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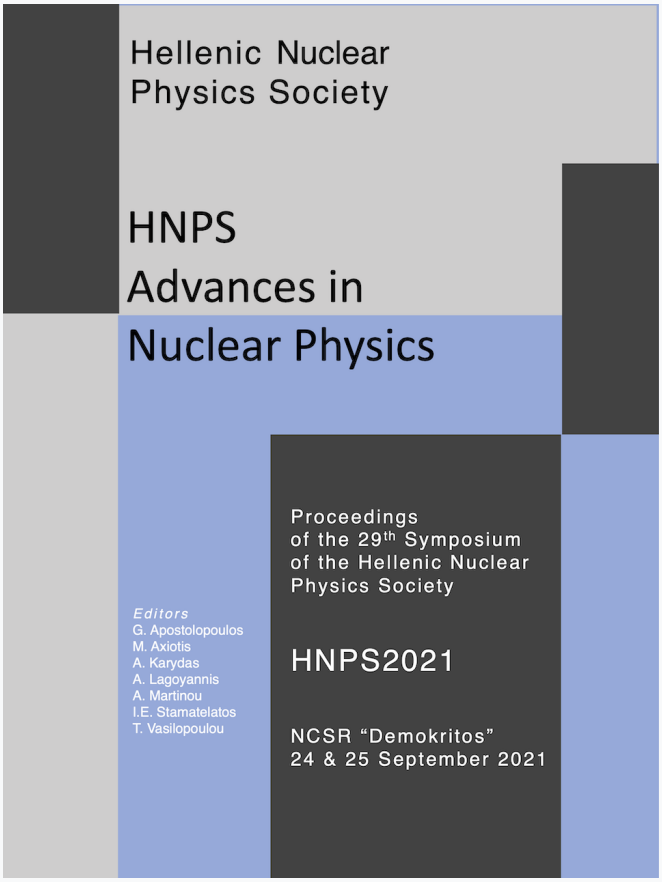

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Comparison of Real and Generated by MCNP Simulation Spectra for Validation of Neutron Activation Calculations

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Abstract The objective for decommissioning planning, is to obtain a radiological understanding of the involved installation. The characterization at this stage could be carried out by means of: (a) neutron activation calculations based on reactor design and neutron flux; (b) dose rate measurements; (c) in-situ gamma spectrometry; (d) sampling for determination of the scaling factors in activated and contaminated components.

Neutron activation calculations contain several uncertainties. These uncertainties are based on the input data - such as material data (composition and impurities), neutron flux and energy, nuclear data libraries - and on the methodology of the process and the simulation codes.

Taking into consideration all these modeling uncertainties, this work is focused on the development of a technique for validation of the calculations. A non-destructive gamma spectrometry technique using MCNP6.1 simulations is under development for interpretation of the resulting gamma-ray spectra of the radionuclides in activated components. In particular, a spectrum will be produced, based on the activities of the main radionuclides in the activated component and the results of MCNP6.1 simulations. This spectrum will be compared with the experimental spectrum.

The radiological characterization of activated components is essential for the decision making process during decommissioning. The cutting techniques to be followed in order to reduce the production of secondary waste and limit the doses to personnel and the selection of decontamination techniques should be based on accurate determination of the radionuclides inside the material and/ or in the surface contamination. The proposed method will facilitate the precise characterization and classification of the waste produced from the decommissioning.

Keywords neutron activation calculation, MCNP6.1 simulation, spectra

INTRODUCTION

Many of the important long lived radionuclides contained in the radioactive waste are difficult to measure (DTM) using non-intrusive techniques because they are low energy, non-penetrating beta or alpha emitting nuclides (i.e. non-gamma emitters) [1]. Identification of these DTM nuclides requires methods that involve analysis of waste samples using radiochemical analysis to separate the various radionuclides for measurement. The approach that is used is the scaling factor (SF) method. The SF method is based on developing a correlation between easily measurable gamma emitting nuclides (key nuclides) and DTM nuclides. The activities of DTM nuclides are then estimated by measuring the gamma emitting nuclides and applying the scaling factors.

The key radionuclides which are also easy to measure (ETM) are usually ^{60}Co and ^{137}Cs. ^{60}Co is an activation product radionuclide produced by the ^{59}Co(n,γ)^{60}Co reaction in the 100% abundant stable cobalt isotope ^{59}Co with a cross-section of 18.7 barns [2]. On the other hand ^{137}Cs is a fission products and due to its high water solubility is easily transported and settled as surface contamination. In this study, the spectrum of these two radionuclides as well as of ^{90}Sr, which is a fission product and a pure β^- emitter is generated by MCNP6.1 code and compared with the corresponding experimental one.

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EXPERIMENTAL DETAILS

The gamma spectrometry system we use consists of the following main parts:

- Detector unit: A Bicron Monoline scintillation detector NaI(Tl) (Model 3M3/3) with a 3" x 3" crystal in a thick aluminium housing, covered with a white reflector, including a photomultiplier tube, an internal magnetic/light shield and a 14-pin connector;
- Electronics and acquisition unit: a digital signal-processing unit (Osprey Digital Tube Base MCA) and a high voltage supply system (850 V);
- GenieTM 2000 spectroscopy software for spectrum acquisition.

In this preliminary study, for both the experimental spectrum and the spectrum produced by the MCNP6.1 code, the point source geometry for the three radionuclides (^{60}Co, ^{137}Cs and ^{90}Sr) is used. The point source is placed at 15 cm distance in front of the scintillation detector NaI(Tl), on the main axis of symmetry.

For production of the MCNP6.1 gamma-ray spectrum is necessary to use the resolution versus gamma-ray energy of the detector. The energy peak for a mono-energetic photon source is broadened at the spectrum. The shape of this peak is approximately Gaussian with the center at the source energy and a width characteristic of the specific detector. By the MCNP6.1 simulations, a single value is calculated and placed in the tally bins without any broadening. Therefore, the calculated spectra should be modified to account for the peak broadening. The peak broadening is dealt with by changing the energy of the particle during the Monte Carlo simulation just before it is tallied by randomly sampling an energy to be deposited from a Gaussian distribution centered at the original particle energy [3]. This is accomplished by using the FTn special treatment for tallies [4].

Regarding the simulated spectra, F8 pulse-height tally combined with the "FT8 GEB card" of MCNP6.1 code is used. This type of tally, provides the energy distribution of the pulses that are created within the cell that models the detector. The tally value corresponds to the counts registered in each energy bin specified by the user and the results are normalized to be per starting particle, ending up giving the resolution of the detector. The Gaussian Energy Broadening (GEB) option defines the energy broadening according to the Gaussian formula (Eq. 1).

$$f(E) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(E-E0)^2}{2\sigma^2}} \quad (1)$$

where: E: broadened energy;
Eo: unbroadened energy;
σ : standard deviation depends on FWHM according to the Eq.2.

$$FWHM = 2\sqrt{2 \cdot ln2} \cdot \sigma \approx 2{,}35482 \cdot \sigma \quad (2)$$

The FWHM is defined experimentally by using the Eq.3.

$$FWHM = a + b\sqrt{E + cE^2} \quad (3)$$

where: E: incident gamma ray energy (MeV);
a, b, c: user provided constants from the fitting function.

A non-linear function adjusted by least-squares procedure is applied to determine the values of a, b and c coefficients [5]. These values are used as input to the "FT8 GEB card" of MCNP6.1 code, in order to consider the energy and resolution of the detector in the simulation. The a, b and c parameters

are functions of the type and the size of the detector [6] with units of MeV, $MeV^{1/2}$ and MeV^{-1}, respectively [7]. In the present work, the adjustment coefficients of the resolution curve for the Na(Tl) detector were obtained by the method of least squares and the values are α= -0.0055 MeV, b=0.06214 $MeV^{1/2}$ and c=0 MeV^{-1} according to the experimental procedure described, using data from four radioactive sources of ^{60}Co, ^{137}Cs, ^{133}Ba, ^{241}Am.

Table 1. *Energy and resolution calibration of NaI(Tl) scintillation detector*

Source	Energy (MeV)	FWHM
Am-241	5.95E-02	0.026139
Ba-133	3.56E-01	0.072639
Cs-137	6.62E-01	0.101197
Co-60	1.17E+00	0.136747
	1.33E+00	0.14613

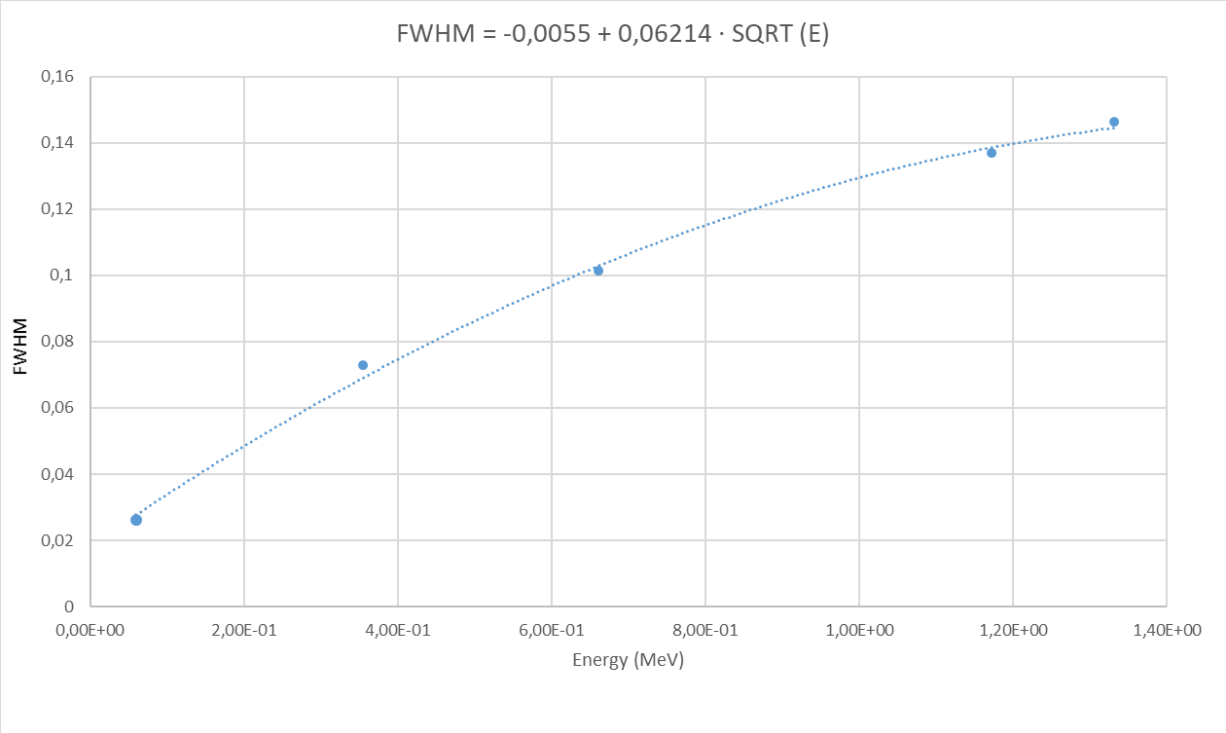

Fig. 1. *Function of FWHM for Bicron Monoline scintillation detector NaI(Tl) (Model 3M3/3) with a 3" x 3" crystal.*

RESULTS AND DISCUSSION

In Fig. 2, Fig. 3 and Fig. 4, the qualitative comparison of simulated and the experimental spectrum of ^{60}Co, ^{137}Cs and ^{90}Sr sources shows that they are in perfect agreement in the region of the characteristic peaks of the radionuclide. The experimental spectrum at the very low energy region in both the ^{60}Co and ^{137}Cs has the same form leading us to the conclusion that the background as well as additional effects of photon collection from the NaI crystal in the real detector are taking place. That form is absent at the simulated spectra.

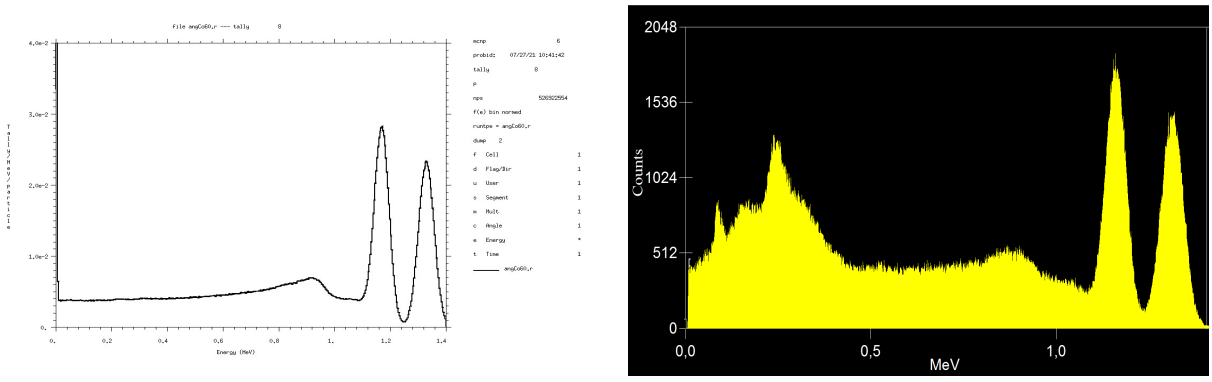

Fig. 2. *Comparison between simulated and experimental pulse height distribution to ^{60}Co source*

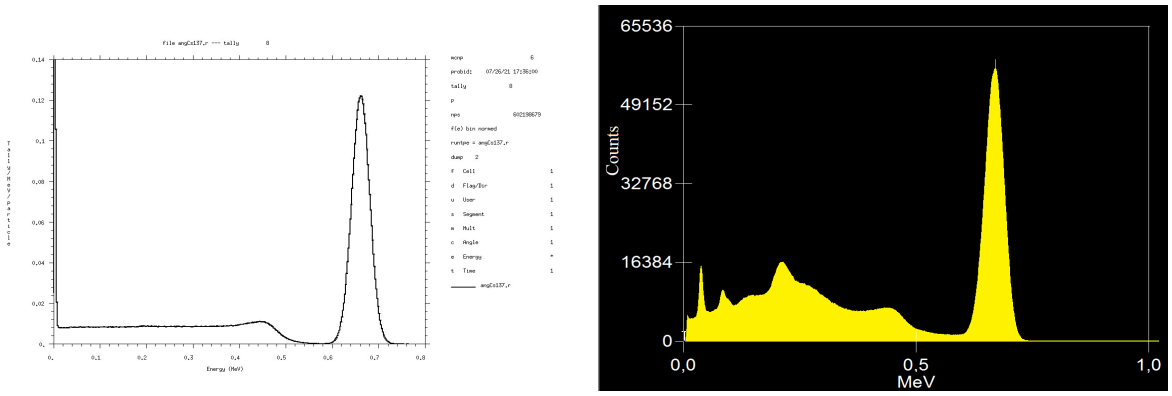

Fig. 3. *Comparison between simulated and experimental pulse height distribution to ^{137}Cs source*

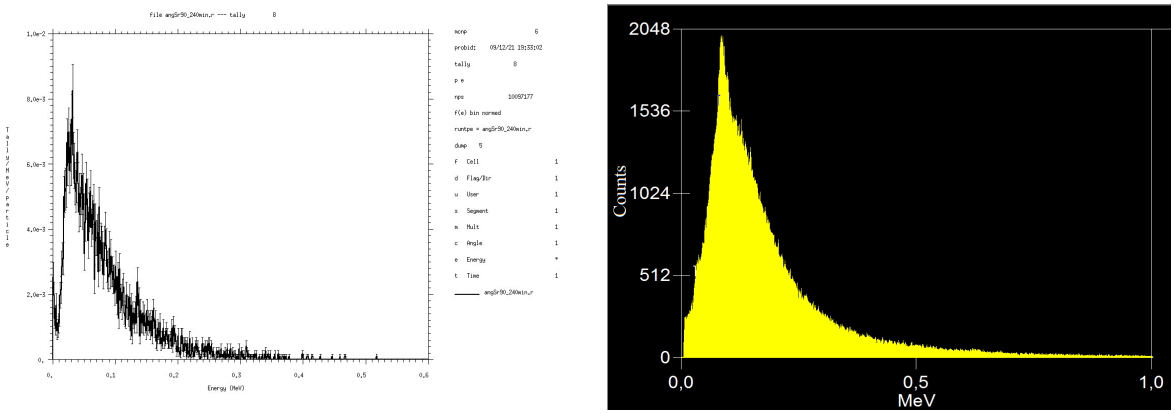

Fig. 4. *Comparison between simulated and experimental pulse height distribution to ^{90}Sr source*

CONCLUSIONS

The qualitative agreement between the simulated and measured spectra justifies the validity of the simulation results for gamma sources. The simulated spectra presented in this work show that not only the gamma peaks are characteristic but also the continuum are representative for each of the radionuclides. The comparison of measured and simulated spectra is a way to validate in the future the gamma-ray spectra generated by the radionuclides in activated and contaminated components and therefore the results of the neutron calculation.

Our next steps include the quantitative comparison of simulated and real spectra in case of complex geometries of sources with multiple radionuclides.

Acknowledgments

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