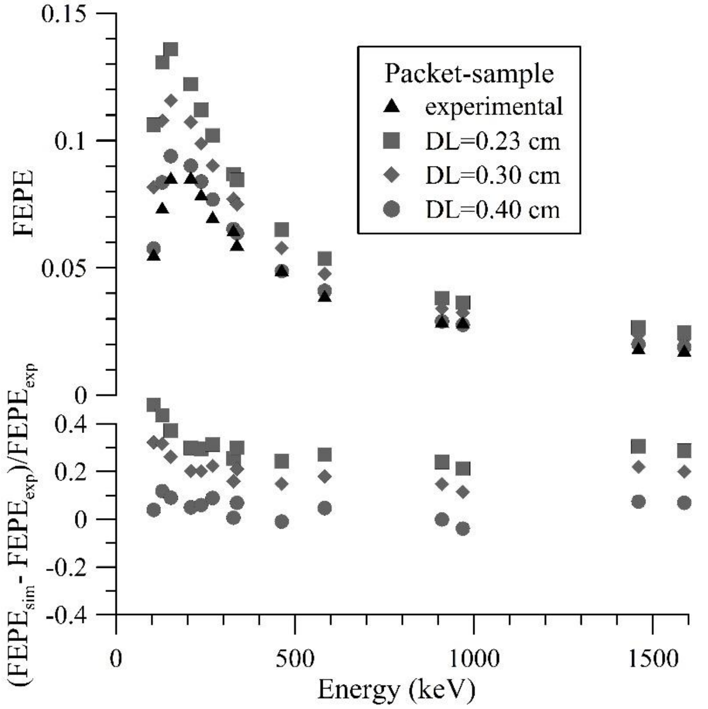

Figure 12. Simulated FEPE values and differences compared to the experimental values for the "packet-sample" geometry. HPGe detector: ORTEC GEM 50195S.

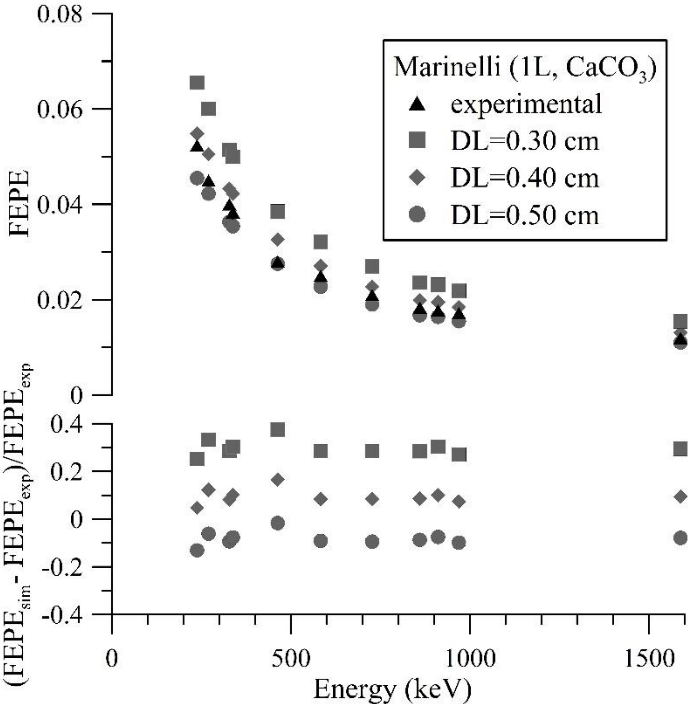

Figure 13. Simulated FEPE values and differences with respect to the experimental values for the 1 L "Marinelli" container filled with calcium carbonate (CaCO3) inert. HPGe detector: ORTEC GEM 50195S

4. Conclusions

The use of PENELOPE code and the equivalent models defined with the comparison with the experimental data, assuming a fictitious value of DL, makes it possible to obtain rapid evaluation of efficiencies for the geometries examined with various materials and different densities. Results obtained with PENELOPE code and the analogous ones obtained with the MCNP5 code are comparable. Moreover, the first is easy to implement and quite fast, so that it can be used at least for rather simple geometries with a normal "personal computer" in Windows environment. Reliability of simulations is reduced, as it happens to most MC codes, for low energy gamma-ray radiations.

Finally, a variation of the characteristics of the detector over time was highlighted, as already indicated by the manufacturer. The models used in the simulations must be continuously verified, and the experimental measurements of efficiency periodically repeated also for the same measurement geometry. However, the use of equivalent models, with the attribution to dead layer of all the uncertainties of detector parameters, makes modeling and realization of the simulation simpler and faster.

Disclosure statement

No potential conflict of interest was reported by the authors.

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