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DEVELOPMENT OF SOFTWARE FOR THE DETERMINATION OF GAMMA-RAY DETECTION EFFICIENCY

Antônio C. O. da Silva, Frederico A. Genezini and Guilherme S. Zahn

Instituto de Pesquisas Energéticas e Nucleares, IPEN - CNEN/SP
Av. Professor Lineu Prestes 2242
05508-000 São Paulo, SP
antonio.carlos.silva@usp.br

ABSTRACT

Gamma spectrometry is frequently used as a tool in analytical chemistry or environmental analyses. The efficiency of the detection setup is one of most important steps of the analyses, but users don't always calculate their own efficiency curve because this procedure is not trivial, and therefore they adapt their measurement geometry to work in a setup that has been previously calibrated, which will often cause limitations. In order to solve this problem, a software was developed that helps a non-experienced user to compute the detection efficiency curve and to determine the detection efficiency at a given gamma-ray energy.

1. INTRODUCTION

The difficulty for the determination of efficiency curves for geometries in a very specific experimental arrangement leads many users of gamma spectroscopy to use pre-determined curves, which sometimes are not very similar to those that best represent the experiment. Due to this a software has been developed to make the fitting of the efficiency function easier. The main purpose of this software is fitting efficiency functions for gamma spectroscopy measurements. Today, there is plenty of mathematical software for this work, but they are too generic and require previous knowledge of fitting methods or even programming skills.

The objective of this work is to develop a software specifically for fitting efficiency functions, making the interface simpler, especially for users who do not have knowledge that other programs require, as programming of computers.

Additional tools are also available, like interpolation using the covariance matrix of parameters and corrections for large sources. A database with some fitted parameters according to the source and detector geometry is also implemented, in order to help the users in choosing initial values for the fit parameters - users are only required to choose the features of their experimental setup and sensible initial parameters for the fit are loaded from this database. Alternatively, the initial values for the fit can also be determined using the gradient method [1]. The fitted curve can be graphically displayed in the screen and saved in disk as an image file.

2. METHODOLOGY

The chosen language for the software development was the Visual Basic .NET framework because this is a language where a friendly environment for a non-technical user can be easily created.

The Gauss-Marquardt [2] method was used for fitting the efficiency functions; this method is known for its fast convergence when good initial parameters are used. The partial derivatives of the functions that are necessary for the method are obtained using Richardson extrapolation [3].

There is a bank of efficiency functions [4-9] for users to choose from when fitting their data, according to the energy range of interest; the user can see the function and a brief description of its characteristics, like who proposed it or its useful range of energy.

To help the user in the choice of initial parameters for the fit, a bank of parameters is being assembled by measuring detection efficiencies with several experimental setups with different detectors and source-detector distance. This bank can be continuously fed by the users.

After the fitting process, its quality can be checked by chi-square and users can view the fitted function in a two-dimensional graph where uncertainty bars are added to the experimental points and this figure can be exported as a graphic file in one of the formats supported by the Visual Basic libraries (jpg, bmp, png, etc.).

Users have the option to fit the data using instrumental uncertainties in both the independent and dependent variables (Y, X), or only in Y. The software uses the covariance matrix in the interpolation process thereby enabling these interpolated data to have correctly calculated uncertainties.

An additional tool of the software is the calculation of solid angle and self-absorption corrections, which make the transference of the geometry used in the efficiency calibration (often using a punctual source) to the interest geometry. The solid angle is corrected by a Monte Carlo simulation and the self-absorption by an analytical calculus, using Eq. 1, obtained by Taylor expansion of the usual self-absorption expression [10], considering the hypotheses of μ(E)H is small and superior order terms do not contribute significantly:

$$\varepsilon_{large}(E) = \varepsilon_{puntual}(E)\,\exp[-\mu(E)\rho H/2] \tag{1}$$

where ε_{large} is the corrected efficiency, $\varepsilon_{punctual}$ is the efficiency measured with a punctual source, μ(E) is the mass attenuation coefficient, obtained from XCOM database [11], and ρ is the density of the source material and H is the height of the source.

To provide for the case when the user wants to fit a simpler function where (linear in the parameters), which is not the generally case of the efficiency functions, the option to use the least squares method was also made available.

Figure 1 shows a snapshot of the software after a fit was performed.

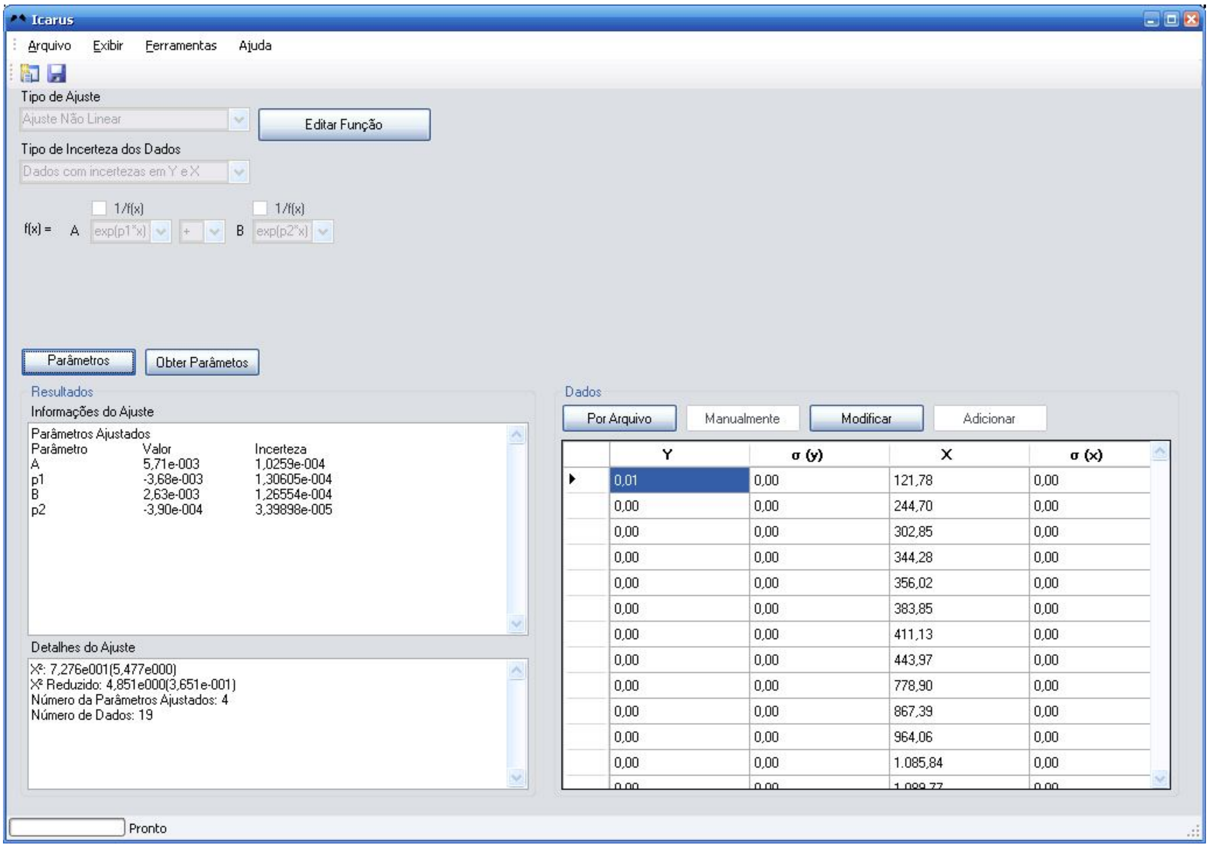

Figure 1. Snapshot of the software screen shown after the fitting process: data, parameters, function and chi-square.

3. RESULTS AND DISCUSSION

To check the reliability and feasibility of the software fit, efficiency data from an HPGe detector (60%) measured using a ^{152}Eu standard point source at 17 cm from the detector end cup was fitted to one of the efficiency functions proposed. The same function was fitted using the MatLab platform as a benchmark, and the solid angle correction was verified using a measurement with a large source and comparing the values corrected by the software to the known activity of the source.

3.1 Fit Example

The peaks from the gamma ray spectrum were fitted using the software IDeFix [12]. The calculated efficiencies were then fitted using a suitable function for the energy range used [13], shown in Eq. 2.

$$\varepsilon(E) = Ae^{p1 \cdot E} + Be^{p2 \cdot E} \tag{2}$$

In Table 1 the four fitted parameters are presented, together with the reduced chi-square and the results obtained in the MatLab fit. The results were identical, but the reduced chi-square was slightly different; this may be due to truncation effects, but will be further investigated.

Table 1. Fitted parameters and uncertainties

Parameters	Software	Matlab
X^2	4.85	4.68
A	0.00571(10)	0.00571(10)
p1	-0.00368(13)	-0.00368 (13)
B	0.00263(13)	0.00263 (13)
p2	-0.00039(03)	-0.00039 (03)

Chi-square and parameters fitted in Matlab and in the Software for the efficiency curve shown in the equation (2).

In Fig. 2 the graph of the fit is shown. The axes and the legend can be easily changed by the user, and the graph can also be seen in logarithmic scales.

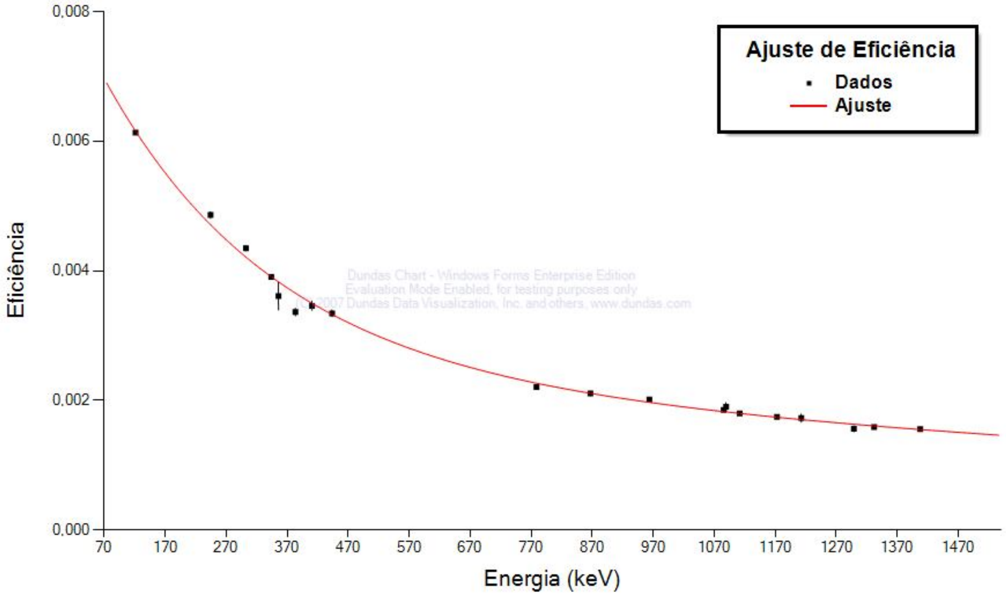

Figure 2. Graph obtained by data fitting of efficiency function.

The solid angle correction was checked by comparing a measurement made with a large source (diameter=50 mm and height=10 mm) with a measurement made with a punctual source and then corrected by software. A small energy range was chosen and the Z-Score test was applied. The default of the program is to run five simulations with $5x10^6$ events each and to get the mean and standard deviation of them. The correction calculated for this test was 0.92878(08). Table 2 contains the results of this test, where were used punctual and large ^{152}Eu standard source. In order to avoid self-absorption effects the low-energy photons were not used. The results obtained from punctual source with the correction calculated by the software led to good agreement with the large source efficiency.

Table 2. Results of the solid angle correction test

Energy (keV)	Efficiency ($x10^{-3}$) Large source	Efficiency ($x10^{-3}$) Punctual source	Efficiency ($x10^{-3}$) Corrected	Z-Score
778.9	2.502 (25)	2.58 (06)	2.40 (06)	-1.6
867.4	2.16 (05)	2.40 (11)	2.23 (11)	0.6
964.1	2.163 (28)	2.24 (05)	2.08 (05)	-1.4
1085.8	2.030 (29)	2.11 (05)	1.96 (05)	-1.2
1089.8	2.14 (09)	2.162 (13)	2.01 (12)	-0.9
1112.1	2.023 (20)	2.08 (04)	1.935 (36)	-2.1
1213.0	1.90 (11)	1.90 (12)	1.77 (11)	-0.9
1299.2	1.73 (07)	1.85 (10)	1.72 (09)	-0.10
1408.0	1.6730 (14)	1.749 (24)	1.625 (22)	-2.2

4. CONCLUSIONS

The software presented in this paper can be of a great help in assisting non-experienced users in the process of correctly determining the detection efficiency of the experimental setup. The fitting algorithm was checked against a well-established algorithm developed in the MatLab platform, and the results were in perfect agreement. The correction for large samples was checked experimentally, also with good results.

The next steps in the development of this software are testing the self-absorption correction, expanding the database of initial parameters, and checking the fits for the other fitting functions.

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