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Second version of the open-source software GSA for gamma-ray spectrum analysis

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The collaboration among the PRESN team, LaMCScI laboratory and CNESTEN center made it possible to implement the first version of the GSA software. Its first version is already available to the public; it is not only free but also an open source, demonstrating the developers' commitment to promoting the open sharing of scientific knowledge. This first version is characterized by its flexibility and non-commerciality, and it is available without any conditions on the following website: https://www.github.com/LAHCEN-EL-AMRI/Gamma-Spectra-Analysis, allowing users to add personal options, making it a particularly adaptable tool to the different requirements of scientific research. This article deals with the second version of GSA, which focuses on a core and complementary feature: the calculation of isotope activity. In order to accomplish this goal, instead of implementing a single efficiency formula, as is often the case in most software, four formulas were integrated. The users can therefore select the one they want to implement. To ensure the accuracy and reliability of this new feature, a validation was performed on GSA. The results obtained with GSA v2 were carefully studied by comparing them to those obtained with the renowned Genie 2000 software. Owing to this comparison step, it was possible to verify and confirm the accuracy of the results of GSA version 2. This second version of GSA is available as a free and open source software on the following site: https://www.github.com/LAHCEN-EL-AMRI/GSA-v2/tree/master.

Introduction

In the field of nuclear physics, gamma spectrum analysis is a fascinating technique. Measuring the energy of gamma rays emitted by radioactive sources is possible because of it.[1] Each radionuclide has its own gamma energy,[2] which can serve as a digital fingerprint for its identification. This method is frequently used in different sectors, such as research, medicine, industry, safety and security.[3] For example, in medicine, it is used to diagnose and treat certain conditions.[4] In science, it contributes to the understanding of nuclear and atomic characteristics. In safety, it focuses on managing severe nuclear accidents.[5] The study of the gamma spectrum is a powerful tool that continues to develop owing to technological advances.

A gamma spectrum is formed by the emission of gamma-ray photons by a radioactive isotope of an element (or several elements) and their interaction with the material.[6] Through the photoelectric effect, Compton effect or pair creation, these photons interact with a germanium crystal, which allows them to give energy to the crystal's electrons. The current produced by this interaction is proportional to the energy deposited in the crystal by the radiation.[7]

The study of gamma-ray spectra presents obstacles. Indeed, each radioactive nuclide has a unique gamma ray spectrum, which allows it to be recognized. In addition, each nuclide has a particular half-life ($T_{1/2}$) and a distinct yield. However, it is often difficult to distinguish the relevant signals, those we want to study, from spurious signals coming from other sources of radiation.

Additionally, in-depth study of this spectrum is commonly employed to determine the identity and quantity of gamma-ray emitters in a sample. It is important to have a good knowledge of nuclear physics and a good command of data analysis techniques for this.[8]

The extreme complexity of the gamma-ray spectra lies in the superposition of the peaks, which makes the identification of specific nuclides difficult.[9] Small peaks, those that are essential for accurate analysis, can be hidden by the often noisy background of the spectrum. Additionally, a gamma spectrum can have many peaks, making it very difficult to analyze them manually. Each peak corresponds to a particular energy emitted by a nuclide, and their superposition can be misleading.

Calibration in gamma spectrum analysis depends heavily on the experiments performed and their adjustment to theoretical models.[10] This combination improves the accuracy of the

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calibration by adapting the parameters to real conditions while taking advantage of theoretical predictions. It is therefore crucial to calibrate the energies in order to guarantee precise identification of peaks according to the energy they represent.[11] It is essential to go through this step in order to differentiate between the various gamma radiations emitted by radioactive sources. Likewise, it is essential to calibrate the efficiency in order to capture the probability of detection of gamma-ray photons by the detector,[12,13] which has a direct impact on the perceived intensity of the peaks.[14]

Finding peaks requires a thorough analysis of each point in the spectrum to identify high intensity elements that indicate the presence of a peak. It is essential to understand the behavior of nuclides and the instrumentation used for the acquisition of the gamma spectrum.

Presently, there is a wide variety of commercial software for analyzing gamma-ray spectra, each with its own characteristics and benefits. HYPERMET-PC is particularly known for its ability to perform precise and detailed analyses.[15] Another popular software Genie 2K[16,17] is popular for its friendly user interface and advanced data processing capabilities. Thanks to its original methodology, k0 software is frequently used in specific neutron activation analysis (NAA) applications.[18] Finally, laboratories frequently use GammaVision[19] because of its robustness and reliability in spectrometric analysis, as well as other software not mentioned here.

Physicists and engineers using gamma spectrometry data need these computational tools. They not only allow for rapid and accurate identification of nuclides, but also allow effective quantification of isotopes present in a sample. These software programs are invaluable resources in the fields of nuclear research and security due to their ability to manage vast volumes of data and provide reliable results.

This software also plays a role in the teaching and training of students in nuclear physics, providing them with the opportunity to become familiar with spectral analysis methods and develop practical skills in data interpretation. In summary, the development of gamma spectrum analysis software remains an essential element in the evolution of nuclear science and the training of the next generation of scientists.

Most commercially available gamma spectrum analysis software is fee-based,[20] *i.e.*, users must pay to use it and generally cannot customize or modify options to suit their particular needs. However, a significant exception is GSA (Gamma-ray Spectral Analysis) software, developed by our PRESN team (Nuclear Reactor Energy and Physics, Nuclear Security and Environment) and LaMCScI laboratory (Laboratory of Condensed Matter and Interdisciplinary Sciences) in cooperation with CNESTEN (National Center for Nuclear Energy, Science and Technology).[21,22] This software is characterized by its free and open source nature, offering users the possibility to adjust and modify it independently.

GSA has already been disseminated in the scientific community in its first version,[1] which was favorably received for its flexibility and accessibility. The second version, which will be presented in this research, presents significant improvements. The main objective of this new version is to accurately calculate the activity, an essential feature for interested users.

GSA v2 software is a tool for nuclear physics researchers and students, offering them an accessible alternative to often expensive commercial solutions. In addition, the possibility of contributing to it establishes a direct collaboration between users and developers, thus promoting innovation and the continuous improvement of the software.

Validation of this new functionality was carried out by comparing the analysis results obtained by GSA v2 with those provided by the reference software Genie 2000. This comparison made it possible to evaluate the accuracy and reliability of the results generated by GSA v2.

General presentation of the first version of GSA

The open source software GSA (Gamma-ray Spectra Analysis) was developed with the aim of providing a powerful and accessible tool for researchers and experts involved in measurement and analysis. The first version offers an intuitive interface (Fig. 1), which makes it possible to efficiently locate peaks in a gamma spectrum, calculate the areas under these peaks and identify associated radionuclides, which is essential for the characterization of radioactive materials and environmental monitoring. Available on GitHub (**https://www.github.com/LAHCEN-ELAMRI/Gamma-Spectra-Analysis**), the source code encourages collaboration and innovation. Through it, users have the ability to customize the software according to their particular needs and make contributions that will benefit the entire community. GSA remains accessible to everyone thanks to its detailed user manual (**https://www.github.com/LAHCEN-EL-AMRI/Gamma-Spectra-Analysis/tree/master/Install/Doc**), making it a valuable resource.

Students and researchers who want to understand the underlying principles of spectral analysis are particularly interested in the clear explanations of the mathematical functions used in GSA. The results obtained are reinforced by this transparency, which promotes learning and the application of these methods in professional practice.

By comparing its performance with renowned software such as Genie 2000, Maestro and FitzPeaks, GSA is rigorously validated for its accuracy and reliability. GSA has proven its ability to replace commercial gamma-ray spectrum analysis software, providing a viable solution for laboratories and institutions with limited resources.

In summary, GSA stands out as a tool for gamma-ray spectrum analysis, combining precision and collaboration. Spectral data processing promises to foster research and innovation through its open and scalable approach.

Second version of GSA

The absence of the activity calculation option in the first version leads to the incompleteness of GSA v1. For this improvement, the development team took the time to fill this gap. The

Fig. 1 Graphical interface of the first version of GSA.

objective of this new feature is to allow users to estimate the activity with precision. To facilitate the analysis and obtain optimal results, four known formulas have been integrated to evaluate the efficiency in the field of gamma spectroscopy:

$$\text{Formula 1: } \ln(\text{efficiency}) = a + b \times \ln(E) + c \times \ln(E)^2 + \ldots + f \times \ln(E)^n \quad (1)$$

It is used by Genie 2000 software,[17] to estimate efficiency using a logarithmic series.

$$\text{Formula 2: efficiency} = a \times E^{(-b)} \quad (2)$$

A simple power-type formula, often used for quick adjustments.

$$\text{Formula 3: efficiency} = a + b \times E + c \times E^2 + \ldots + f \times E^n \quad (3)$$

A polynomial formula that provides great flexibility in adapting to data.

$$\text{Formula 4: efficiency} = \exp(a + b \times E + c \times E^2) \quad (4)$$

An exponential relationship makes it easier to understand the complex fluctuations of efficiency with energy.

It is important to note that GSA v2 allows the user to select the degree of the formula from (2) to (5) for formulas (1) and (3) ($n = 2$, 3, 4 or 5).

These formulas provide the possibility to compare different methods and select the one that best fits the experimental data (Fig. 2). E is the energy of the radiation detected. The coefficients a, b, c, d, e and f are calculated using the least squares method, using experimental data consisting of energies and their efficiencies. The values of the coefficients a, b… in each formula are independent of the other formulas. These coefficients play an essential role because they modify the formula in order to adapt to the particular characteristics of the detector and the radiation concerned.

When the user taps on an efficiency formula, a window appears, displaying all the information required for an optimal efficiency calibration (Fig. 3), as well as a flexible graph. This interface provides a clear view of the information. Efficiency coefficients are automatically calculated by pressing the "Select the calibration nuclides" button (Fig. 3). To do this, GSA v2 uses energy and efficiency data corresponding to the radioactive sources previously entered by the user. Among the most commonly used radioactive sources for efficiency calibration are ^{137}Cs (Cesium-137) and ^{60}Co (Cobalt-60).

These data can also be easily modified, added or deleted by the user, allowing great flexibility in adjusting the parameters (Fig. 4 and 5). This feature ensures effective customization of the tool, thus offering the user the possibility to quickly adapt it

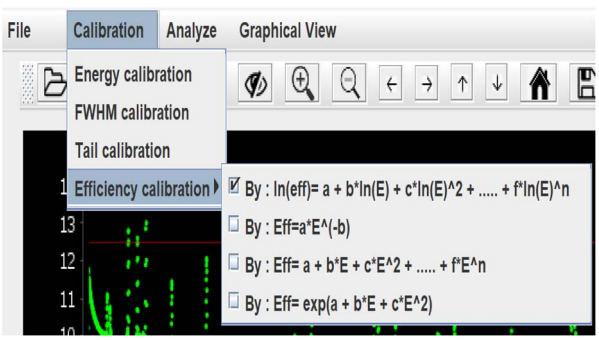

Fig. 2 Efficiency formulas in GSA v2.

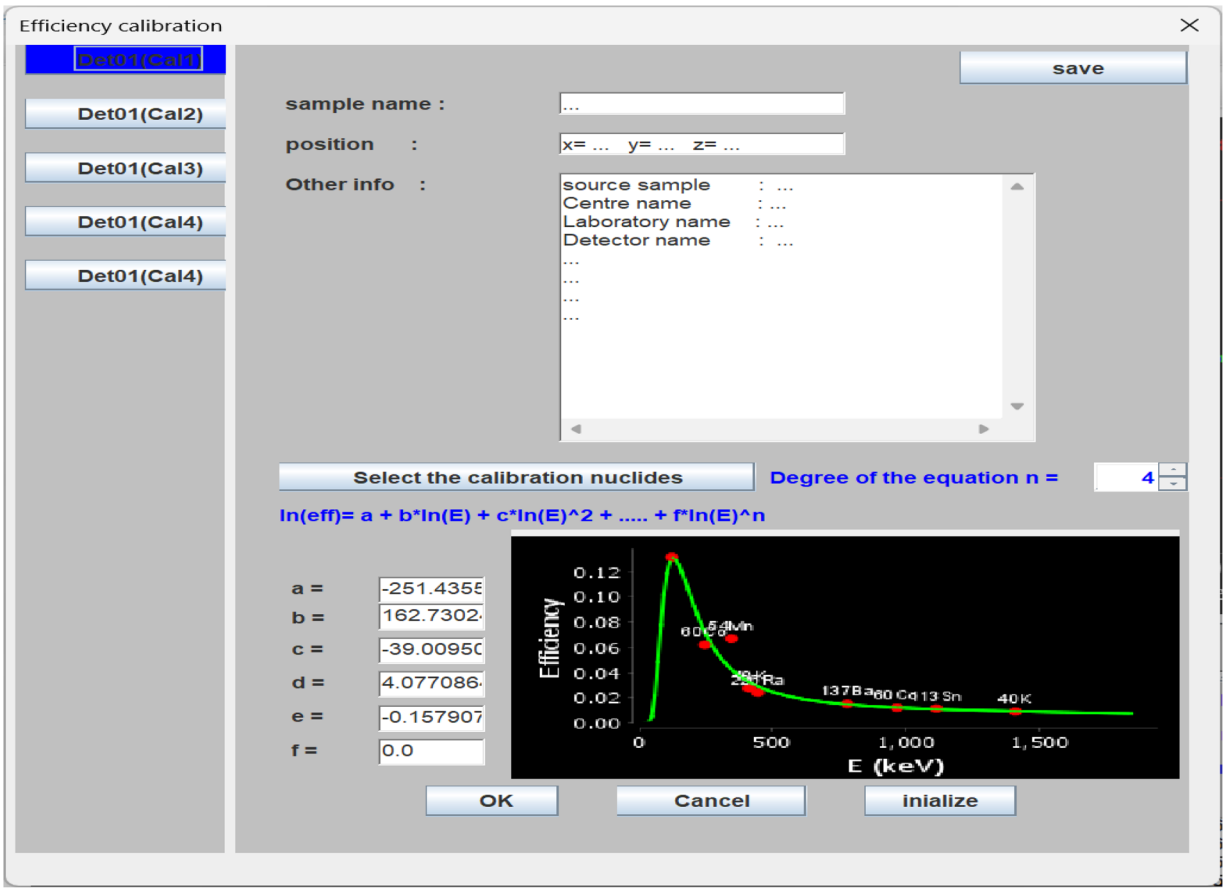

Fig. 3 Efficiency calibration window.

Nuclide	Energy (keV)	EmissionProbability(%)	Efficiency (effl)
137Cs	121.78	85.1	0.1315287711
60Co	244.0	99.9	0.06221250025
54Mn	344.28	100.0	0.06716867823
40K	411.0	10.7	0.02775032853
226Ra	443.96	100.0	0.02425373938
137Ba	778.9	85.5	0.0153877396
60Co	964.0	99.9	0.01240755308
113Sn	1112.07	100.0	0.01161158858
40K	1408.0	11.1	0.0092600542

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Fig. 4 An example of the energies and efficiencies used in GSA v2 to calculate the coefficients of the efficiency formula.

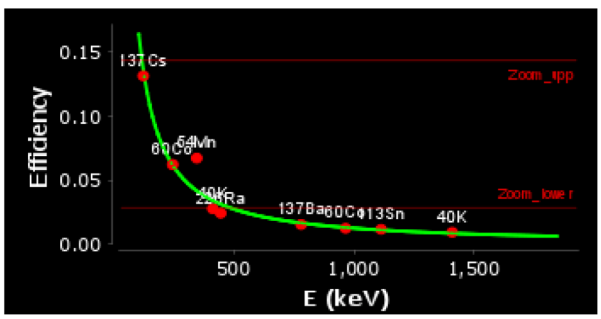

Fig. 5 An example of the efficiency curve found by GSA v2 using formula (2) and the data from Fig. 4.

to their particular needs. In addition, the use of a user-friendly interface simplifies the interaction with the data, making the whole process accessible even to unfamiliar users.

Efficiency allows us to calculate the activity using the well-known formula (5)

$$A = \frac{N}{\varepsilon \times R \times t} \quad (5)$$

where N is the net peak area, ε is the absolute efficiency (GSA v2 chooses the values of ε which correspond to the efficiency formula chosen by the user), R is the yield or branching ratio and t is the live time in seconds. This formula, well known in the field, has been directly integrated into GSA v2. The activity value of each nuclide found appears in the software's graphical interface (Fig. 6). In addition, the result report automatically integrates the activity values and their errors for each nuclide, ensuring a complete and accurate analysis of the data (Fig. 7).

Note here that a becquerel (Bq) corresponds to a disintegration per second, while a curie (C_i) is equivalent to 3.70×10^{10} becquerels (1 Bq = 1 decay per s and 1 $C_i = 3.70 \times 10^{10}$ Bq).

Fig. 6 Graphical interface of GSA v2.

	Channel	Energy	FWHM	Net area	Background	Error(%)	nucleides	Activity±Error(Bq)
007M	21,80E01	50,77E00	10,02E-01	21,43E03	14,73E04	26,23E-01	TH227	23.62063 ± 0.002891006 Bq
008S	26,10E01	60,49E00	10,27E-01	27,68E03	13,49E04	19,71E-01	AM241	8.660473 ± 6.167519E-4 Bq
009S	31,70E01	73,15E00	10,56E-01	36,11E02	14,90E04	21,62E000	BI211	43.02927 ± 0.257679400 Bq
010S	32,70E01	75,41E00	10,61E-01	55,54E02	16,10E04	14,36E000	PB212	8.517585 ± 0.022016050 Bq
011S	37,80E01	86,94E00	10,85E-01	15,37E05	20,97E04	91,00E-03	PB212	4273.871 ± 2.530458E-4 Bq
012S	46,00E01	10,55E01	11,21E-01	12,24E05	21,72E04	10,52E-02	U235	26459.10 ± 0.002275370 Bq
013S	47,80E01	10,96E01	11,29E-01	55,32E02	20,88E04	11,76E000	U235	83.28255 ± 0.177029670 Bq
014S	51,10E01	11,70E01	11,42E-01	14,70E03	19,95E04	43,77E-01	TE132	187.7866 ± 0.055926670 Bq

Fig. 7 An example of the result report containing activity and its error.

Validation of GSA v2

GSA v2 was validated using the reference software Genie 2000. This program, recognized for its reliability in the analysis of gamma spectra, served as the basis for the evaluation of the performance of GSA v2. The results obtained by GSA v2 were compared to those provided by Genie 2000, which confirmed the accuracy of the activity.

Methodology

Before validating the activity calculation option, it is necessary to confirm that the four efficiency formulas are well coded. For this reason we used the same data for each formula, and then we compared the efficiency figures created by GSA v2.

The "CERNIPF.CNF" spectrum file of the "CERNOBYL" sample was used as a case study to further validate GSA v2 software. This is a very information-rich file, available in Genie 2000 software, which contains a wide variety of peaks, including overlapping peaks and small peaks, making it a very powerful test for evaluating the performance of the spectral analysis algorithm.

The format.cnf (binary file) is specific to Genie 2000 and cannot be used directly with other software such as Maestro. A first analysis was carried out using Genie 2000, and then a manual reanalysis was carried out in order to correct any possible errors, such as negative areas or those with high uncertainty. With these adjustments, it was possible to obtain a reliable reference data set for future comparisons.

To ensure consistency of results, during the GSA v2 analysis, the same energy calibration coefficients, Full Width at Half Maximum (FWHM), Tail shape parameters, and efficiency parameters were used. Live time is already provided by the file, $t = 150\,000$ s.

On the other hand, it is difficult to use the same nuclide library for several software, because each software has its own nuclide library. The diversity of libraries makes the standardization of data and results more complex. To facilitate the

validation of GSA v2, a nuclide library similar to that of Genie 2000 was created and then integrated into GSA v2.

Finally, we compared the activity measured by Genie 2000 to that obtained by GSA v2 using the four efficiency formulas.

Results and discussion

The determination of activity begins with the selection of the appropriate efficiency formula. In this situation, the four formulas mentioned above were considered. In order to verify their performance, the information in Fig. 4 was applied to each formula. The corresponding curves for all formulas were provided by GSA v2 software (Fig. 8).

It is evident that all four formulas are correctly implemented, as the plotted curves are consistent and logical, as shown in Fig. 8. The proximity or alignment of the calibration nuclides on the efficiency curve, as well as the comparison of the reference values in Fig. 4 with their positions on the curves in Fig. 8, highlights the correct integration of the formulas into GSA v2.

The peak search was performed with Genie 2000, and then with GSA v2, taking care to maintain the same configuration parameters in both software to obtain as similar results as possible. However, a manual reanalysis of the peak search results was performed to correct any anomalies and ensure increased accuracy. Then, peaks that were not part of both software, Genie 2000 and GSA v2, were removed to ensure a reliable and relevant comparison of the final results.

Because the detector efficiency depends on the energy, we grouped these peaks into three energy intervals, to adjust them to the sensitivity of the efficiency for each interval. Each group therefore represents an energy range where the efficiency remains relatively stable, which facilitates the analysis and comparison of the results. The detected peaks are presented in Table 1 and are classified according to these energy intervals.

Table 1 Peak search results by GSA V1

Energy group	A	B	C
Number of peaks	29	81	48

Table 2 Common peaks between the two results

Energy group	A	B	C
Number of peaks	26	76	42

Group A represents the range from 0 to 300 keV, Group B from 300 to 1000 keV, and Group C covers energies above 1000 keV up to the highest observed energy. Using these categories, it is possible to study the activity based on detector efficiency fluctuations for each energy range.

Another methodical approach was implemented to better understand the disparities in activity values between the reference and GSA v2 results. After identifying the nuclides using the same nuclide library, the study excluded all nuclides that were not common between the two results. Using this method ensures a consistent and reliable baseline. The results in the previous table become as follows (Table 2):

The implementation of this approach ensures that the variations observed in activity values are the result of variations between the software themselves and not anomalies or absence of detection.

The absolute efficiency must be calibrated to measure the activity of the nuclides. This measurement is based on the same reference in terms of energy/efficiency. Using these sources, it is possible to establish the coefficients of the efficiency formulas. Subsequently, these coefficients are used to develop the absolute efficiency curve, which is essential for accurate

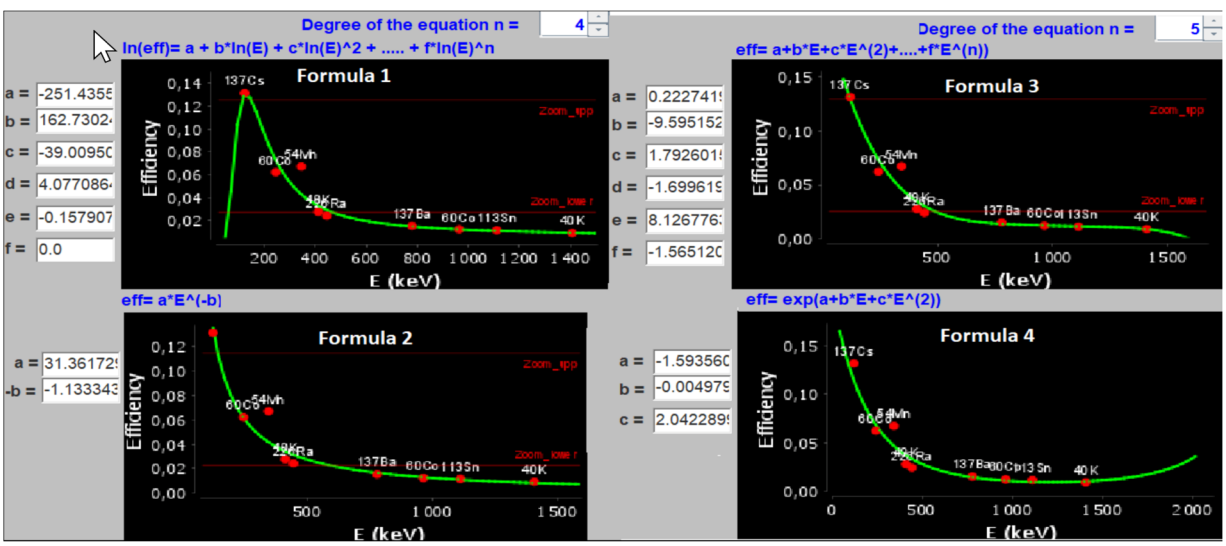

Fig. 8 Efficiency curves generated by GSA v2 corresponding to the efficiency formulas.

Nuclide	Energy (keV)	EmissionProbability(%)	Efficiency (effI)
57Co	121.78	28.67	0.00224516754
152Eu	244.0	7.61	0.00161887349
60Co	344.28	26.6	0.00134114445
152Eu	443.96	3.12	0.00106684368
152Eu	778.9	12.97	6.7849855E-4
152Eu	867.32	4.16	6.2792094E-4
152Eu	964.0	14.6	5.9291584E-4
152Eu	1085.8	9.96	4.3798047E-4
60Co	1112.07	13.41	5.3238512E-4
152Eu	1212.12	1.38	4.783175E-4
152Eu	1298.49	1.61	4.6246128E-4
152Eu	1408.0	20.8	4.1278E-4

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Fig. 9 Sources used for efficiency calibration in this analysis.

measurements. Fig. 9 represents the nuclides used by Genie 2000 and GSA v2 to calibrate the efficiency in our analysis.

Due to the inclusion of only one efficiency formula in Genie 2000 (formula (1)), it is not possible to use the other three efficiency formulas. Therefore, activity was only measured with the first formula for Genie 2000. However, for GSA v2, all four formulas were used. Fig. 10 shows the efficiency curves for each formula, generated by GSA v2.

The gamma spectrum used in this study has many peaks, which would make it difficult to compare each reference activity value with each activity value measured by GSA v2.

As such, averaging the relative standard deviation of the activity of each Group (A, B and C) is recommended. In practice, we calculate the relative standard deviation of the mean of the RSD_i activity for each activity i, using eqn (6).

Once we have calculated the RSD_i, we move on to averaging these relative standard deviations for each group RSD_j. Eqn (7) makes it possible to obtain this average by synthesizing the variations of all the peaks of the same group into a single representative value. Using this method, it is possible to perform a comprehensive and statistically robust comparison of the performance of GSA v2 software, thus overcoming the difficulty of comparing a large number of activity values.

$$\mathrm{RSD}_i = \frac{\sigma_i}{\overline{A}_i} \times 100 = \frac{\sqrt{\left(A_{r_i} - \overline{A}_i\right)^2 + \left(A_i - \overline{A}_i\right)^2}}{\sqrt{2} \times \overline{A}_i} \times 100 \quad (6)$$

$$\mathrm{RSD}_j = \frac{1}{N} \sum_{i=1}^{N} \mathrm{RSD}_i \quad (7)$$

where j = A, B and C, σ_i is the standard deviation, A_{r_i} is the reference activity value of nuclide i, A_i is the activity value of nuclide i found by GSA v2 software, $\bar{A}_i$ is the average of A_{r_i} and A_i, and N is the number of activities in group j.

The conclusions of this study, presented in Table 3, provide a clear overall view of GSA v2 software performance. By focusing on RSD_j, it is possible to identify the characteristics of the efficiency formulas that provide more consistent activity measures.

The mean of relative standard deviation level between the efficiency calibration formulas compared to the reference (Genie 2K) is represented by the percentages of RSD_j in the table. A lower value indicates a higher match with the reference, suggesting that the formula is effective in assessing activity.

Genie 2K (formula (1), degree $n = 3$): all three groups (A, B and C) have an RSD_j of 0%, which means that it is the reference.

Formula (1) (degree $n = 3$), GSA v2: in all three groups, the relative deviations are small (0.15% for A, 0.30% for B and 0.40% for C), suggesting a high precision for efficiency measurement, close to the reference. It seems that this formula is suitable for general use in all energies.

Formula (2), GSA v2: Group A shows a significant deviation (15.34%), suggesting lower accuracy for low energies. However, the differences are significantly smaller in Groups B and C (0.81% and 4.12%, respectively), suggesting that this formula is more suitable for medium and high energies.

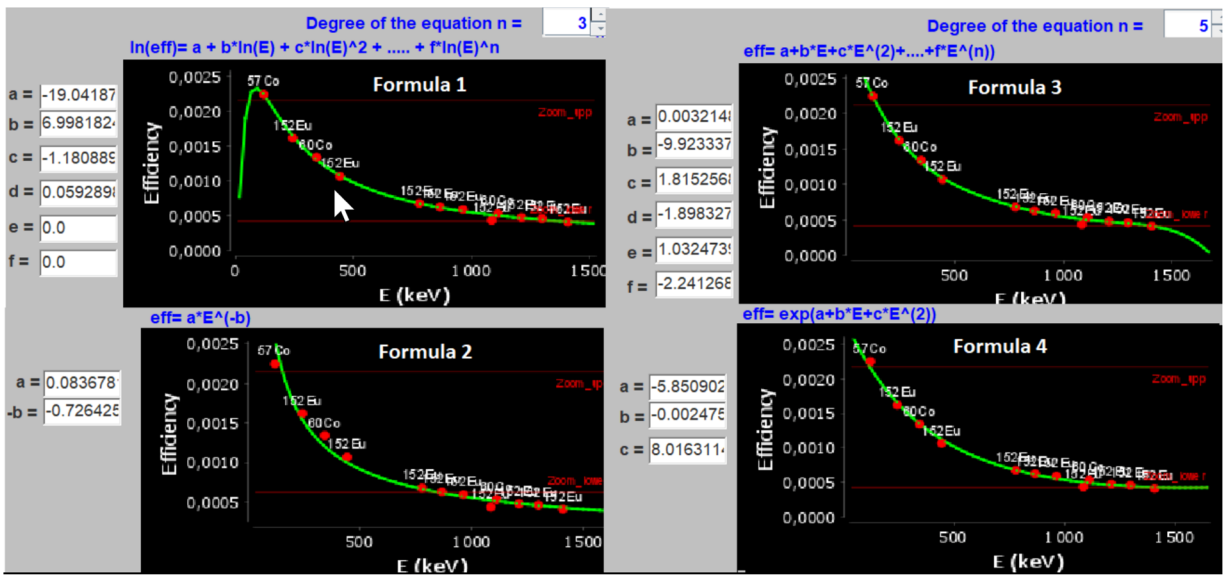

Fig. 10 Efficiency curve for the four formulas by GSA v2.

Table 3 Results for the mean RSD_i of each group (RSD_j)

	RSD_j		
Group of activities	A	B	C
Reference (using Genie 2K), formula (1), degree $n = 3$	0.00%	0.00%	0.00%
GSA v2: formula (1), degree $n = 3$	0.15%	0.30%	0.40%
GSA v2: formula (2)	15.34%	0.81%	4.12%
GSA v2: formula (3), degree $n = 5$	14.72%	0.77%	6.16%
GSA v2: formula (4)	16.95%	0.69%	5.43%

Formula (3) (degree $n = 5$), GSA v2: the deviation is also high for low energies (Group A), but it decreases in Groups B and C (0.77% and 6.16%, respectively). This suggests that this formula is better suited for medium energies, although it still has a larger deviation in Group C.

Formula (4), GSA v2: the deviation is highest among the formulas in Group A (16.95%), indicating limited accuracy for low energies. However, this formula provides satisfactory accuracies for Groups B and C (0.69% for B and 5.43% for C), making it a suitable option for medium and high energies.

Formula (1) is the most efficient in terms of accuracy for low energies (Group A), with the lowest RSD_j. All formulas are efficient for medium energies (Group B), although formula (4) has the lowest RSD_j. Formula (1) remains the best option for high energies (Group C), although formula (3) also provides adequate accuracy. The results indicate that in most energy ranges formula (1) remains the most reliable, while the other formulas differ in accuracy depending on the energy group.

Conclusions

In the second version of GSA software, a feature was added to calculate the activity of isotopes. This evaluation is based on an efficiency assessment, for which four formulas were included. This is intended to offer the user the best possible option, thus ensuring maximum accuracy. Graphical analysis confirmed the validity of these four formulas and the results of the activity calculation were validated by comparison with those obtained with Genie 2000. GSA v2 is free and open source software, available on the site mentioned above, under the GNU Affero General Public License. This offers users great flexibility, without any limitations of use.

Data availability

The software developed for this study, including the Java code and data visualization functionalities using the JFreeChart library, is available at **https://www.github.com/LAHCEN-EL-AMRI/GSA-v2/tree/master**. The analysis scripts utilized in this research are included in the repository, with the version of the code employed for this study being version 2.0.

Author contributions

Conceptualization: Lahcen El Amri, Hamid Amsil, methodology: Lahcen El Amri, software: Lahcen El Amri, validation: Lahcen El Amri, Hamid Amsil, Omar El Bounagui, Abdelouahed Chetaine, formal analysis: Lahcen El Amri, Hamid Bounouir, investigation: Lahcen El Amri, Omar El Bounagui, Hamid Bounouir, Brahim Elmokhtari, data curation: Abdessamad Didi, Hamid Amsil, writing – original draft: Lahcen El Amri, writing – review & editing: Hamid Amsil, Omar El Bounagui, Abdelouahed Chetaine, visualization: Hamid Bounouir, Abdessamad Didi, supervision: Omar El Bounagui, Hamid Bounouir, project administration: Lahcen El Amri, funding acquisition: Lahcen El Amri.

Conflicts of interest

There are no conflicts to declare.

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