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Comparison of the Number of Particle History for Monte Carlo Codes in Gamma-Ray Spectroscopy

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Keywords

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History Number
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Number of Runs
PHITS

Abstract

Monte Carlo is a numerical computation algorithm that is widely used in many fields of science and is used to obtain numerical results with a large number of repeated random samplings. Radiation transport with Monte Carlo simulation continues to increase its popularity in the fields of radiation measurement. The high accuracy and precision measurement of radionuclide activity amounts in gamma-ray spectrometry depends on the efficiency calibration of the detector. Efficiency calibration is carried out in two ways, using certified reference materials, by experimental method or Monte Carlo simulation method. The experimental method is expensive, procedurally complex and time-consuming due to the supply of reference material. The use of the Monte Carlo technique in a reliable way without the need for a standard radioactive source in determining the detector efficiency is becoming common. The most critical step for accurate and precise results in getting the response of a detector with the Monte Carlo method is modeling the detector with its realistic dimensions. Another parameter as important as detector modeling is the number of histories in the simulation code examined in this study. The effect of the number of histories on efficiency was examined in detail using PHITS, GESPECOR and DETEFF Monte Carlo simulation codes. Since there is no definite number about this effect, which is important for obtaining meaningful and realistic results, the change in the efficiency value was examined by increasing the number of stories from 105 to 108. The results obtained in this work showed that at least 107 particle numbers should be used in all three programs where the uncertainty is below 1%. If the existing facilities are sufficient, it can be increased to 108s in case of having a more equipped and fast computer. However, going higher than this value does not make any sense as seen from the study.

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1. INTRODUCTION

Monte Carlo (MC) simulation is a statistical technique for directly simulating a physical process. The basis of the MC method is a random number generator consisting of random numbers in the range (0, 1). Since such numbers are generated by deterministic algorithms, they are untruly random. However, such pseudo-random numbers are statistically indistinguishable from real random numbers that are evenly distributed in the range (0, 1) and are independent of each other (Kroese & Rubinstein, 2012). Simulating particle transport in MC codes is widely used in a wide variety of fields such as radiotherapy, radiation shielding, detector modeling, medical physics, nuclear technology, accelerator design, astrophysics applications (Iwamoto et al., 2017; Lépy et al., 2019). The MC simulation technique is increasingly used in gamma-ray spectrometry due to advances in technology and a variety of simulation codes (Cebastien Joel et al., 2018; Ordóñez et al., 2019). Accurate modeling of the detection chain via the MC method is crucial for obtaining quality data from detectors and for the design of experiments. MC modeling of radiation detectors is a widely accepted numerical method for detector characterization. For example, MC programs are a excellent guide for the characterization of the

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detectors by determining the dead layer thickness, which is a time-varying parameter in HPGe detectors (Uyar & Bölükdemir, 2022). In gamma-ray spectrometric studies, the MC method is mostly used to obtain the detector efficiency (Sima, 2012; Mrdja et al., 2018; Ordóñez et al., 2019). In addition to the efficiency, MC simulation programs are used to acquire the true coincidence summing correction factor, which is an important correction factor (Vidmar et al., 2011; Yoon et al., 2020). Since this method is a statistical process in which random numbers are used, keeping the number of histories as high as possible allows us to obtain more meaningful results.

The principle of the Monte Carlo method consists in simulating the history of a certain number of photons passing through the HPGe crystal. Therefore, these photons should interact with the Ge crystal in an appropriate number for the photoelectric effect, compton scattering and pair production mechanisms at energies greater than 1022 keV to take place. The number of these photons is called the history number in Monte Carlo simulations. But there is no exact value regarding the number of histories. For example, Ordonez et al. in order to obtain a statistical error of less than 1.5%, they set the number of histories in each simulation at 20 million (Ordóñez et al., 2019). Azli & Chaoui (2015) used 100 million particles to achieve a relative error of less than 1% in the calculated efficiency. Subercaze et al. (2022) used 3 million and Miroslav et al. used 1 million particles in their study (Ješkovský et al., 2019). Therefore, as can be seen from the literature, a number of histories ranging from 1 million to 100 million were used. Here, the performance and features of the computer used in the calculation are very important.

In this study, the effect of history number on efficiency calculation with the MC method was investigated using three different MC programs. For this purpose, the effect of history number was examined in a wide energy range using 59.5 keV, 383.9 keV, 661.7 keV, 1173.2 keV and 1332.5 keV gamma energies. 10^5, 10^6, 10^7 and 10^8 were chosen as history numbers.

2. MATERIAL AND METHOD

MC codes used in HPGe detector response fall into two categories: specialized codes in gamma-ray spectrometry, mostly written specifically for efficiency calculations, and multi-purpose MC codes for a wide variety of applications. The PHITS used in this study is a multi-purpose code for all kinds of applications; GESPECOR and DETEFF are specialized purpose MC codes.

2.1. PHITS Monte Carlo simulation code

PHITS is a multi-purpose MC simulation code for particle transport that was created in cooperation between JAEA, KEK, RIST, and numerous other institutions. With the use of several nuclear reaction models and nuclear data libraries, it can be interested in the transport of all particles over various energies (Sato et al., 2018). The parameters for the history number in PHITS are maxcas and maxbch (Figure 1). The total number of histories is equal to the product of maxcas, the number of particles per batch, and maxbch, the number of batches. It is recommended to set the maxbch value greater than or equal to 10 to obtain reliable results. A larger maxbch provides more reliable statistical uncertainties, but may require a longer computation time.

```
[ Parameters ]
 icntl    =           0     # (D=0) 3:ECH 5:NOR 6:SRC 7,8:GSH 11:DSH 12:DUMP
 maxcas   =     1000000     # (D=10) number of particles per one batch
 maxbch   =          10     # (D=10) number of batches
```

Figure 1. *Defining the number of histories in the PHITS MC code*

2.2. GESPECOR

GESPECOR is a special-purpose Monte Carlo-based code used for calculating true coincidence summing and self-absorption effects, especially full energy peak efficiency in gamma-ray spectrometry. In GESPECOR, variance reduction techniques are applied to improve the statistical accuracy of the computation versus the computation time. The number of histories is determined by the number of runs entered in the window that opens automatically in the system before starting the simulation (Figure 2). This window opens for each quantity desired to be calculated by defining the detector, material, geometry, and prompts the user to enter a random number and a history number.

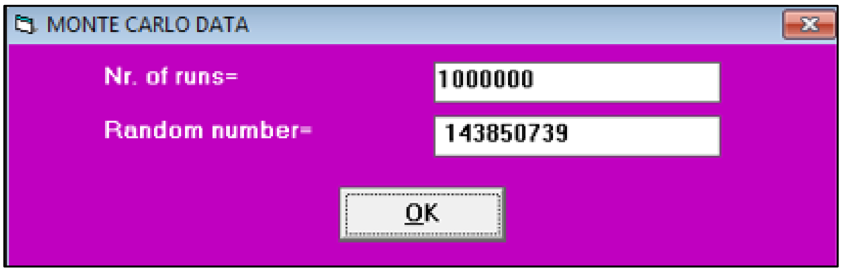

Figure 2. *Defining the number of histories in the GESPECOR MC code*

2.3. DETEFF

DETEFF; it is a user friendly MC program for calculating the full energy peak efficiency in gamma-ray detectors such as NaI, CsI, Ge(Li), HPGe and Si(Li) (Díaz & Vargas, 2010). In DETEFF, the parameters for the number of histories are experiments and number of photons in the Statistics tab (Figure 3). The total number of histories is equal to the value in the experiments multiplied by the number of photons.

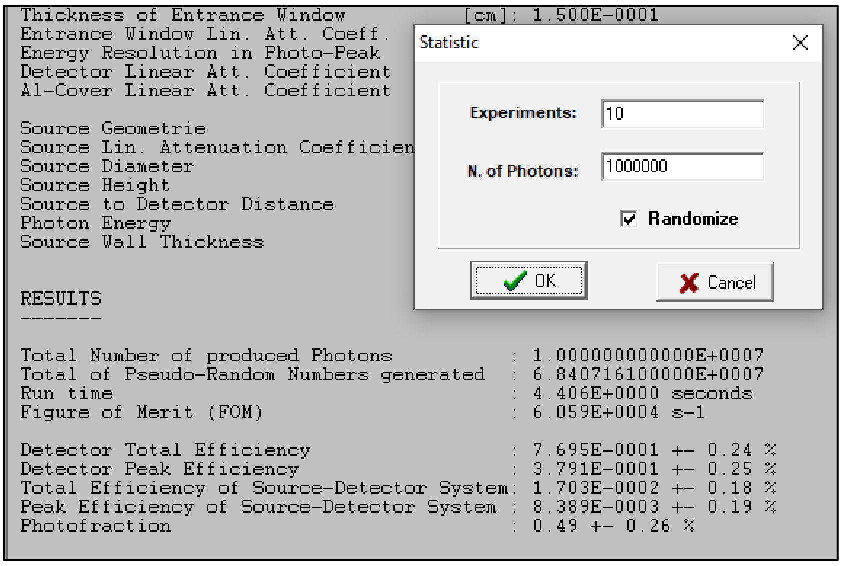

Figure 3*. Defining the number of histories in the DETEFF MC code*

3. RESULTS AND DISCUSSION

Measurements were taken at 10^5, 10^6, 10^7,10^8 using PHITS, GESPECOR and DETEFF MC codes and ^{241}Am (59.54 keV), ^{133}Ba (383.85 keV), ^{137}Cs (661.66 keV) and ^{60}Co (1173.23 keV and 1332.49 keV) peaks. The efficiency values taken at different particle numbers, with their uncertainties, are given in Table 1.

As shown in the Table 1, the increase in the number of history does not cause a linear change in the efficiency. While the increase in the number of histories decreases the efficiency in some energies, the efficiency increases in some energies. However, the percentage uncertainty values decrease as the number of history increases in all MC codes, that is, they improve. According to Table 2, where the relationship between the history numbers is examined, the percentage difference decreases as the number of particles increases in all MC codes. The percentage difference values between the history numbers (n) were calculated according to the Equation 1.

$$\frac{|10^n + 10^{n+1}|}{10^n} \times 100 \qquad (1)$$

For example, when the percentage difference value according to the efficiency values obtained with 10^5 and 10^6 history numbers with an energy value of 59.54 keV is calculated according to Equation 1; $\frac{|0.00455-0.00475|}{0.00455}\times 100=4.37$ is obtanied.

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Table 1. *Efficiency values obtained with PHITS, GESPECOR and DETEFF for different particle numbers*

Particle Number	Nuclide	Energy (keV)	PHITS (Uncertainty %)	GESPECOR (Uncertainty %)	DETEFF (Uncertainty %)
10^5	^{241}Am	59.54	0.00455 (0.047)	0.00539 (0.057)	0.00529 (0.840)
	^{133}Ba	383.85	0.01095 (0.030)	0.01086 (0.270)	0.01150 (1.770)
	^{137}Cs	661.66	0.00766 (0.036)	0.00803 (0.360)	0.00855 (2.440)
	^{60}Co	1173.23	0.00568 (0.042)	0.00592 (0.510)	0.00628 (3.780)
	^{60}Co	1332.49	0.00517 (0.044)	0.00552 (0.370)	0.00611 (3.410)
10^6	^{241}Am	59.54	0.00475 (0.015)	0.00539 (0.012)	0.00534 (0.440)
	^{133}Ba	383.85	0.01082 (0.010)	0.01089 (0.110)	0.01115 (0.830)
	^{137}Cs	661.66	0.00796 (0.011)	0.00807 (0.160)	0.00848 (0.420)
	^{60}Co	1173.23	0.00589 (0.013)	0.00594 (0.140)	0.00616 (1.000)
	^{60}Co	1332.49	0.00543 (0.014)	0.00550 (0.120)	0.00577 (0.910)
10^7	^{241}Am	59.54	0.00483 (0.005)	0.00539 (0.006)	0.00530 (0.130)
	^{133}Ba	383.85	0.01090 (0.003)	0.01089 (0.024)	0.01126 (0.270)
	^{137}Cs	661.66	0.00815 (0.004)	0.00807 (0.042)	0.00842 (0.210)
	^{60}Co	1173.23	0.00599 (0.004)	0.00593 (0.068)	0.00615 (0.250)
	^{60}Co	1332.49	0.00557 (0.006)	0.00551 (0.042)	0.00571 (0.150)
10^8	^{241}Am	59.54	0.00483 (0.001)	0.00539 (0.004)	0.00530 (0.050)
	^{133}Ba	383.85	0.01091 (0.001)	0.01088 (0.012)	0.01125 (0.070)
	^{137}Cs	661.66	0.00815 (0.001)	0.00807 (0.011)	0.00838 (0.060)
	^{60}Co	1173.23	0.00600 (0.001)	0.00592 (0.015)	0.00616 (0.100)
	^{60}Co	1332.49	0.00559 (0.001)	0.00551 (0.011)	0.00571 (0.100)

Table 2. *Percentage difference values between history numbers from PHITS, GESPECOR and DETEFF*

History Number	Nuclide	Energy (keV)	PHITS	GESPECOR	DETEFF
n:5	^{241}Am	59.54	4.37	0.02	0.98
	^{133}Ba	383.85	1.21	0.25	3.04
	^{137}Cs	661.66	3.90	0.53	0.78
	^{60}Co	1173.23	3.84	0.30	1.85
	^{60}Co	1332.49	5.11	0.36	5.57
n:6	^{241}Am	59.54	1.75	0.01	0.64
	^{133}Ba	383.85	0.79	0.04	0.99
	^{137}Cs	661.66	2.34	0.05	0.70
	^{60}Co	1173.23	1.50	0.25	0.19
	^{60}Co	1332.49	2.59	0.15	1.04
n:7	^{241}Am	59.54	0.05	0.01	0.08
	^{133}Ba	383.85	0.25	0.06	0.09
	^{137}Cs	661.66	0.25	0.04	0.32
	^{60}Co	1173.23	0.37	0.04	0.16
	^{60}Co	1332.49	0.42	0.03	0.14

The biggest difference in the PHITS MC code occurred at n:5, that is, between 10^5 and 10^6 history numbers (up to 5.1%). When 10^6 and 10^7 data are examined, it is seen that the difference values are smaller and close to each other (Figure 4).

When the percent difference values between the particle numbers calculated according to the Equation (1) were examined for GESPECOR, an uncertainty of less than 1% was obtained in all particle numbers. The lowest uncertainty was obtained between 10^7 and 10^8, as expected (Figure 5).

The biggest difference in the DETEFF MC code occurred at n:5, that is, between the historical numbers 10^5 and 10^6 (up to 5.6%). When the 10^7 and 10^8 data are examined, it is seen that the difference values are less than 1% (Figure 6).

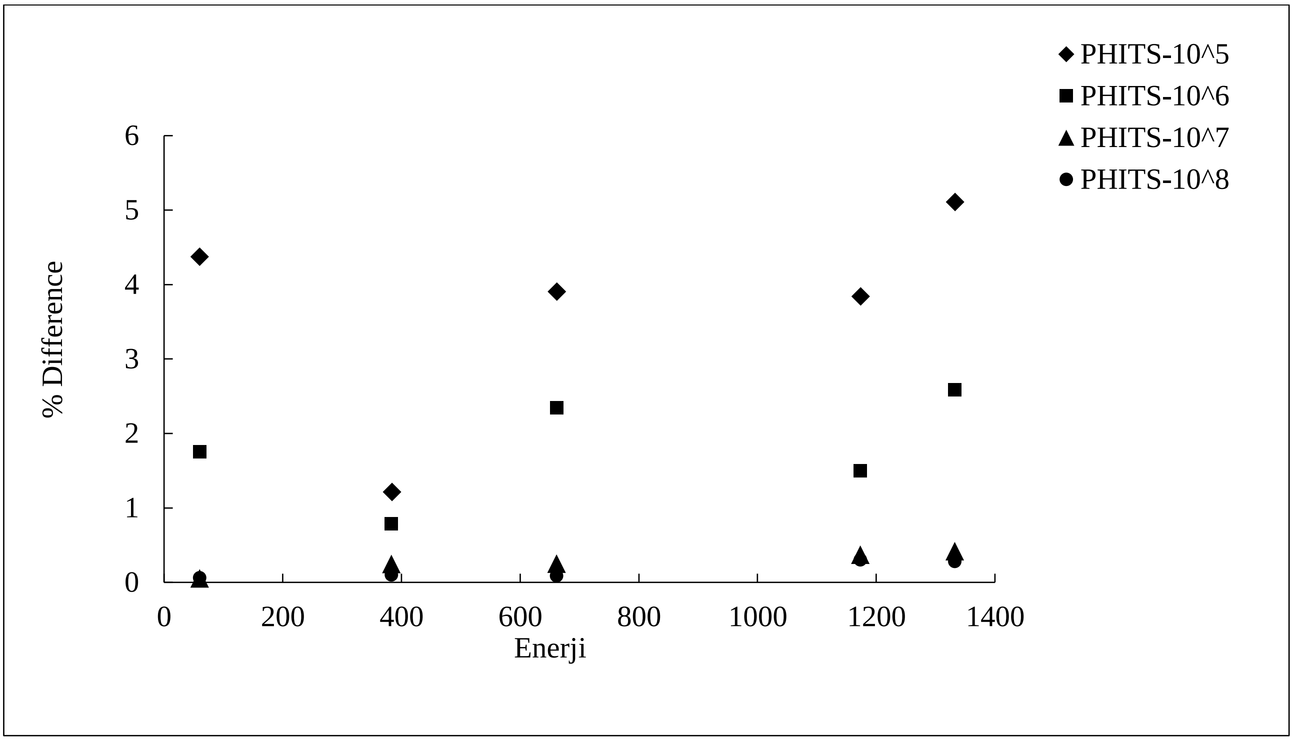

Figure 4. *Variation of percent difference values between particle numbers obtained with PHITS according to energy*

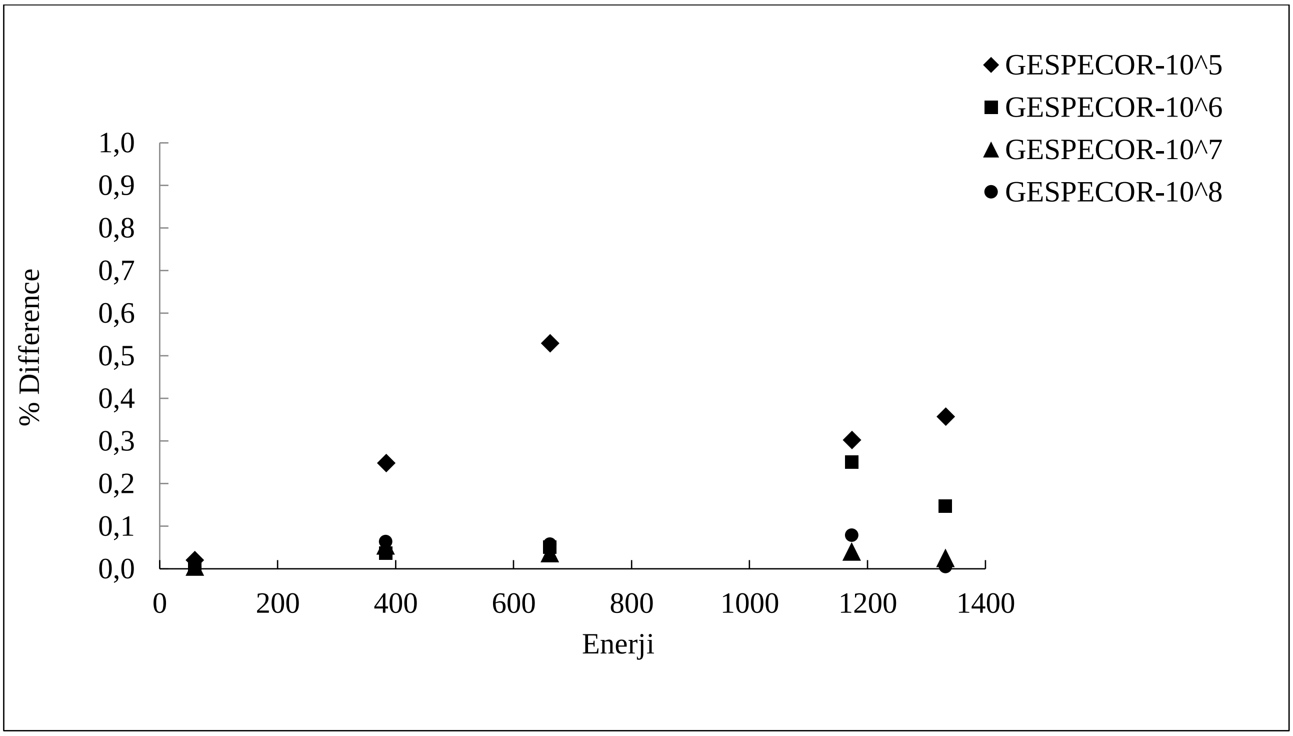

Figure 5. *Variation of percent difference values between particle numbers obtained with GESPECOR according to energy*

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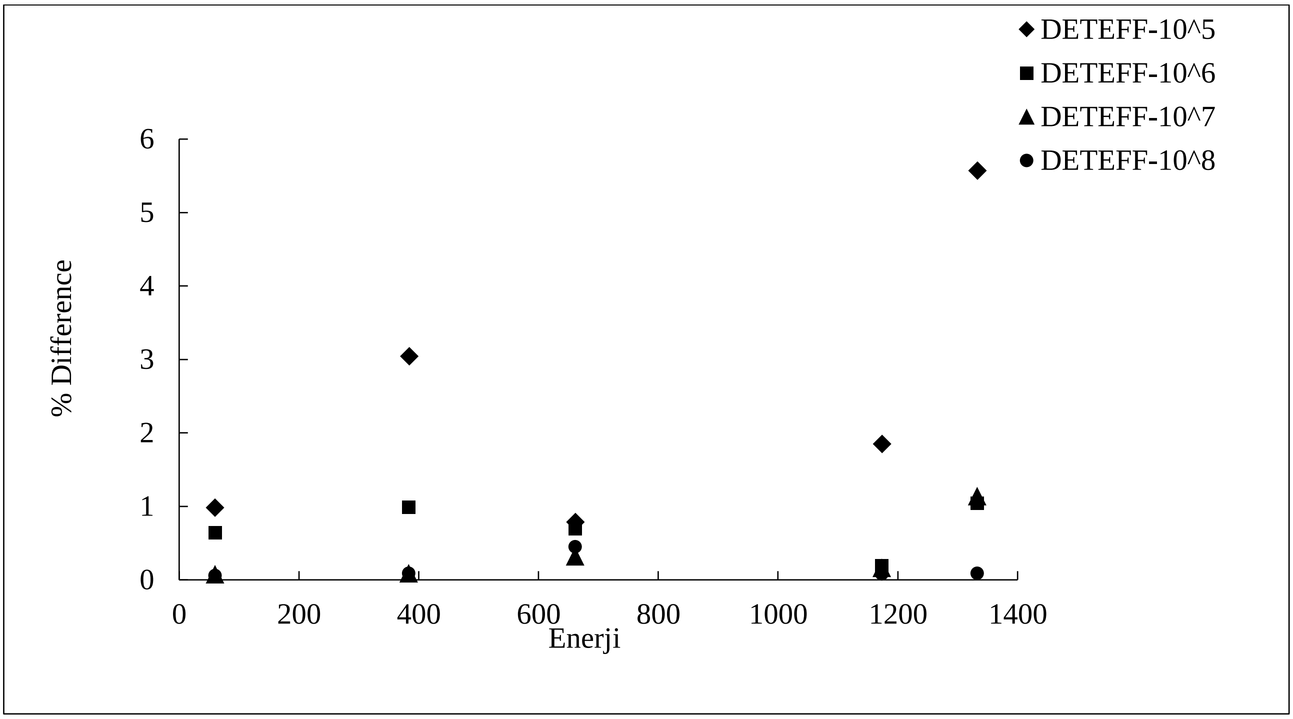

Figure 6. *Variation of percent difference values between particle numbers obtained with DETEFF according to energy*

4. CONCLUSION

In this study, the effect of the number of histories on the efficiency was investigated with different Monte Carlo codes. Efficiency values were obtained at energies in the range of 59.5-1332.5 keV by using 10^5, 10^6, 10^7 and 10^8 particle numbers. Efficiency values were obtained for each code at the same particle count and the same energy at varying times ranging from a few seconds to several hours. Therefore, it is seen that the execution times of each code is different from each other. It has been observed that the dedicated packages GESPECOR and DETEFF give much faster results on average than general-purpose MC code PHITS. In MC programs, faster results are obtained by applying reduction techniques to the variance value, which is the mean of the square of the differences from the mean, also known as the standard deviation. MC programs such as GESPECOR and DETEFF, which are specially developed for gamma-ray spectrometric studies, cause faster results due to the algorithms developed by applying these techniques. General-purpose packages like PHITS are at a disadvantage in terms of speed to get results due to their more complex physics and particle tracking. In DETEFF and GESPECOR the percentage difference between particle counts is less, but repeatability is low. In other words, different values were obtained in each repeated simulation.

When the efficiency values in all MC programs are examined according to Table 1, it is seen that the efficiency value in low history numbers is determined with a difference of up to 8% from what it should be. Therefore, while uncertainty contributes to the efficiency value from many factors, we should avoid increasing the uncertainty by keeping the number of histories low. In conclusion, it was determined that at least 10^7 particle numbers should be adjusted to obtain good statistics in simulations where gamma-ray spectrometric calculations are made.

CONFLICT OF INTEREST

The authors declare no conflict of interest.

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