

Development and Optimization of Geometric Models of a HPGe Detector for Numerical Efficiency Calculation

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ABSTRACT

This paper presents the development, optimization, and validation of a numerical model of the coaxial HPGe detector ORTEC GEMC100 for the determination of full-energy peak efficiency required in gamma-spectrometric activity measurements. The model was developed to support the needs of “Nuclear Facilities of Serbia”, LLC during the decommissioning of hangars H1 and H2 and the RA research reactor, where complex and non-standard source geometries often make direct experimental efficiency determination impractical and, in some cases, impossible. Particular emphasis was placed on achieving a level of reliability such that the uncertainty of simulated efficiencies is comparable to the measurement uncertainty of certified radioactive calibration sources.

The detector modeling was based on crystal geometry and construction parameters from the manufacturer’s technical documentation, and a detailed three-dimensional model was implemented in the MCNP-5 Monte Carlo code. Model optimization was performed through iterative adjustment of dead-layer thicknesses and related structural parameters, using measurements with certified point sources, a certified 1500 cm³ Marinelli beaker, and a certified CBSS2 reference source. Additional cross-verification was carried out by comparing efficiencies calculated with MCNP-5 and FLUKA 4-4.1.

The validated detector model was then used as input for the EFFTRAN software in an operational test case, and the obtained results were compared with full Monte Carlo calculations and with the ISOCS software for the Canberra GX5020 detector. The results showed good agreement between simulated and experimental data, as well as close consistency among the different computational approaches. The developed methodology therefore provides a reliable basis for practical numerical efficiency determination and a foundation for future software solutions applicable to semiconductor and scintillation detectors of various types and manufacturers.

Keywords: *HPGe detectors, detection efficiency, numerical calibration, MCNPX-2.7, FLUKA-4-4.1*

1 INTRODUCTION

High-purity germanium (HPGe) detectors have become the standard instrumentation for high-resolution gamma-ray spectrometry. Their superior energy resolution enables accurate radionuclide identification and quantitative activity determination. Such applications are particularly relevant in the work carried out at the Vinča site, where the decommissioning of hangars H1 and H2 and the RA research reactor required reliable radionuclide inventory assessment under demanding measurement conditions. These activities must be performed in accordance with the recommendations of the International Atomic Energy Agency (IAEA), particularly those related to the decommissioning strategy of shut-down nuclear reactors and the characterization of radioactive waste [1,2]. In practice, however, many of the measured objects encountered in these campaigns, as well as in routine laboratory work, deviate significantly from standard calibration geometries. In

such cases, experimental calibration alone is generally insufficient for accurate full-energy peak efficiency determination.

For complex and non-standard source geometries, Monte Carlo simulations are widely used for full-energy peak efficiency calculations. Accurate detector modeling is of critical importance in this process, requiring a detailed and realistic representation of crystal dimensions, dead-layer thicknesses, endcap structure, and all surrounding materials. Dead-layer parameters are particularly critical because they strongly influence calculated efficiencies, especially in the low-energy region. Inaccurate geometric modeling can lead to significant systematic deviations between simulated and measured efficiencies, ultimately compromising the accuracy of derived radionuclide activities. Therefore, detector models must be carefully optimized and experimentally validated against certified calibration sources before they can be used with confidence in practical applications.

Our laboratory has extensive experience in the numerical calibration of laboratory and in-situ spectrometric systems [3, 4, 5, 6]. In our methodology, the principal purpose of a validated detector model is the generation of a precomputed library of point-source efficiencies in air around the detector. These data constitute the basis of an in-house approach conceptually analogous to Canberra's ISOCS [7] methodology, in which efficiencies for arbitrary source geometries are obtained from previously generated detector-specific response data rather than by performing a full Monte Carlo simulation for each individual case. The validated geometric model is therefore used to calculate efficiencies in air at a dense set of points in space and over the energy range of interest, and the results are stored in a dedicated database for subsequent operational use. Although the initial generation of these libraries demands considerable computational resources and time, once prepared for densely selected points in air across the entire energy range of interest, they provide the foundation for the rapid operational determination of full-energy peak efficiencies for any extended radioactive source. The procedure used to calculate this data involves numerical averaging of the point-source efficiencies in air over the actual source volume and the detector surface (including both frontal and lateral areas), while properly accounting for photon attenuation and self-absorption along the trajectories through the source material and its biological shielding. This approach is particularly important in our laboratory because ISOCS cannot be used for non-Canberra detectors, nor does it allow direct integration of externally generated detector libraries into its framework. Accordingly, the long-term objective is to establish a domestic software solution capable of performing detector-specific efficiency calculations for the detectors used in our practice.

In addition to this primary role, validated detector models are also used in two other ways. First, they enable direct efficiency determination for rare and geometrically complicated source configurations that are difficult to treat by standard calibration or simplified analytical approaches, such as clusters of radium needles, multiple industrial sources in a common container, uranium bullets, and similar non-standard objects. Second, they provide reliable reference efficiencies for standard laboratory geometries, which can then be used in efficiency transfer procedures such as EFFTRAN [8]. In this context, the model makes it possible to generate a denser and more consistent set of reference values than is available from direct experimental calibration alone, thereby improving interpolation quality and extending the applicability of transfer methods for typical source geometries used in laboratory measurements.

Within this framework, the development of an accurate model of the ORTEC GEMC100 detector had a clear practical motivation. In addition to restoring the detector to full operational use after vacuum loss and semiconductor reprocessing, such a model was required as a reliable basis for the future generation of detector-specific efficiency libraries and for broader numerical-calibration tasks in routine work. Accordingly, a detailed three-dimensional geometric model of this coaxial HPGe detector was developed and implemented in the Monte Carlo MCNP-5 code [9]. The model was optimized through iterative tuning of the dead layer thicknesses and other structural parameters based on systematic comparisons with experimentally determined efficiencies obtained using certified point sources at multiple source-to-detector distances and a certified 1500cm³ Marinelli beaker. Model validation was performed by comparing simulated and experimentally obtained

efficiencies for the CBSS2 bulk source. Furthermore, a comparative analysis of simulation results from the MCNP-5 and FLUKA-4-4.1 [10] codes was performed to assess consistency and provide cross-verification between the two platforms. Once the detector model was successfully validated, its practical applicability was demonstrated by using it as input for the EFFTRAN code. The resulting efficiencies were compared with those obtained using the ISOCS software for the Canberra GX5020 detector.

2 METHODOLOGY AND VALIDATION

2.1 Energy calibration

Following detector repair, the detector response was first checked against the manufacturer's original parameters using certified reference sources. The agreement was not adequate for reliable efficiency determination, which indicated that recalibration and model re-optimization were required. Energy calibration of the detector was performed by measuring certified point sources placed at a fixed source-to-detector distance of 12 cm. The radionuclides used were: ^{54}Mn , ^{57}Co , ^{60}Co , ^{109}Cd , ^{133}Ba , ^{137}Cs , ^{152}Eu , ^{228}Th . In addition, a certified 1500 cm³ Marinelli beaker was measured in order to test the detector model in an extended-volume geometry. The same measurements were used to determine the energy dependence of the full width at half maximum (FWHM), shown in Figure 1. Figure 1 shows that the post-repair energy resolution is poorer than the manufacturer-specified values prior to the intervention.

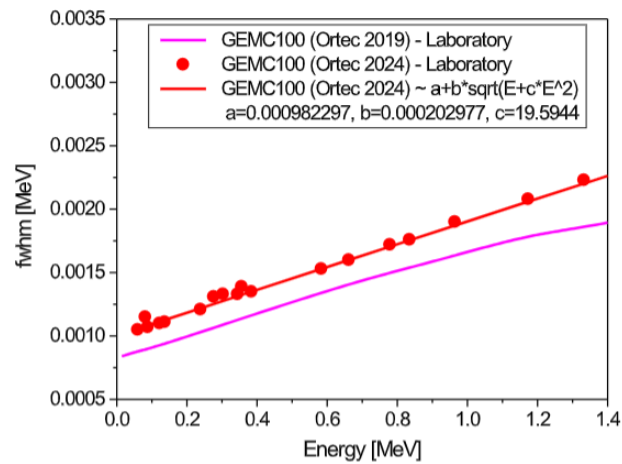


Figure 1: Energy dependence of the FWHM

The measured FWHM-energy dependence was incorporated into the MCNP-5 model through the Gaussian Energy Broadening (GEB) function, in order to reproduce the experimental peak shapes realistically. The same response broadening was introduced in FLUKA-4-4.1 to enable direct comparison of simulated spectra. The adopted relation is given by:

$$FWHM = a + b \sqrt{E(1 + cE)} \quad (1)$$

where a, b and c are fitting coefficients determined from the measured FWHM values. Values of these coefficients for MCNP-5 and FLUKA are shown in Table 1.

Table 1: FWHM fitting coefficients used for detector response broadening

Coefficients	Codes	
	MCNP-5 (FWHM in MeV)	FLUKA-4-4.1 (FWHM in GeV)
a	$9.82297 \cdot 10^{-4}$	$9.82297 \cdot 10^{-7}$
b	$2.02977 \cdot 10^{-4}$	$6.41870 \cdot 10^{-6}$
c	19.5944	$1.95594 \cdot 10^4$

A validated detector model is important not only for the calculation of full-energy peak efficiencies, but also for the realistic reproduction of the detector amplitude response through the Gaussian Energy Broadening (GEB) function. This is particularly important for sources surrounded by absorbing or shielding materials of different compositions and geometries, where commercial efficiency-determination software often cannot provide satisfactory accuracy. Simulated spectra obtained in this way make it possible to derive quantities such as the peak-to-total ratio and compare them with experimentally measured values. Such comparisons are especially useful for radionuclides characterized by a single prominent full-energy peak, and in measurement situations where Compton scattering in the source matrix, container, or surrounding shielding prevents reliable determination of full-energy peak efficiency. Under these conditions, agreement between simulated and measured spectra, including spectral-shape indicators, provides an additional and practically important basis for assessing the adequacy of the detector model.

2.2 Detector model development

In the initial stage of MCNP-5 model development, the crystal thickness and diameter were varied, while the cavity dimensions were kept at the manufacturer-specified values. This step was guided by comparison with measured efficiencies of the point sources at energies above 150 keV, where the influence of the dead layer is less pronounced. In the second stage, the dead-layer thickness was adjusted to improve agreement in the energy region below 150 keV, where the detector response is particularly sensitive to inactive germanium layers. After agreement with the certified point sources had been achieved, the model was further refined using a certified 1500 cm³ Marinelli beaker containing a mixed radionuclide solution, in order to test the model under an extended-volume measurement geometry. A cross-sectional view of the detector model with the Marinelli beaker is shown in Figure 2.

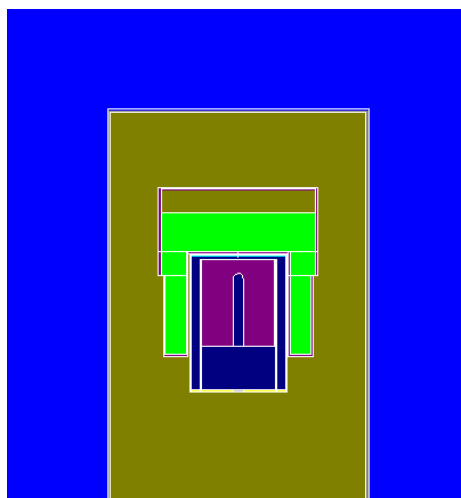


Figure 2: Cross-sectional view of the GEMC100 detector model with the 1500 cm³ Marinelli beaker

2.3 Model optimization and validation

After multiple iterations, the final optimized model corresponded to a top dead-layer thickness of 0.45 mm. For the investigated geometries, the optimized MCNP-5 model reproduced the measured efficiencies within $\pm 3\%$ for energies above 150 keV, which is within the uncertainty range of the certified sources. At lower energies, the deviations were approximately $\pm 5\%$. The comparison for point sources at 12 cm and for the 1500 cm³ Marinelli geometry is shown in Figure 3 and Figure 4, respectively.

Validation of the MCNP-5 detector model was performed using the certified CBSS2 reference source (250 cm³). This geometry was selected because it is representative of liquid-sample measurements in plastic containers and is therefore suitable as a reference geometry for subsequent efficiency-transfer applications. The corresponding MCNP-5 model is shown in Figure 5, while the comparison with experimental data is given in Figure 6. The agreement between simulated and measured efficiencies for the CBSS2 source supports the use of the optimized detector model as a reference for efficiency-transfer calculations in routine sample measurements.

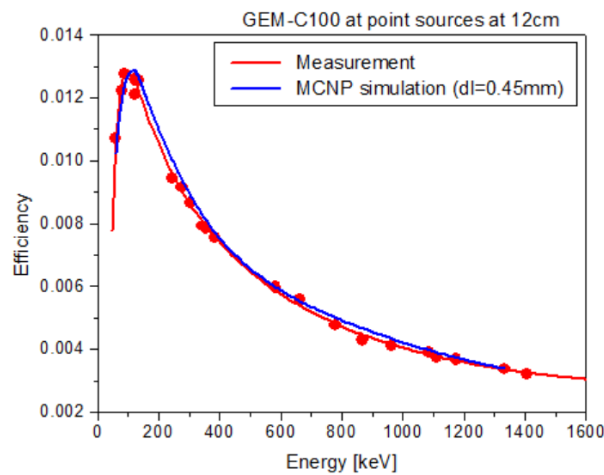


Figure 3: Comparison of measured and MCNP-5-calculated full-energy peak efficiencies for certified point sources

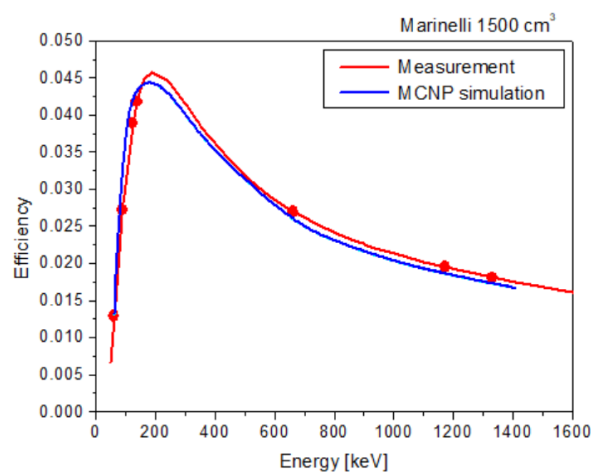


Figure 4: Comparison of measured and MCNP-5-calculated full-energy peak efficiencies for the 1500 cm³ Marinelli beaker

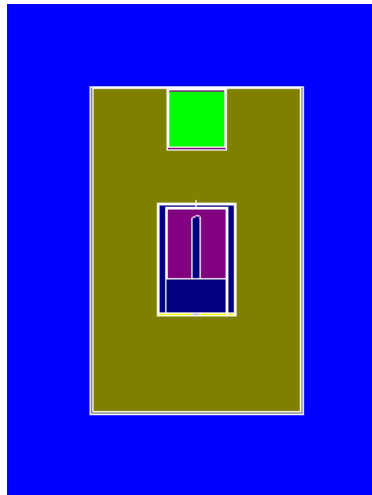


Figure 5: Cross-sectional view of the GEMC100 detector model with the CBSS2 reference source

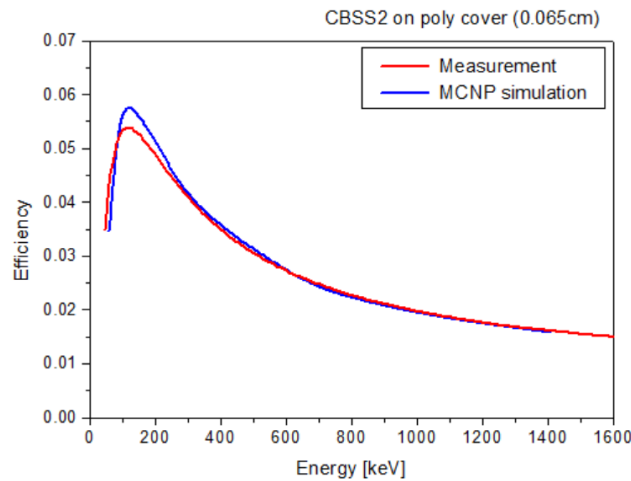


Figure 6: Comparison of measured and MCNP-5-calculated full-energy peak efficiencies for the CBSS2 reference source

Following the final verification of the detector model in MCNP-5 code, the same set of detector parameters was implemented in FLUKA-4-4.1 for cross-validation between the two Monte Carlo codes. Table 2 shows the full-energy peak efficiency values calculated using MCNP-5 and FLUKA-4-4.1 Monte Carlo simulations for the certified point sources placed at 12 cm, while * Statistical uncertainty obtained with MCNP-5 and FLUKA-4-4.1

Table 3 presents the results for the CBSS2 source. The differences between the two codes are minor and remain well within the statistical uncertainties of the simulations.

The Monte Carlo simulations performed with FLUKA-4-4.1 and MCNP-5 show excellent agreement for the certified point sources, with relative differences in full-energy peak efficiency not exceeding 0.5% at all energies. For the CBSS2 source, the relative differences are below 1% for all energies. Although MCNP codes use photon interaction libraries based on ENDF/B evaluations and FLUKA employs its own internal libraries, the two codes show excellent agreement. For the bulk-source case, the maximum relative difference for the identical model geometry does not exceed 1%.

Table 2: Full-energy peak efficiencies calculated for certified point sources

Energy [keV]	Efficiency	
	FLUKA-4-4.1	MCNP-5
59,54	$1,006 \cdot 10^{-2} \pm 0,07\%*$	$1,010 \cdot 10^{-2} \pm 0,29\%*$
88,03	$1,331 \cdot 10^{-2} \pm 0,08\%$	$1,328 \cdot 10^{-2} \pm 0,29\%$
122,06	$1,358 \cdot 10^{-2} \pm 0,09\%$	$1,352 \cdot 10^{-2} \pm 0,16\%$
136,47	$1,329 \cdot 10^{-2} \pm 0,09\%$	$1,322 \cdot 10^{-2} \pm 0,10\%$
185,71	$1,188 \cdot 10^{-2} \pm 0,09\%$	$1,183 \cdot 10^{-2} \pm 0,13\%$
356,01	$7,986 \cdot 10^{-2} \pm 0,12\%$	$7,970 \cdot 10^{-2} \pm 0,16\%$
661,66	$5,324 \cdot 10^{-3} \pm 0,22\%$	$5,320 \cdot 10^{-3} \pm 0,17\%$
778,90	$4,817 \cdot 10^{-3} \pm 0,19\%$	$4,806 \cdot 10^{-3} \pm 0,21\%$
1173,23	$3,718 \cdot 10^{-3} \pm 0,26\%$	$3,710 \cdot 10^{-3} \pm 0,26\%$
1332,49	$3,438 \cdot 10^{-3} \pm 0,27\%$	$3,410 \cdot 10^{-3} \pm 0,31\%$
1408,01	$3,308 \cdot 10^{-3} \pm 0,27\%$	$3,298 \cdot 10^{-3} \pm 0,32\%$

* Statistical uncertainty obtained with MCNP-5 and FLUKA-4-4.1

Table 3: Full-energy peak efficiencies calculated for the CBSS2 reference source

Energy [keV]	Efficiency	
	FLUKA-4-4.1	MCNP-5
59,54	$8,028 \cdot 10^{-3} \pm 0,06\%*$	$8,104 \cdot 10^{-3} \pm 0,05\%*$
88,03	$1,201 \cdot 10^{-2} \pm 0,06\%$	$1,201 \cdot 10^{-2} \pm 0,05\%$
122,06	$1,278 \cdot 10^{-2} \pm 0,06\%$	$1,281 \cdot 10^{-2} \pm 0,06\%$
136,47	$1,287 \cdot 10^{-2} \pm 0,06\%$	$1,273 \cdot 10^{-2} \pm 0,06\%$
185,71	$1,171 \cdot 10^{-2} \pm 0,07\%$	$1,171 \cdot 10^{-2} \pm 0,06\%$
356,01	$8,359 \cdot 10^{-3} \pm 0,10\%$	$8,368 \cdot 10^{-3} \pm 0,08\%$
661,66	$5,877 \cdot 10^{-3} \pm 0,13\%$	$5,902 \cdot 10^{-3} \pm 0,07\%$
778,90	$5,395 \cdot 10^{-3} \pm 0,15\%$	$5,409 \cdot 10^{-3} \pm 0,10\%$
1173,23	$4,346 \cdot 10^{-3} \pm 0,17\%$	$4,343 \cdot 10^{-3} \pm 0,10\%$
1332,49	$4,056 \cdot 10^{-3} \pm 0,20\%$	$4,046 \cdot 10^{-3} \pm 0,10\%$
1408,01	$3,958 \cdot 10^{-3} \pm 0,20\%$	$3,915 \cdot 10^{-3} \pm 0,10\%$

* Statistical uncertainty obtained with MCNP-5 and FLUKA-4-4.1

3 RESULTS

To demonstrate the practical applicability of the validated detector model, the detector dimensions were implemented in EFFTRAN for the determination of the specific activity of ^{137}Cs in a water sample collected from the spent-fuel storage pool of the RA reactor. The analysed sample had a mass of 70 g and was measured in a plastic container. In the EFFTRAN calculation, the detector dimensions were combined with the reference point-source data and the corresponding reference efficiencies previously obtained from the MCNP-5 model. Specific activity values for the water sample were then determined using efficiencies calculated by EFFTRAN, MCNP-5, and FLUKA-4-4.1 for the sample geometry shown in Figure 7. The resulting values are summarized in Table 4.

As an additional practical benchmark, the same water sample was also measured using a Canberra GX5020 detector, and the activity was determined using the ISOCS efficiency-calculation methodology. Although this does not represent a strict one-to-one comparison on the same detector, it provides a useful reference against an established commercial approach. The corresponding ISOCS result is included in the Table 4.

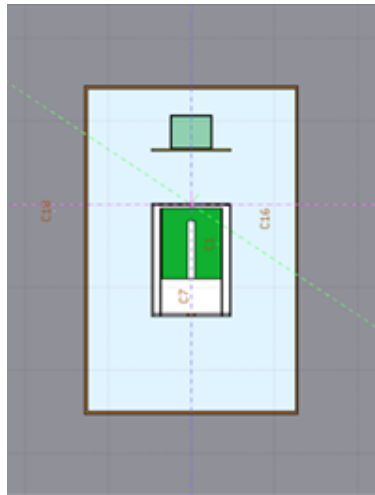


Figure 7: FLUKA-4-4.1 model of the GEMC100 detector and water-sample measurement geometry

Table 4: Specific activity of ^{137}Cs in the water sample

Detector	Code / software	Specific activity [Bq/g]
GEMC100	EFFTRAN	$149,1426 \pm 6,1977$
GEMC100	MCNP-5	$150,6282 \pm 6,2594$
GEMC100	FLUKA-4-4.1	$150,7996 \pm 6,2665$
GX5020	ISOCS	$156,1709 \pm 4.7003$

The results obtained with EFFTRAN, MCNP-5, and FLUKA-4-4.1 are in very close agreement, while the ISOCS-based value is somewhat higher. Nevertheless, the differences among all four approaches remain within about 3–5%, which supports the practical applicability of the validated model and the efficiency-transfer approach for rapid activity determination.

Figure 8 compares the measured spectrum of the water sample with the spectra simulated using the MCNP-5 and FLUKA-4-4.1 models. In both cases, detector response broadening was introduced through the GEB function using the coefficients given in Table 1. The comparison shows that the simulated spectra reproduce the main features of the measured amplitude response satisfactorily, which provides additional support for the adequacy of the detector model under the investigated measurement conditions.

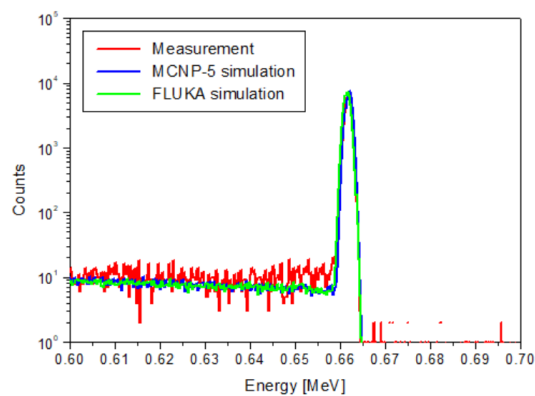


Figure 8: Comparison of measured and simulated spectra for the water sample

4 CONCLUSION

A detailed geometric model of the ORTEC GEMC100 HPGe detector was developed, optimized and validated for use in numerical efficiency determination under non-standard measurement conditions. The optimization procedure, based on comparisons with certified point sources, a 1500 cm³ Marinelli beaker, and the CBSS2 reference source, resulted in good agreement between simulated and measured efficiencies over the investigated energy range. Additional cross-verification between MCNP-5 and FLUKA-4-4.1 showed very close agreement, confirming the consistency of the developed detector model across two independent Monte Carlo platforms.

The practical applicability of the validated model was further demonstrated through its use in the EFFTRAN efficiency-transfer method for the determination of the specific activity of ¹³⁷Cs in a water sample. The results obtained with EFFTRAN were in very close agreement with those obtained using the full Monte Carlo models, while comparison with the ISOCS methodology also showed acceptable consistency for operational purposes. These findings support the use of a carefully validated geometric detector model as a reliable basis for rapid activity determination in routine laboratory practice, particularly under time constraints that do not allow full Monte Carlo calculations for every individual sample. More broadly, they confirm the practical value and robustness of efficiency-transfer methods when supported by an accurate detector model.

Future work will focus on further improvement of the GEMC100 model, particularly through the introduction of a conical front (bulletization) of the germanium crystal. This refinement is expected to improve agreement at both low and high gamma-ray energies and further reduce the overall uncertainty of calculated efficiencies.

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