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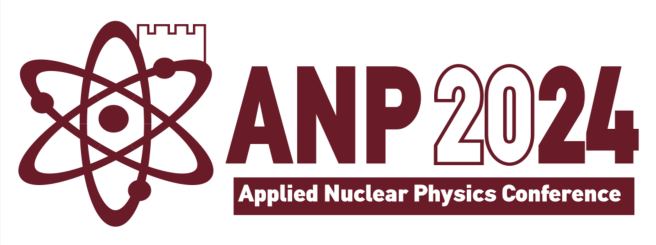

Development of an automated method for analysis of environmental gamma spectra collected with HPGe detectors

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Development of an automated method for the analysis of environmental gamma spectra collected with HPGe detectors

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Abstract Gamma ray spectrometry is one of the most valuable tools in interdisciplinary research work based on radioactivity. Although a multitude of software packages for gamma ray spectra analysis are available on a large scale, only a few of them are oriented towards environmental applications. To improve the investigation protocol, we designed software with features meant to respond to specific needs of archaeological and geological samples. We present a newly developed program meant to enhance precision with emphasis on the low energy part of the spectrum, including features such as autocalibration, especially with a focus on high-purity germanium detectors. The software was tested against commercially available packages for calibration and environmental sample spectra, providing very good results. The algorithm proved to be robust and efficient, while using simple procedures based on the physics of the interactions of interest. Currently our team is working on adding more functions albeit keeping the program user-friendly, before making it available online.

Keywords: Gamma spectrometry, environmental samples, interdisciplinary research, software development

INTRODUCTION

Interdisciplinary and environmental research often requires an accurate understanding of the radioactive processes involved in the samples to be studied. Among the dedicated experimental protocols, gamma ray analysis is the most widely spread and easy to use, still not uniformly straightforward in terms of result obtention [1-3]. The reasons behind this vary from sample preparation issues or detector calibration procedures, which often introduce a serious bias in the results, to the software for spectrum analysis, which is not always adapted to the situation; this paper addresses this particular need in terms of software. Indeed, there is always a trade-off between versatility and precision in specific situations, and our environmental samples (mainly geological and archaeological) are no exception, in the sense they require special attention for spectrum analysis, especially for the low energy part of the spectrum.

The software we are developing is called GaDeTool-Geo (acronym for Gamma Decision Tool Geoscience) and it is mostly meant to be used for spectra collected with High-Purity Germanium (HPGe) detectors, although any kind of detector with a linear response in energy suits. Several packages are widely available, from the ones developed by the main detector manufacturing companies, such as Ortec's Gamma Vision 32 [4], or Canberra's Genie 2000 [5] to the numerous solutions developed by universities or research institutes or NGOs such as InterSpec [6], Xtrack, open-source such as GSA [7], to cite only a few. However, the analysis of environmental sample spectra requires sometimes a lot of interventions from the user, which are time consuming and enhance the chances of human errors. What is needed here is a program which eliminates most of those issues, although it keeps the decisions on the human side. The first advantage is the self-calibration, which is independent on the calibration sources, on electronic parameters post the preamplification stage, and even on the source of the spectrum on a general ground, as all is needed is an ASCII file input containing the counts in each energy channel, without any other information. Then follows a series of features, such as flexible background channels selection in (semi)automated or manual mode, peak symmetrization procedure for the situations in which the peak shape is distorted and so on, as described in the next section.

MATERIALS AND METHODS

In order to obtain a simple, robust, still versatile tool, the first thing to establish was a minimum set of prerequisites for a minimized set of features which lead to a complete and accurate analysis of the spectrum. For the vast majority of the detection systems used in gamma interdisciplinary spectroscopy, the detector parameters are clear and stable, the preamp circuit is stable, but while performing *in situ* spectrometry, one can encounter instabilities in terms of energy calibration due to vibrations, temperature changes and any other parameters that may influence electronics for signal analysis. Additionally, it is not unusual to stand in need of comparing spectra which were not calibrated, or were calibrated with different sources in different setups, so that little changes on the energy axis may lead to a different interpretation of the data, especially if the user is not an expert.

Consequently, the purpose is to have a tool which autocalibrates the spectrum in first place. This is achieved in the simplest and most natural way possible: any environmental sample contains elements such as elements of the U series, Th series, ^{40}K and some β^+ emitters; those lead to clearly set energies in the spectrum, which are given by parameters depending solely on nuclear structure (or the annihilation energy). This means the ratios of some well-known pairs of energies present in the spectrum will be approximately the same as the ratios of some pairs of centroids (expressed in channels) from the linear part of the plot. In other words, by making use of two pairs of energies, e.g. 1460 keV of ^{40}K, 2614 keV of ^{208}Tl and 511 keV for an omnipresent annihilation peak, a linear regression provides the calibration curve for the high energies. A second step is to convolute with the lower part, as most likely this straight line would not lead towards 0 keV for channel 0, and to make use for example of the U-Ra 186 keV peak and some low energy Thorium lines, of which energy ratios will slightly bend the slope in order to correct the curve towards the origin.

The predefined algorithms are simple and clear, and they allow the user to change different parameters, according to their needs (if the full widths at half-maximum (FWHM), are unusual, or if background variations are severe), although this time the user has to be skilled for data analysis and interpretation. For most gamma software packages, the graphical user interface is a complex one, and often involves interaction with databases which provide precise energies, but which do not match perfectly spectrum calibration - or worse, assign radionuclides which have very close energies, but actually have nothing to do with the sample under analysis. The approach here was to identify all the natural and the usual, well-known anthropogenic emitters in the automated process, and then let the spectrometrist decide what to assign further.

The code was written in Python, based on the principle "less is more", in the sense the algorithms involve strictly necessary data and provide strictly necessary output: peak centroid in keV, peak area, radioelement identification for the usual ones, and FWHM. Scanning the spectrum is performed with a minimum of operations, a single time, right and left of the global maximum, once the latter is identified. One particularity of this software is that in its default operating mode peak areas are calculated just over half-height. This is done while assuming the event distribution is Gaussian and then the result is divided by 0.761, which is the numerical integration result for a normal distribution considering a unit total area. The reason behind this is the more the analysed channels are distanced from the centroid, the less the information they contain is relevant, as they may be affected by Compton interactions (left side of the peak), true coincidence summing with soft X-rays (right side) and various background effects. In case of significant deviation of the peak FWHM or anomalous background (e.g. higher background on the high energy side of the peak), the code asks for human decision; this is useful mostly at low energies. The main logic steps involved are as follows:

- reading the input file (ASCII);
- selection of the global maximum from the histogram;
- finding the next maximum on the right and left side;

- finding the background areas for left and right of the global maximum;
- deleting analysed channels from the search list and consider the next local maxima as global for their areas;
- calculation of the typical FWHM and reiteration till search intervals are comparable;
- peak centroid assignment;
- regression for energy calibration;
- plotting the spectrum;
- peak energy assignment and area calculation;
- printing analysis report.

RESULTS AND DISCUSSION

The algorithm structure for this software consists of four main functions that perform the stages of the analysis, facilitating the understanding and optimal maintenance of the code. There is a function for eliminating successive descending channels near the identified maxima from the search interval, a function for identifying next local maxima and peaks in the spectrum, a function dedicated to identifying the centers of the peaks based on the difference between the average background levels, and a function for identifying the peaks corresponding to predefined energy ratios depending strictly on the associated nuclear disintegration schemes which allows a precise calibration.

The secondary functions are used for plotting the spectrum, displaying the peaks, finding the coefficients of the calibration equation, calculating peak areas, full widths at half-maximum and uncertainties. All of them are implemented from the Python libraries and recalled recursively for each iteration, allowing calibration, peak identification and calculations.

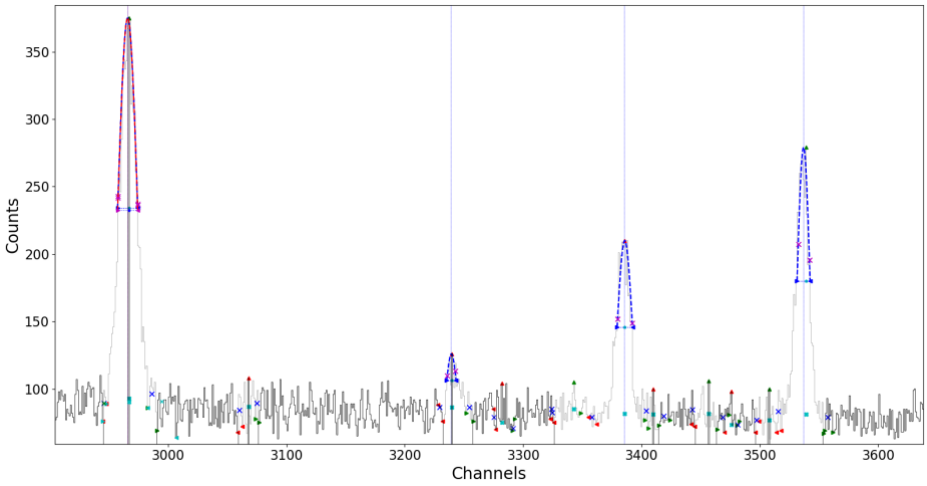

Figure 1. *Peak analysis over half height in GaDeTool. Channel number on the horizontal axis shows the energy in some 0.17 keV per unit; the markers are automatically assigned to local min/max analysis*

The user does not have to set any regions of interest (ROIs), unless a particular energy is sought for, and the centroid for the latter is not automatically assigned (generally a matter of detection limit). Peak identification is always successful for the natural series and common anthropogenic radionuclides (e.g. ^{137}Cs). The code was tested on environmental gamma spectra against commercial packages, providing overall the best results in poor statistics. The criterion for deviation from the best calculated value was comparison with manual analysis, performed channel by channel. In case anything is unclear in the analysis procedure, the code asks for human decision. Before making GaDeTool available online, the steps to be further validated are the peak symmetrization procedure, the automated detector type identification (particular p- or n-type HPGe), reporting potential reasons for anomalous peak width and

certain ratios of peak areas in order to help ^{210}Pb dating procedures -as a lot of samples under analysis in this field originate from sediment cores. Fig. 1 displays an example of peak analysis over half height as shown by the software GUI. One important advantage of such software solutions is the fact automated calibration reduces the time for analysis in a significant manner, which is of great benefit for batches of samples measured in different laboratories. This will also allow handling the data and its uncertainty calculation by a very small group, ensuring unitary protocols.

CONCLUSIONS

The proposed program was designed to perform automatic energy calibration, by recursively using predefined functions and energy ratios which are independent of the sample, shielding, electronics or detector type, as long as the latter has a quasi-linear response with respect to the incident gamma ray energy. Subsequent peak identification, area and peak width calculations provided results in very good agreement with the expected values, with a notable performance for low energies and poor statistics.

Several protocols currently under validation will be added to the code in order to return more than just peak areas, namely additional information on peak FWHM and shape, the reasons behind it, and potential clues for dedicated environmental analysis procedures. All the resulting data requires just a simple ASCII input, without the need of ROI selection from the user side. The goal is to make it available online, first for free testing of environmental sample spectrum analysis, then for sediment database building of geological, biological or archaeological sample investigation.

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