LIBRARIAN DRIVEN ANALYSIS OF GAMMA RAY SPECTRA

V. Kondrashov
Drew University,
Los Angeles, California, United States of America

I. Petersone
Ellat,
Riga, Latvia

Abstract. For a set of *a priori* given radionuclides extracted from a general nuclide data library, the authors use median estimates of the gamma-peak areas and estimates of their errors to produce a list of possible radionuclides matching gamma ray line(s). The identification of a given radionuclide is obtained by searching for a match with the energy information of a database. This procedure is performed in an interactive graphic mode by markers that superimpose, on the spectral data, the energy information and yields provided by a general gamma ray data library. This library of experimental data includes approximately 17,000 gamma ray energy lines related to 756 known gamma emitter radionuclides listed by the ICRP.

Introduction

At present there are two different approaches to gamma ray spectra processing. The first approach is based on a traditional peak search routine [1], and the second one on a so-called "librarian" routine. Our approach falls into the second category. The two different approaches are driven by the requirements of two major groups of tasks. The first group deals with analysis of any gamma spectra with randomly distributed gamma peak locations on the energy axis. For example, observations of gamma spectra obtained from any astrophysical experiment, from satellite observations of gamma bursts or gamma-sources on Earth surface, etc. In this case, we have to fix the gamma ray peaks automatically by a routine such as peak-search, by calculating the first or second derivatives from the spectrum acquired with multichannel analyser. The other group is related to the need to identify gamma ray emitting nuclides. In this case peak locations are not distributed randomly but instead they depend on the set of isotopes. Of course, it would be useful to know this set *a priori*. In that is the case, it would not be necessary to check the full energy region for peak locations. This means that we can reduce the number of regions of interest in any real spectrum emitted by radioisotopes.

For the librarian approach, energy calibration should be sufficiently good in a way that deviation between any reference energy and one calculated from the calibration curve should be within one or two channels for the full energy region under scrutiny. Suppose we have a gamma ray line with reference value energy E. From our energy-channel calibration curve we can calculate the line position N_E expressed in channels. Following our assumption, we can accept only calibrations with maximum deviation of about FWHM/2 in real line position. This means that we have a real line location within $N_E \pm \Delta$, where Δ is about FWHM/2 for a gain normally within 0.3-0.7 keV/ch. By using this curve we can estimate a line position with accuracy ±500 keV/ch, but that is not enough for reliable nuclides identification.

To adjust the line \ peak \ position we could apply any standard fitting procedures - for example fitting this region by an iterative least-squares procedure using Gaussian shape for the peak area and a linear function for the background representation. In this way we can simultaneously estimate peak parameters more precisely, but that is valid only for peaks with good (just near Gaussian) shape and/or good statistics. To decrease the influence of some distortion factors such as outliners, peak position drift, overlapping with another peaks, etc. it would be reasonable to decrease the number of peak parameters (including those of the background) under scrutiny. We can evaluate resolution as a function of energy by creating the resolution-energy dependence from the calibration routine. Due to the complexity of real spectra we sometimes loose convergence of the iteration procedure. To

overcome these difficulties and adjust the peak position on the analysis interval we apply the median estimate of net peak area with simultaneous calculation of area's dispersion [2,3]. As the reader can see from the above explanation, our approach is based on the interaction of the database of nuclides with spectra processing. The approach has been implemented into the codes DIMEN [2] and WinDIMEN [4] for isotope identification and quantification.

Median estimate formalism

The definition of the median estimate and the method for its evaluation for gamma-lines processing can be found in [2], while more details on multiplet deconvolution is given in [3]. Only brief introduction to the method will be given here. The central point is to find a more effective way to develop an elementary estimates population that is as large as possible. Our choice is the method of *finite differences* [3], because in this way we can eliminate (or substantially reduce) a linear background influence and obtain a large number of elementary estimates on the Region of Interest (ROI) selected.

We denote the *second finite difference* of any discrete function f_i as:

$$\Delta^{(2)} f_i = f_{i+2p} - 2f_{i+p} + f_i \tag{1}$$

where, $i \in (i_1, i_2)$, i_1 and i_2 are initial and final numbers of f_i realization, p - is an integer size step for a second finite difference.

We will use the following terms and definitions:

- G_{ij} - the Gaussian function (which represents the gamma peak shape) for i -th channel and j -th peak in multiplet on ROI selected, j=1 in the case of a single peak.
- S_j - net area of j -th peak.
- B_i - linear background in the i -th channel on ROI selected. The background for the entire spectrum can be considered as a set of consecutive linear functions.

The number of pulses in the ROI within $i \in (i_1, i_2)$ is:

$$\|Y_i\| = \|G_{ij}\| \|S_j\|^T + \|B_i\| + \|\xi_i\| \tag{2}$$

where, $\|Y_i\|$, $\|S_j\|$, $\|B_i\|$ and $\|\xi_i\|$ are column matrices with size $[n \times 1]$ and $\|G_{ij}\|$ is a matrix with size $[n \times m]$, $n = i_2 - i_1 + 1$ - number of ROI's channels and m -numbers of peaks in the multiplet.
ξ_i - is the error of measurement in the i -th channel, which in general is not described by the Gaussian distribution, but has limited dispersion and a mean value equals to zero.
In order to eliminate the linear background, the second finite difference has been applied for Y_i:

$$\|\Delta^{(2)} Y_i\| = \|\Delta^{(2)} G_{ij}\| \|S_j\|^T + \|\Delta^{(2)} \xi_i\| \tag{3}$$

To obtain one elementary estimate for peak area we need m second differences. We can get the total set of elementary estimates by choosing different combinations of m second differences from the full set of second finite differences.

To achieve the maximum number of second finite differences we can vary the step size of the second difference from p=1 to $p = \text{int}[n/3] + 1$. For example, the total number of elementary estimates (or combinations) for p=1 is [3]:

$$L = \frac{(i_2 - i_1 - 1)!}{m!(i_2 - i_1 - 1 - m)!} \tag{4}$$

Following [3] we can represent the matrix of net peak area elementary estimates as:

$$\left\| S_j \right\|_l = \left\| \Delta^{(2)} G_{i(k)j} \right\|^{-1} \left\| \Delta^{(2)} Y_{i(k)} \right\| \tag{5}$$

where $i(k) \in (i_1, i_2)$ and $k \in (1, m)$, l is the l -th combination by m elements on the full set of finite differences for any specified step size p.

Finally, we can express the median estimate of j -th peak area $\widetilde{S}_j$:

$$\left\| \widetilde{S}_j \right\| = \underset{L}{med} \left\| S_j \right\|_l \tag{6}$$

where $l \in (1, L)$ or more detailed form:

$$\left\| \widetilde{S}_j \right\| = \underset{L}{med} \left(\left\| \Delta^{(2)} G_{i(k)j} \right\|^{-1} \left\| \Delta^{(2)} Y_{i(k)} \right\| \right)_l \tag{7}$$

We can easily reduce the last formula for singlet and doublet, where:

singlet:
$$S_{1S} = \underset{L}{med} \left(\frac{\Delta^{(2)} Y_{i(1)}}{\Delta^{(2)} G_{i(1)1}} \right) \tag{8}$$

doublet (first peak):
$$\widetilde{S}_{1D} = \left[\frac{\dfrac{\Delta^{(2)} Y_{i(1)}}{\Delta^{(2)} G_{i(1)2}} - \dfrac{\Delta^{(2)} Y_{i(2)}}{\Delta^{(2)} G_{i(2)2}}}{\dfrac{\Delta^{(2)} G_{i(1)1}}{\Delta^{(2)} G_{i(1)2}} - \dfrac{\Delta^{(2)} G_{i(2)1}}{\Delta^{(2)} G_{i(2)2}}} \right] \tag{9}$$

Implementation of the library driven analysis with a graphic user interface as a Windows application

The software package DIMEN, originally developed in Riga Research Radioisotope Institute (Latvia) by V.S. Kondrashov and Z.D. Moroz and initially contributed to Radiation Shielding Information Center (RSIC) at Oak Ridge National Laboratory (USA) in 1996, has been modified and transformed.

The identification of a given radionuclide is obtained by searching for a match with the energy information of a database. This procedure is performed in an interactive graphic mode by markers that superimpose, on the experimental spectra data, the energy information provided by a previously elaborated data library. This library of gamma- and x rays data includes 16712 gamma ray energy lines related to 756 known gamma emitter radioisotopes (749 currently listed by the ICRP and new 7 by C.Lederer and V.Shiriey ,Table of Isotopes , 7th edn.,1978).

Since DIMEN has been originally developed on Pascal programming language it looks naturally to make above mentioned transformation to Windows environment by object-oriented software platform DELPHI. The translation of analytical part of DIMEN has been mainly carried out by replacing the DOS-functions by the similar Windows-functions and adapting all DIMEN's

algorithms to the new Windows environment. The most significant transformation has been done to create the Graphic User Interface by developing the Main Graphic Window of WinDIMEN. WinDIMEN has been programmed by using the Borland Delphi Professional, Version 4.0 (Build 5.104) Update Pack 2, and Borland Delphi 4.0 for Windows 98,95 and NT. Minimal Computer Requirements are: PC-based machine, 486-processor (100 MHz), 16 Kb RAM, 1 Gb HDD. O/S: Windows 98,95 or NT.

GUI description

The translation of the Analytical part of DIMEN was realized by replacing DOS-functions with similar Windows-functions and adapting all of DIMEN's algorithms to the new Windows environment.

A view of the GUI is shown on the Figure 1.

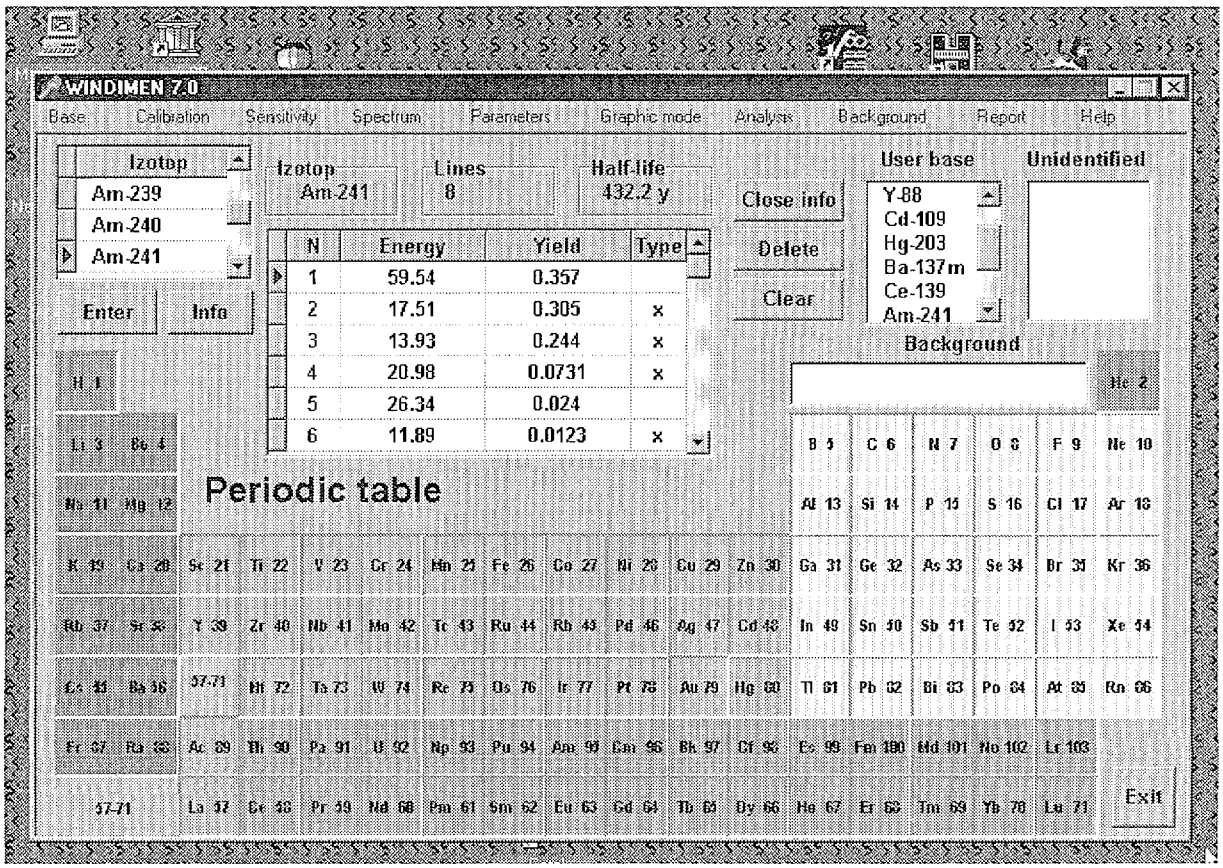

Fig. 1. Main Graphical User Interface (GUI) for WinDIMEN.

The main field of the User Interface is the Periodic Table of Elements. By clicking the left mouse button on the chosen element, the user displays all gamma ray emitted isotopes contained in the WinDIMEN Library in the upper left window. For user reference, the gamma ray lines (energies and yields) of these isotopes are shown in a separate window. On the top of GUI window the reader can find the pop-up menu, which performs the main WinDIMEN's functions and options.

The program has the following steps:

1. Create a nuclide table (user base) according to the preliminary information for the spectrum to be identified.

2. Energy calibration (processing of calibrated peaks and computation of the parameters of the curve "channel number-energy"). The calibration parameters can be kept in a file and then used to process other spectra of the given run. Calibration is recommended before the beginning of each run of measurements by using the spectrum GUI window, see Figure 2.
3. Calibration with respect to absolute sensitivity (efficiency calibration).
4. Processing of the background and storing its parameters to a file.
5. Direct processing of analysed spectrum: identification of analysed lines, computation of peak areas and activities, accounting for the background, printing of the output data.

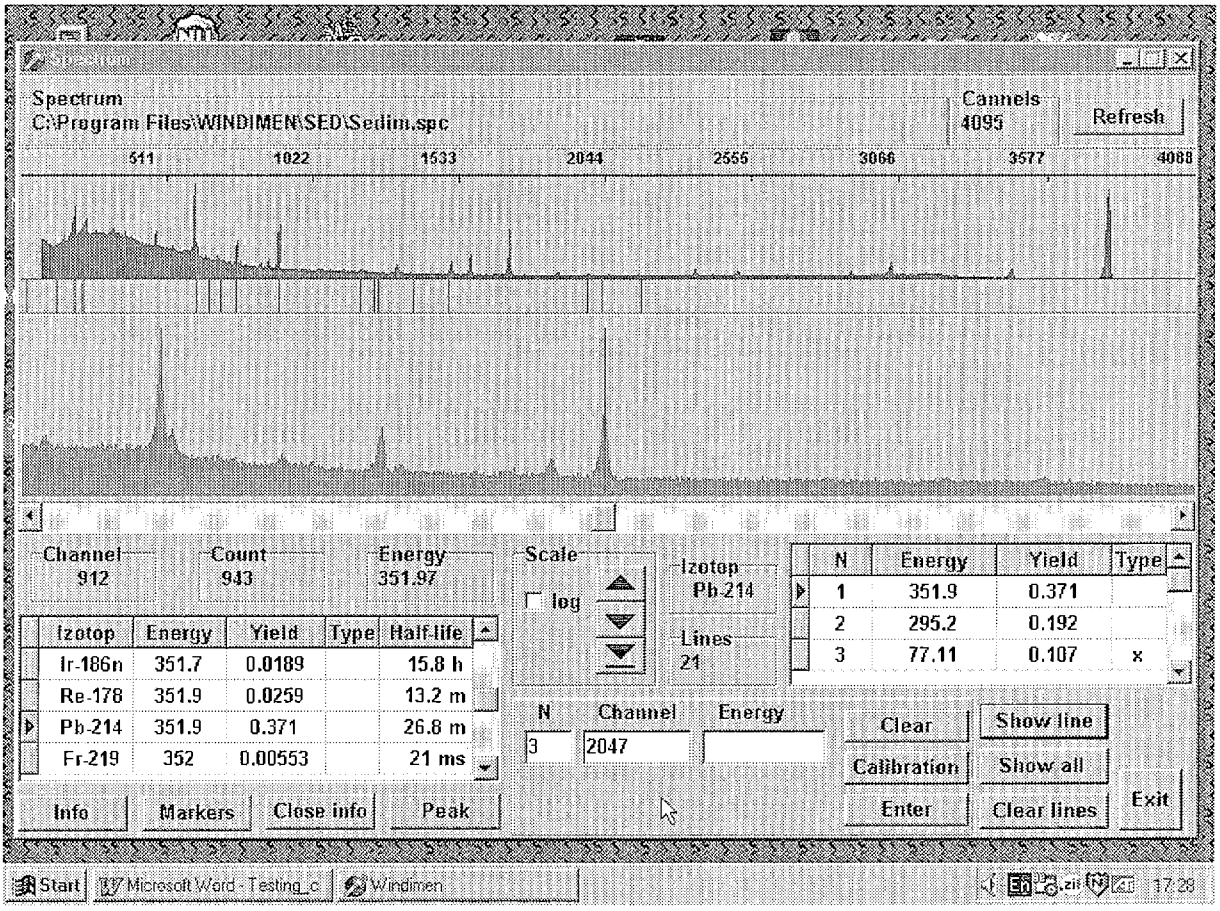

Fig. 2. The spectrum GUI window.

The WinDIMEN reads spectra in two formats: binary (Canberra format) and ASCII (common text format). It reads main parameters such as the file name, energy range, spectrum collecting time, measurement date, probe number, probe mass. Interaction time between WinDIMEN's Data Base and the main program has been optimised and typical program running time is less then for DOS DIMEN version.

Co-operation between the two packages WinDIMEN and ANGES has been elaborated.

- both program use the same spectrum format.
- WinDIMEN graphics option was modified under ANGES spectra performance.
- WinDIMEN can use common ANGES's utilities: energy calibration and efficiency calibration .

In co-operation with National Environmental Health Center in Latvia we have been included in the intercomparison exercise in the BOK 1.1 sub-project, under the Nordic Nuclear Safety Research Programme for 1998-2002, together with a total of 35 laboratories from another countries [5]. The results of intercomparison were discussed at the meeting in Skagen. In the December 2000 the results

of the intercomparison were distributed as NKS-19, ISBN 87-7893-069-3. The intecomparison confirmed that our approach provides a convenient and rapid solution for identifying and quantifying radioisotopes by gamma ray spectra analysis.

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