Applied Radiation and Isotopes xxx (xxxx) 110227

Contents lists available at ScienceDirect

Applied Radiation and Isotopes

journal homepage: www.elsevier.com/locate/apradiso

Review

New open-source software for gamma-ray spectra analysis

Lahcen El Amri [a,*], Abdelouahed Chetaine [a], Hamid Amsil [b], Brahim El Mokhtari [a], Hamid Bounouira [b], Abdessamad Didi [b], Abdelfettah Benchrif [b], Khalid Laraki [b], Hamid Marah [b]

[a] Nuclear Reactor Energy and Physics, Nuclear Security and Environment Team (PRESN), Faculty of Sciences, Mohammed V University, 4 Avenue Ibn Battouta, B.P., 1014, Rabat, Morocco

[b] National Centre for Nuclear Energy, Science and Technology (CNESTEN), B.P. 1382, R.P., 10001, Rabat, Morocco

ABSTRACT

Many commercially available software packages have been created to analyze gamma-ray spectra, but their source code has generally not been shared, although some users may wish to add or modify certain functionality, which is impossible without access to the source code. This study therefore presents a new open-source software package for the analysis of gamma-ray spectra. The name of the software is GSA (Gamma-ray Spectra Analysis), the source code of which is freely available through the GitHub website (https://github.com/LAHCEN-EL-AMRI/Gamma-Spectra-Analysis). The main function of this initial version of the software is to locate peaks, calculate areas, and identify corresponding radionuclides. A future version will complement this by measuring the concentrations of radionuclide elements. The software was validated by comparing its analysis results with those generated by three other software programs, namely Genie 2000, Maestro, and FitzPeaks. All the formulas used are explained in this work, which could be useful for researchers or students looking to create their own software packages for analyzing gamma-ray spectra.

1. Introduction

Analyzing the gamma-rays emitted during radionuclides decay represents a way to analyze a sample. This approach is widely used in many fields, such as industry, geochemistry, archeology, and materials science (El Amri et al., 2021). It is used to identify and quantify the radionuclides present in a sample, including elements that have been previously irradiated in a nuclear reactor. The latter is known as NAA (Neutron Activation Analysis). The NAA is an analytical technique with several advantages, namely: Simple sample preparation, Ease of use of analytical measurement systems, Non-destructiveness of Samples, Accuracy of analysis results (3–5%), Characterization of the majority of matrices …

Gamma rays are usually measured using high-resolution, hyperpure germanium detectors (Ibrahim, 2011), with the measured values being converted into a gamma-ray spectrum. Spectrum analysis then leads to identifying and quantifying elements (Tickner et al., 2016).

On the other hand, gamma-ray spectra often feature a large number of peaks that take a long time to process manually. It is therefore necessary to process them using special software in order to save time and simplify calculations while achieving satisfactory results. Currently, many software packages exist to meet this need, such as GammaVision (GammaVision® 2017.), Maestro (MAESTRO® Multichannel Analyzer Emulation Software.), HYPERMET-PC (Hypermet PC.), K0_IAEA (Kubešová and Jan, 2011), GENIE 2000 (GenieTM, 2021) …

Gamma spectrum analysis generally follows four steps: calibration, peak localization, calculation of net peak areas, and identification of radionuclides. The existing software packages generally cannot be modified; on the contrary, this article presents a new open-source software package presents for the analysis of gamma-ray spectra, named GSA (Gamma-ray Spectra Analysis), the source code of which is freely available through the GitHub website (https://github.com/LAHCEN-EL-AMRI/Gamma-Spectra-Analysis). There is also a detailed user manual (https://github.com/LAHCEN-EL-AMRI/Gamma-Spectra-Analysis/tree/master/Install/Doc). GSA performs the different analysis steps and is available to everyone on the aforementioned website. All the mathematical functions used are explained, and the Java programming language with the JFreeChart library were used to create the software. Consequently, users can modify these or add their own features.

2. Formulas and methods used

An analysis of gamma-ray spectra aims to identify and quantify radionuclides, so the extraction of the energies and areas of full-energy peaks is necessary. For this reason, locating the peaks is the first task to perform. Most gamma-ray spectra are represented by a number of counts as a function of channel, so a mathematical formula must be

* Corresponding author.
E-mail address: lahssenelamri@gmail.com (L. El Amri).

https://doi.org/10.1016/j.apradiso.2022.110227
Received 2 November 2021; Received in revised form 24 March 2022; Accepted 4 April 2022
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available to transform the values of the channels into energy values (i.e., energy calibration). After locating peaks, the energy of each peak is compared to the energies of the radionuclides present in the software library in order to identify the radionuclide corresponding to each peak. Generally, the procedure for analyzing a spectrum follows the four steps presented below.

2.1. Calibration

Before starting the analysis, it is necessary to perform the calibration for energy (E), FWHM (full width at half maximum), and Tail. Energy calibration is accomplished by measuring the spectrum of a source that emits gamma rays with a precisely known energy and comparing the measured peak position (Gilmore, 2008). The energy calibration equation is a second-order polynomial (Eq. (1)), where the variable (C) is the channel number. A first-order equation can also be used. Coefficients a, b, and c are usually taken from the input file, but sometimes the user may wish to modify them for analytical reasons, so he can manually choose the a, b, and c coefficients or select the channels of certain peaks and their corresponding energies. In addition, the graphical calibration works by right clicking on the centroid of the peak. Only well-defined peaks can be used to perform a more precise calibration, and at least two distant peaks are needed. This operation automatically calculates the a, b, and c coefficients.

$$E = a + b * C + c * C^2 \tag{1}$$

Even with high resolution detectors, the full-energy peaks spread over several channels, between three and ten channels. The energy resolution of a detector is expressed by the FWHM of the full-energy peaks. Fig. 1 illustrates this parameter. The photon energy distribution is theoretically associated with a Gaussian law of the form (Eq. (2)):

$$G(x) = Ae^{-\frac{(x-m)^2}{2*\sigma^2}} \tag{2}$$

Where:

- A is the amplitude of the peak
- x represents the energy
- the centroids m corresponds to the initial energies of the γ photons
- σ is standard deviation.

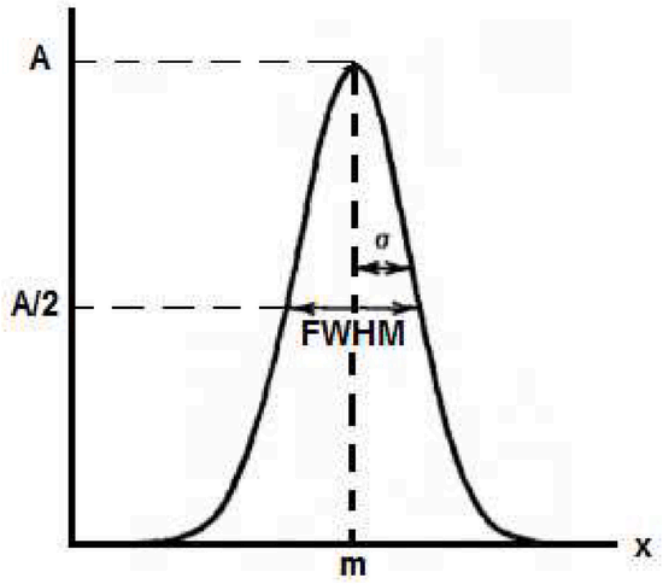

Fig. 1. The Gaussian form and its parameters.

The peak shape depends on FWHM (FWHM = 2355 σ), so the calibration of FWHM versus the energy is important in the peak search algorithm and in the calculation of the region of interest. In addition, it plays an important role in extracting the backgrounds under peaks.

Eq. (3) is used for FWHM calibration, where a' and b' are constants that are taken from the input file. For energy calibration, the user can modify them however he or she sees fit.

$$FWHM = a' + b' * \sqrt{E} \tag{3}$$

practically, the full-energy peaks are slightly different from Gaussian function. The low energy side is often slightly tilted, so Eq. (4) was included in the software to adjust the peak shape (Fig. 2). In addition, the Gaussian function was modified to make it more practical (Eq. (5)).

$$Tail = a'' + b'' * E \tag{4}$$

$$Fi = \begin{cases} Ae^{-\frac{(Ci-Cp)^2}{2*\sigma^2}}, & if\ Ci > Cp - Tail \\ Ae^{\frac{Tail*(2*Ci-2*Cp+Tail)}{2*\sigma^2}}, & if\ Ci \le Cp - Tail \end{cases} \tag{5}$$

Where, a'' and b'' are constants, Fi is the value of the peak model function at channel Ci, A is the amplitude of the peak, Cp is the peak centroid, and σ is the width of the Gaussian (2.355 σ ≃ FWHM).

2.2. Peak search

Peak searching is one of the most sensitive issues in spectrum analysis due to the complex spectral shapes which require specific methods. The peak search method currently used in this software is based on Mariscotti's method (Mariscotti, 1967), which is also called the second derivative method. It can find overlapping peaks, which can present a problem for some methods like the recurrence method, so it is used in almost all gamma-ray spectra analysis software, such as HYPERMET-PC (Révay et al. 2005), K0_IAEA (Rossbach and Blaauw 2006), GENIE 2000 (Suárez-Navarro et al., 2018), and GammaVision (2017).

The smoothed second derivative of count N at channel i is calculated using the following function:

$$N''_{i\,smoot}(z,\omega) = \sum_{k=i-z*m-1}^{i+z*m+1} C_{k-i}(z,\omega) * N_k \tag{6}$$

$$C_{k-i}(z,\omega) = \sum_{j=i-m}^{i+m} C_{k-j}(z-1,\omega) \tag{7}$$

$$C_{ki}(0,\omega) = \begin{cases} 0 & if\ |k-i| \ge 2 \\ 1 & if\ |k-i| = 1 \\ -2 & if\ k = i \end{cases} \tag{8}$$

The standard deviation on $N''_{i\,smoot}(z,\omega)$ is:

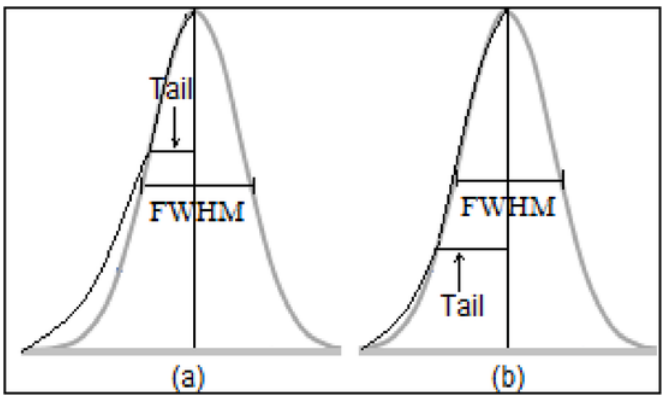

Fig. 2. The effect of the Tail on the shape of the peak.

$$E\left[N''_{i\ smoot}(z,\omega)\right] = \left[\sum_{k=i-z*m-1}^{i+z*m+1} C^2_{k-i}(z,\omega) * N_k\right]^{1/2} \quad (9)$$

Where N_k is the original spectrum count at each channel k. By default, $z = 5$ and $m = 1$. Also, $\omega = 2 * m + 1$.

$$\begin{cases} \frac{|N''_{i\ smoot}(z,\omega)|}{E\left[N''_{i\ smoot}(z,\omega)\right]} \geq threshold\ ,\ the\ peaks\ are\ acceptable. \\ \frac{|N''_{i\ smoot}(z,\omega)|}{E\left[N''_{i\ smoot}(z,\omega)\right]} < threshold,\ the\ peaks\ are\ not\ taken\ into\ account. \end{cases}$$

The standard threshold value is 2 (Fig. 4). To get good peak search results, two additional parameters l_{min} and l_{max} are entered in the peak search parameters window, and these represent the minimum and maximum, respectively, number of negative points of $N''_{smoot}(z,\omega)$ for accepting a peak (Fig. 3).

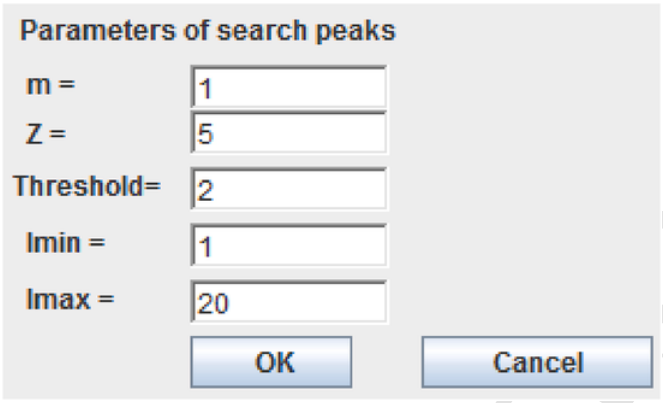

Fig. 3. Software window for peak search parameters.

2.3. Peak area calculation

The radionuclide quantification is based on the net area of full-energy peaks, which are considered as Gaussian functions superimposed to a continuous background. Determining the background of each peak is necessary in order to calculate its net area. The software considers the peak background to be linear, the average of five counts is taken at each base of the peak (left B_l and right B_r). The software automatically takes the average of three counts if less than five channels are available (Fig. 5), or it just takes a count if less than three channels are available.

The peak area calculation depends if the peak is well isolated or is part of a group of overlapping peaks. The factor k was used in the software to distinguish overlapping peak (The software uses k = 8 by default). Two peaks overlap if the distance between them is less than k.σ.

Peaks are non-overlapping if the distance between them is greater than k.σ. In this case, the background B and the net peak area A of peak with centroid C are calculated using the following formulas (GammaVision® 2017):

$$B = a' * C_j + b' \quad (10)$$

where $a' = \frac{B_r - B_l}{C_r - C_l}$ and $b' = B_r - a' * C_r$

$$A = \sum_{i=l}^{r} N_i - B \quad (11)$$

Where B_l and B_r are the averages of the background counts for the low (C_l) and high (C_r) end of the centroid C, $l = \text{int}\left(C - \frac{k*\sigma}{2} + 0.5\right)$ and $r = \text{int}\left(C + \frac{k*\sigma}{2} + 0.5\right)$.

In case of overlapping peaks, it is necessary to separate the n candidate peaks. The equation for the background calculation is the same both for isolated or overlapping peaks, only the limiting channels are

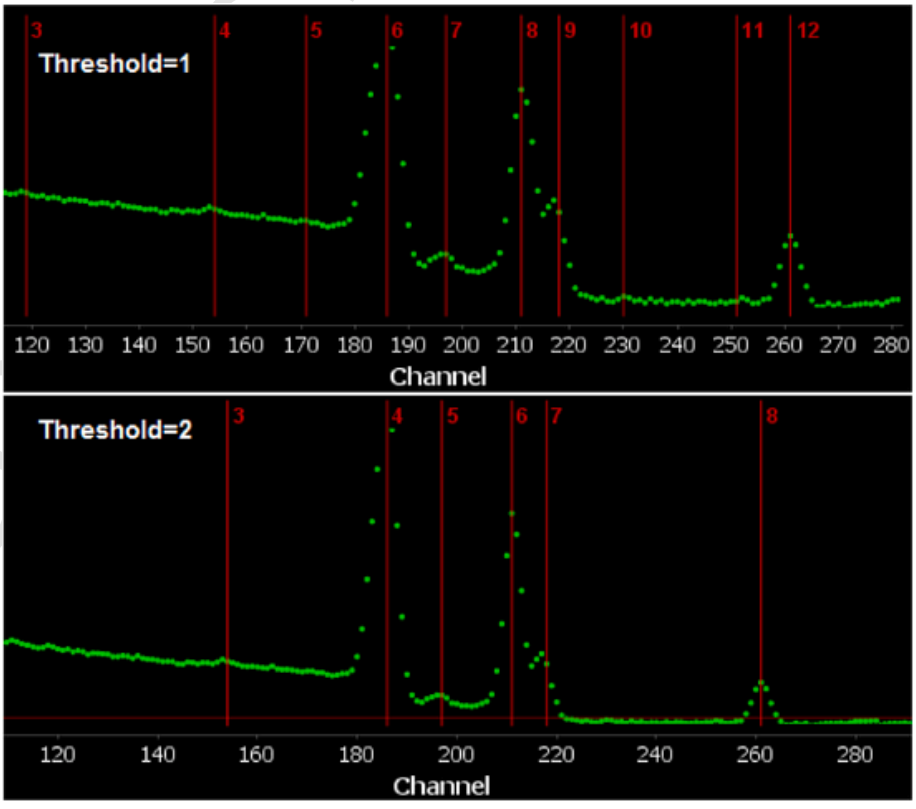

Fig. 4. The threshold effect.

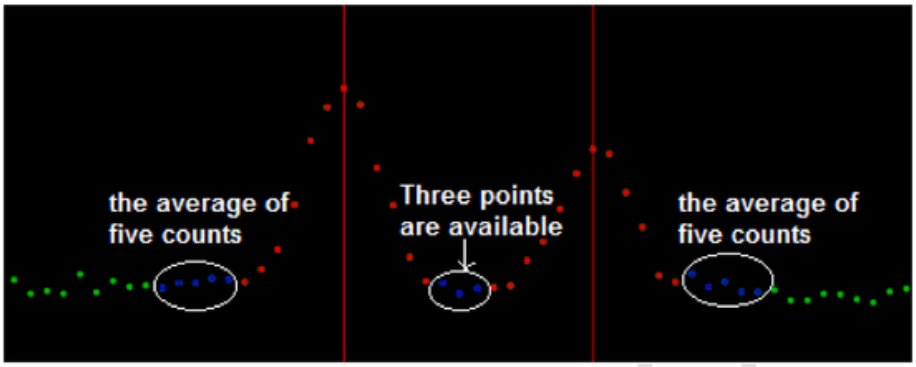

Fig. 5. Peak bases (blue color). (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

different. The background $(B_{j,i})$ from peak j to channel i and the area of the peaks are calculated using the following formulas:

$$B_i = a * C_i + b \tag{12}$$

where $a = \frac{B_{mr}-B_{ml}}{C_{mr}-C_{ml}}$ and $b = B_{mr} - a * C_{mr}$.

Where B_{ml} and B_{mr} are the averages of the background counts at the low and high ends of the first multiple peak C_{p1} and the last multiple peak C_{pn}, successively, while C_{ml} is the lowest channel of centroid C_{p1} and C_{mr} is the highest channel of centroid C_{pn} (Fig. 6 and Fig. 7).

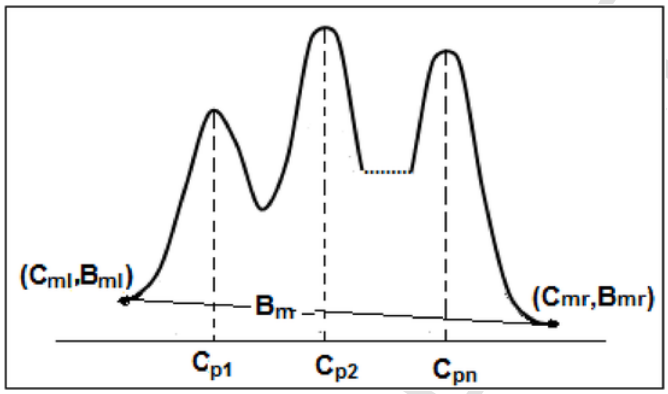

Fig. 6. Overlapping peaks.

$$A_j = \sum_{i=l_j}^{r_j} H_j e^{-\frac{(C_i-C_{pj})^2}{2*\sigma_j^2}} - B_{j,i} \tag{13}$$

Where $l_j = \text{int}\left(C_{pj} - \frac{k*\sigma_{pj}}{2} + 0.5\right)$ and $r_j = \text{int}\left(C_{pj} + \frac{k*\sigma_{pj}}{2} + 0.5\right)$.

In addition, $j = 1,2 \ldots n$, where n is the number of overlapping peaks with the same background B_m, while H_j is the value of the origin count N_j corresponding to centroid C_{pj} and $B_{j,i}$ is the value of the background corresponding to the channel C_i.

2.4. Radionuclide identification

The peak search algorithm identifies the energy, FWHM, and peak areas for the gamma-ray spectrum. It then attempts to match the identified energies to those listed in a library that is selected for analyzing that sample. Energy calibration is sufficient if any deviation between a reference energy and one calculated from the calibration curve is within one or two channels for the full energy region under scrutiny (IAEA 2002). The libraries selected relate to the radionuclides most likely to be found in a particular sample can be easily identified. Knowledge of the source (origin) of the sample and which gamma-emitting radionuclides are likely to be present are necessary in order to minimize the chances of incorrectly identifying a radionuclide that is not present.

Libraries provided by a manufacturer are still insufficient (Griggs, 2019), because software manufacturers do not know what all the poten-

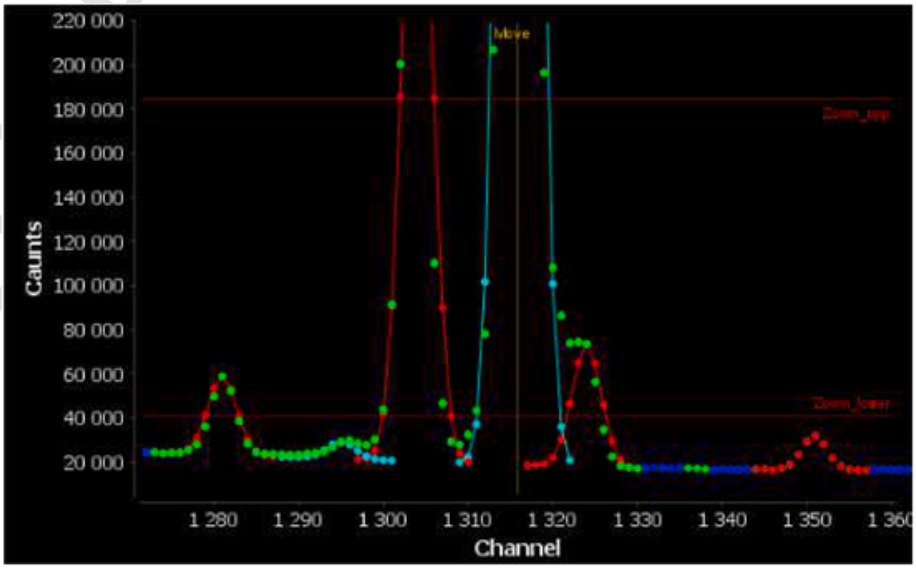

Fig. 7. Software interface following spectrum analysis (zoom is on part of the overlapping peaks).

tial applications are and cannot cover every possibility, so they supply libraries with a convenient framework for users to make additions, deletions, or edits as they see fit for their particular application (Griggs, 2019).

In this regard, this software has an example standard library of 514 different radionuclides. The current library was created in ASCII form, so users can modify, add, or delete radionuclides and their dependencies, and there is also the option to create personal library files. A created library file must have five columns for the name of the radionuclide, energy, intensity, half-life, and its unit.

3. Software validation

Three popular software packages were used to validate GSA namely Genie 2000, Maestro, and FitzPeaks by comparing the results of their analyses with those found by GSA.

3.1. Methodology

The spectrum file "CERNIPF.CNF" for the "CERNOBYL" sample available in the GENIE 2000 software was used to validate our software. It contains all sorts of desirable peaks (e.g., overlapping peaks, small peaks, etc.) for learning about the performance of a software package's algorithm. The.cnf input file format is proprietary and cannot be directly read by Maestro, so it was inputted into Genie 2000 and then exported to.chn format. The different software packages could read the (.chn) input file without problems.

The spectrum was analyzed using the Genie 2000 spectrum analysis software before being manually reanalyzed in order to correct errors, such as negative areas, areas with large uncertainty, and so on. The results of this processing were used as the reference.

The software analysis was performed using mainly the same energy calibration coefficients, FWHM, and Tail to calculate the areas. Finally, the results obtained were compared to evaluate the performance of the new software for different sorts of peaks (overlapping peaks, small peaks, etc.). The software used for this comparison were Genie 2000, Maestro and FitzPeaks with the same library. The first comparison involved the search for peaks, while the second was for the areas of regions of interest.

3.2. Results and discussion

The abovementioned spectrum analysis of 4096 channels revealed that the spectrum contains 169 peaks. However, the shapes and sizes of the peaks can generally have an impact on an analysis of gamma-ray spectra, so it is necessary to separate the peaks into three groups to consider the results:

A: single peak with big size that is well defined.

B: single peak.

C: overlapping peaks.

The goal here is to evaluate the performance of the search method (second derivative) that was employed in the GSA software. To this end, Table 1 shows the results of the four software programs' searches for peaks.

Peaks in group A are found by all software packages, because thanks to their size and isolation, they do not pose any difficulties for any peak search method. In contrast, the peaks of groups B and C were not exhaustively found, with each software package finding a different number of peaks, although these numbers are relatively similar. For example, Genie 2000 found 158 peaks and 25 false positive, but it missed 11 peaks. Maestro detected 152 peaks, 15 false positive and 17 false negative. FitzPeaks found 151 out of 169 peaks and 10 false positive but missed 18 peaks. GSA detected 156 peaks and 17 false positive but missed 13 peaks. All false negatives were either very small peaks or significantly overlapping, because overlapping peaks can be too hard to find algorithmically. For example, if two peaks have energies very close to each other, a graph will show a single peak rather than two peaks (Vigineix, 2012), so the software will conclude it is a single peak. What is more, low intensity peaks are at the background level, so analysis software is more likely to confuse them with the background. In such cases, some users increase the peak search threshold value to find smaller peaks, but this runs the risk of detecting many false positive. Many users prefer to fix a threshold that will minimize the number of false positive at the risk of missing some peaks. For these reasons, the results in Table 1 differ slightly.

Table 1
Peak search results.

Group of peaks	Number of peaks found			The false negative			The false positive		
	A	B	C	A	B	C	A	B	C
Reference (169 peaks)	3	44	122	0	0	0	0	0	0
Genie 2K (183 peaks)	3	41	114	0	3	8	0	18	7
Maestro (167 peaks)	3	37	112	0	7	10	0	10	5
FitzPeaks (161 peaks)	3	38	110	0	6	12	0	7	3
GSA (173 peaks)	3	40	113	0	6	7	0	11	6

On having validated the peak searching functionality, another study was performed to validate the calculation of the peak areas. In this study, any peaks that were not found in the first study were ignored, and only the peaks that were reflected in the reference's peaks were considered. The best way to evaluate performance when calculating many regions of interest in the spectrum through software is to calculate the average of the relative standard deviation of each group. Genie 2000 was withdrawn from this study at this point because the reference peak areas had already been calculated using it.

The relative standard deviation of the mean area of each peak i is calculated using Equation (14). Next, the average of RSD_i for each group was calculated using Equation (15). The results of this are shown in Table 2.

$$\mathrm{RSD}_i = \frac{\sigma_i}{\bar{A}_i} * 100 = \frac{\sqrt{(A_{ri}-\bar{A}_i)^2 + (A_i-\bar{A}_i)^2}}{\sqrt{2} * \bar{A}_i} * 100 \tag{14}$$

$$\mathrm{RSD}_j = \frac{1}{N}\sum_{i=1}^{N} \mathrm{RSD}_i \tag{15}$$

Where i is the peak number in its group, j = A, B, and C, A_{ri} is the net area of reference peak i, A_i is the net peak area for i found by the software, $\bar{A}_i$ is the mean of A_{ri} and A_i, and N is the number of peaks in group j.

All the mean RSD_j for group A are less than 0.09%, indicating that their areas are considerably larger than their backgrounds. In such cases, subtracting the background does not pose any difficulties. In contrast, the RSD_j of groups B and C are somewhat higher but all less than 2.41%. When the peak region is smaller, the software is more likely to

Table 2
The results for the mean RSD_i of each group.

Group of peaks	Peaks in common with reference peaks			$\mathbf{RSD}_j$		
	A	B	C	A	B	C
Reference	3	44	122	0%	0%	0%
Maestro	3	37	112	0.09%	1.77%	2.41%
FitzPeaks	3	38	110	0.05%	1.98%	2.05%
GSA	3	40	113	0.07%	2.10%	1.78%

accumulate errors during the analysis. Due to the presence of weak peaks, subtracting their backgrounds becomes complicated. This is why the RSD_j means in group A are considerably lower than those of groups B and C. However, all three programs yield values that are broadly similar, suggesting that GSA has equivalent performance.

4. Conclusion

On presenting a new open-source software package and its algorithms, a study was carried out to evaluate its performance in finding peaks and calculating their net areas. Its analysis results were compared with those produced by three other popular programs, namely Genie 2K, Maestro, and FitzPeaks. A comparison revealed that all their spectrum analysis results were broadly similar. This means that the software presented in this work has been adequately verified as being suitable for peak identification and peak area calculation.

To improve this program, further functionality will be incorporated in a future version, and this open-source software will be updated progressively.

An updated version, which will also be open source, will include elemental analysis, which aims to determine the proportion of each chemical element in the composition of a substance. Our team is currently developing algorithms to integrate into this software based on two methods: the K0 method (Revay and Kennedy n.d 2012.) and the comparative method (Glasgow, Dyer, and Robinson n.d. 1995).

Uncited references

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CRediT authorship contribution statement

Abdelouahed Chetaine: Supervision. **Hamid Amsil:** Validation, Methodology, Formal analysis. **Brahim El Mokhtari:** Data curation. **Hamid Bounouira:** Data curation. **Abdessamad Didi:** Data curation. **Abdelfettah Benchrif:** Data curation. **Khalid Laraki:** Data curation. **Hamid Marah:** Data curation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Annex

General presentation of the software

The installation process is routine and without any complications. Unfortunately, the current version is limited to English only. The Gamma-ray Spectra Analysis (GSA) software's graphical interface was created with simplicity and clarity in mind, and many options were included to assist the user. To simplify the software's presentation, the graphical interface is divided into the following six areas (Fig. 8): the menu bar, the icon bar, a space for graphs, a space for information extracted from the file, a space for markers and analysis information, and a space of results. (The user manual goes into more detail.)

Fig. 8. GUI (Graphical User Interface of GSA).

Menu bar (Fig. 9): This has four menus: **File**, **Calibration**, **Analyser,** and **Graphic view**. Each of these has sub menus with specific options. In summary, the **File** menu is used to open the spectrum file, and it includes some options for comparing spectra and freeing up space for graphs and results. Currently accepted file formats are.Chn, Spc, and Spe. **Calibration** is used to perform energy, FWHM and Tail (See Fig. 2) calibrations. The energy calibration curve is also available in this menu. The **Analyser** menu is essentially for analyzing the gamma spectrum in a good quality manner, with peak search and surface calculation submenus being available. It also has options for displaying the analysis results through the GUI or in a report. The **Graphic view** menu is used to show or hide certain graphs (e.g., graph of peaks, peak bases, background, etc.).

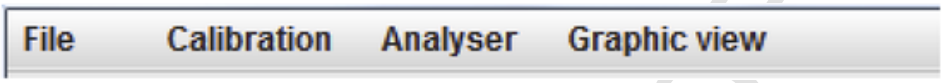


Fig. 9. Menu bar.

Icon bar (Fig. 10): The icon bar has fifteen icons, with each having various functionality. These are mostly shortcuts to functionality on the menu bar, but they also include options for zooming and manipulating, graphics.

Fig. 10. Icon bar.

The Space for Graphs: This is the area in Fig. 8. Through the menu options, mouse, and icons, the user can view graphs in this area. Currently, this is the only such area. Once a graph is displayed, users can manipulate it by using either the icons or the mouse. A right click on the area reveals certain options, such as graphical energy calibration, color modification, graph recording, and so on.

Space for information extracted from the file: There is a hidden space under the gray program panel. To display it, the user must double click on the white bar under the graph space then drag it down. This displays information extracted from the file, such as start time, start date, calibration equation, and such like (Fig. 11).

Fig. 11. Space for information extracted from file.

Space for markers and analysis information (Fig. 12): This space is useful after finding peaks or calculating areas, and it serves two functions. First, it displays the necessary information for each peak found, namely channel, energy, FWHM, area, uncertainty, nuclide, energy, gamma intensity, and half-life. Second, it clarifies and simplifies the visualization of the peaks. Four buttons manage these two functions: The **Next** button moves the peak marker to the next peak, while the **Previous** button moves the peak marker to the previous one. **Range** is used to make the peak marker appear on the complete graph. This button then becomes **Not Range** to dismiss this functionality. **Clear Marker** is used to clear the marker.

The uncertainty in the net area is the square root of the sum of the squares of the uncertainty in the adjusted gross area and the weighted error of the adjusted background. The background uncertainty is weighted by the ratio of the adjusted peak width to the number of channels used to calculate the adjusted background (GammaVision® 2017).

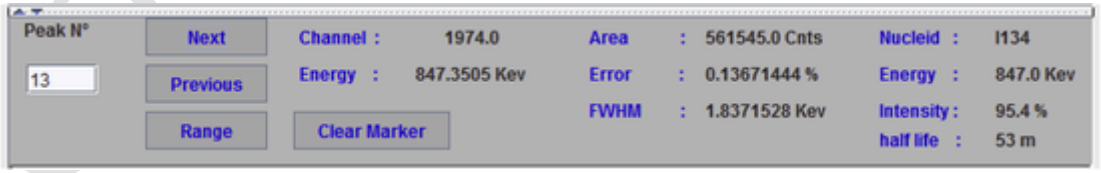
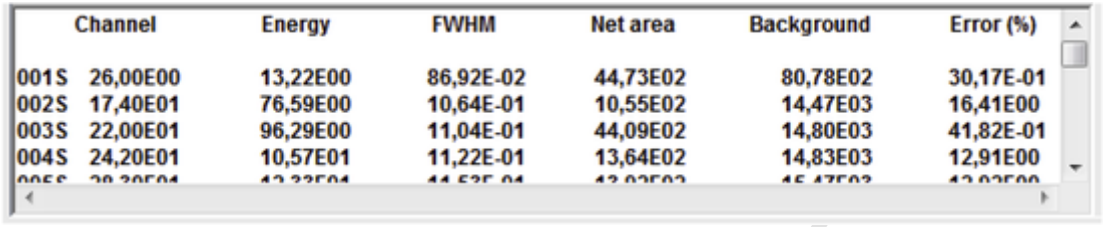


Fig. 12. Space for markers and analysis information.

The space for results (Fig. 13): This space is reserved for displaying the results of the analysis, including the spectrum data and identified peaks. The copy and cut options work, and the operator can delete or modify.



	Channel	Energy	FWHM	Net area	Background	Error (%)
001S	26,00E00	13,22E00	86,92E-02	44,73E02	80,78E02	30,17E-01
002S	17,40E01	76,59E00	10,64E-01	10,55E02	14,47E03	16,41E00
003S	22,00E01	96,29E00	11,04E-01	44,09E02	14,80E03	41,82E-01
004S	24,20E01	10,57E01	11,22E-01	13,64E02	14,83E03	12,91E00

Fig. 13. Space for the results.

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