

## A package for gamma-ray spectrum analysis and routine neutron activation analysis

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**Abstract.** A package for gamma spectrum analysis (PGSA) was developed using object-oriented Borland C++ design for MS-windows. This package consists of five programs which can be used for gamma-ray spectrum analysis and routine neutron activation analysis. The advantages of PGSA are its simple algorithms and its need for only minimum amount of input information.

**Keywords.** Gamma spectrum analysis; neutron activation analysis; nuclide identification; elemental concentration.

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### 1. Introduction

In the early 1990s the Experimental Nuclear Physics Department focused its attention towards investigating neutron activation analysis (NAA) using 14 MeV neutron generator and radioactive neutron sources (Am-Br). From that period the conditions of the measuring technique have changed and the computer systems have become faster and more precise. So the analysis programs should be qualified to meet the new conditions.

The PGSA package was designed to analyse gamma-ray spectra detected by germanium detectors. The sequence of operations of all programs is shown in figure 1. It consists of the following programs:

- Gamma wavelet transform model (GWTM.EXE);
- Gamma identification model (GIM.EXE);
- Concentration gamma model (CGM.EXE);
- Neutron flux calculation code (NFC.EXE);
- Detector efficiency calculation code (EFF.EXE);
- Library of isotopes produced when the sample is irradiated by a neutron beam for a short time (from seconds to hours) (SHORT.LIB);

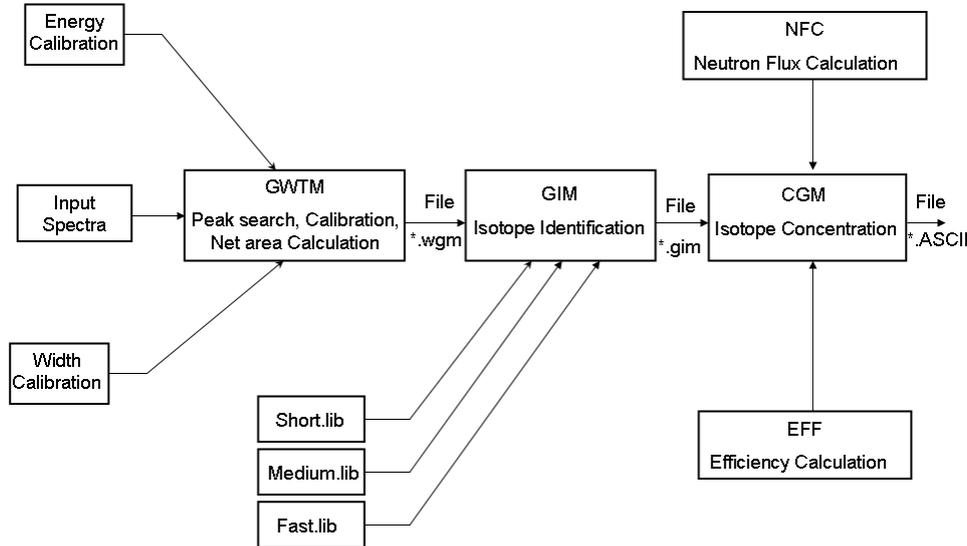


Figure 1. Sequence of operations in PGSA package.

- Library of isotopes produced when the sample is irradiated by a neutron beam for medium time (from hours to a few days) (MEDIUM.LIB);
- Library of isotopes produced when the sample is irradiated by a neutron beam for a long time, more than few days (LONG.LIB).

## 2. Gamma wavelet transform model (GWTM)

It was designed to analyse a gamma-ray spectrum to determine the position, gamma-ray energy, width and area of each peak component.

### 2.1 Energy and width calibration

GWTM code reads several gamma-ray lines with their energies and centroids or widths and then a least-squares fit is done for every  $(x_i, y_i)$  data points to obtain fitting coefficients. This method will distribute the deviations between the actual and computed energies more uniformly and also will reduce the sensitivity of the results to the particular choice of peaks and their location in the spectrum. The fitting coefficients are calculated as

$$\sum_{n=0}^N \left( \sum_{i=1}^M x_i^{n+k} \right) a_n = \sum_{i=1}^M x_i^k y_i, \quad k = 0, 1, 2, 3, \dots, N, \quad (1)$$

where  $M$  is the number of data points. Equation (1) can be rewritten in more detail as

$$\begin{pmatrix} M & \sum_{i=1}^N x_i & \sum_{i=1}^N x_i^2 & \dots & \sum_{i=1}^N x_i^N \\ \sum_{i=1}^N x_i & \sum_{i=1}^N x_i^2 & \sum_{i=1}^N x_i^3 & \dots & \sum_{i=1}^N x_i^{N+1} \\ \sum_{i=1}^N x_i^N & \sum_{i=1}^N x_i^{N+1} & \sum_{i=1}^N x_i^{N+2} & \dots & \sum_{i=1}^N x_i^{2N} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \dots \\ \dots \\ a_N \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^N y_i \\ \sum_{i=1}^N y_i x_i \\ \dots \\ \sum_{i=1}^N y_i x_i^N \end{pmatrix}. \quad (2)$$

The coefficients,  $a_n$ ,  $n = 0, 1, 2, 3, \dots, N$  are determined by solving eq. (2) using Gauss elimination.

### 2.2 Peak search

The first main operation in analyzing gamma spectra is peak searching. Several methods have been developed for peak search [1,2].

The searching method of GWTM depends on wavelet theory for analyzing signals [3,4]. Since any spectrum is often discrete, its discrete form of wavelet transform is necessarily used, which can be expressed as [5]:

$$W_\Psi(a, b) = \frac{1}{N} \frac{1}{\sqrt{|a|}} \sum_{i=1}^N \frac{1}{\sqrt{C_\Psi}} \Psi\left(\frac{i-b}{a}\right) \cdot A(i), \quad (3)$$

where  $\Psi\left(\frac{i-b}{a}\right)$  is the basis wavelet function,  $a$  and  $b$  are the dilation and translation parameters, with  $a > 0$  and  $b$  having arbitrary values,  $C_\Psi$  is a normalization constant and  $A(i)$  is the count number at channel  $i$ .

Since gamma spectra are in Gaussian shape it will be a good choice if the basis wavelet is from the family of Gauss functions. One of them is called Mexican Hat, which can be used for searching peaks in the investigated gamma spectra. Mathematically, this type of basis function can be written in the form,

$$\Psi(x) = (1 - x^2) \exp(-x^2/2). \quad (4)$$

Once the mother wavelet is chosen, the computation starts with different  $a$ , depending on the full-width at half-maximum (FWHM), and wavelet transform is computed for all values of  $a$ . The wavelet with scale  $a$  is then shifted towards the right by  $b$  amount. Each spectrum count is multiplied by the corresponding value of the wavelet function. This procedure is repeated until the wavelet reaches the end of the spectrum. This generates a spectrum in which the peaks are emphasized and the background is smoothed. When the process is completed, the sum of these products is then a point of the wavelet spectrum which is expressed as

$$W(a, b)f = \frac{1}{N} \frac{1}{\sqrt{|a|}} \sum_{i=1}^N \frac{1}{\sqrt{C_{\Psi}}} \left(1 - \frac{(i-b)^2}{a^2}\right) \exp\left[-\frac{(i-b)^2}{2a^2}\right] A(i). \quad (5)$$

The wavelet algorithm for searching peaks has an iterative process as follows:

1. Scanning the whole spectrum with arbitrary default values of the dilation parameter  $a$  equals FWHM/2.353 and the window width equals 3\*FWHM.
2. Evaluating peaks.
3. Repeating step 1 with the new generation of FWHM according to a width calibration function.
4. Selecting all peaks.

This algorithm can select all peak singlets or multiplets with a good sensitivity to avoid statistical fluctuations which are part of the spectral background. During the process of peak search, each consecutive peak is compared to its neighbor to see if a multiplet should be formed or not. If peaks  $i$  and  $i + 1$  satisfy the condition ( $X_{i+1} - X_i < P \cdot \text{FWHM}$ ), where  $X_i$  and  $X_{i+1}$  are centroid of peaks in units of channels, and  $P$  is a user selectable separation parameter, then they are considered to be part of the multiplet. When a 2-peak multiplet is found, the next inter-peak distance from peak  $i + 1$  to peak  $i + 2$  is checked in the same way until the condition is no longer satisfied.

### 2.3 Peak shape model

GWTM code theorizes a modified representation of the photopeak by the sum of two components, a Gauss function and low energy tailing function, which ride on a polynomial background. The exponential tail is joined smoothly to the Gaussian function; the function and its first derivative are continuous. The peak shape with low energy tailing has the form:

$$f(x_i) = \begin{cases} B_1 + B_2(x_i - X) + he^{\left(\frac{-(x_i - X)^2}{2\sigma^2}\right)}, & x_i > X - T \\ B_1 + B_2(x_i - X) + he^{\left(\frac{T(2x_i - 2X + T)}{2\sigma^2}\right)}, & x_i < X - T \end{cases}, \quad (6)$$

where  $f(x_i)$  is the value of the peak model function at channel  $x_i$ ,  $B_1$  is a constant in the continuum approximation,  $B_2$  is the slope in the continuum approximation,  $h$  is the height of the peak,  $X$  is the peak centroid,  $\sigma$  is the width of the Gaussian function, and  $T$  is the joining point of the additional tailing exponential. The value of tail parameter  $T$  has some effect on the peak. If the tail parameter is small, the tailing is quite pronounced.

#### 2.4 Peak area determination

The peak area is calculated using a linear least squares fit algorithm. The area of each photopeak is calculated from the best fit. In each case, the peak area may be expressed as

$$\Sigma_{\text{Total}} = \Sigma_{\text{Gauss}} + \Sigma_{\text{Tail}}. \quad (7)$$

The area under the Gaussian portion,  $\Sigma_{\text{Gauss}}$  is defined as

$$\Sigma_{\text{Gauss}} = \int_{X-T}^R h \exp \left[ -\frac{(x-X)^2}{2\sigma^2} \right] dx, \quad (8)$$

where  $h$  is the height of the peak,  $X$  is the peak centroid,  $\sigma$  is the width of the Gaussian function,  $T$  is the distance in channels for the tail, and  $R$  is the last channel of the peak in the right of the peak region of interest. The integration is calculated using the Gauss-quadrature integration technique [6].

$$\Sigma_{\text{Gauss}} = h\sigma\sqrt{2\pi}. \quad (9)$$

The area under the tail portion,  $\Sigma_{\text{Tail}}$ , is defined as

$$\Sigma_{\text{Tail}} = \int_L^{X-T} h \exp \left[ \frac{T(2x - 2X + T)}{2\sigma^2} \right] dx, \quad (10)$$

where  $L$  is the first channel of the peak in the left of the peak region of interest. The area under the tail portion,  $\Sigma_{\text{Tail}}$  is calculated by solving the integral in a closed form.

#### 2.5 Working with GWTM

To start working with GWTM without problems, all PGSA package should be installed in the hard disk. The main window of GWTM program consists of three main parts, menu bar, control bar and status bar as shown in figure 2.

The first step in the program is to do energy/channel and width calibration. It reads a data file containing the energy of each gamma-lines with their centroids. Then a least square fitting was done for the data to get the calibration equation. Width calibration is done automatically by the same way but the user can control it from the Setting Menu.

The second step is to import spectrum data for processing. We supported our program with different binary formats to be able to read various spectra. From File Menu, spectrum data can be read from the dialog window as shown in figure 3.

The third step is locating the peaks. The program can scan the whole spectra by using three types of wavelet functions, viz., Mexican Hat, Gauss and Morlet basis wavelet function. Each one of them makes filtering for peaks from background with different sensitives. From the Setting Menu, one can select one of them as shown in figure 4. After selecting the wavelet, user should choose from the Analyze Menu wavelet scanning to locate all peaks in the spectrum.

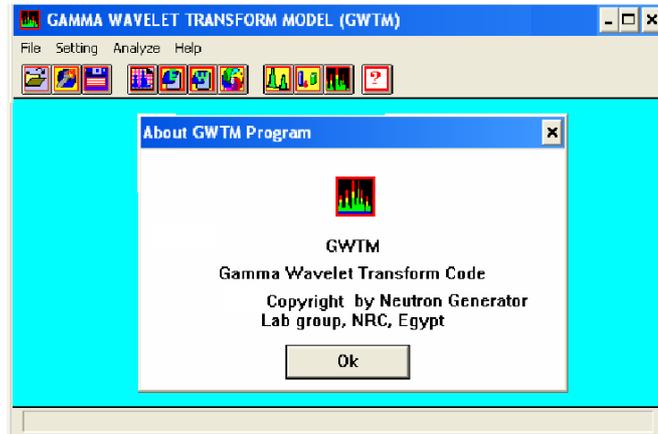


Figure 2. Main window of GWTM program.

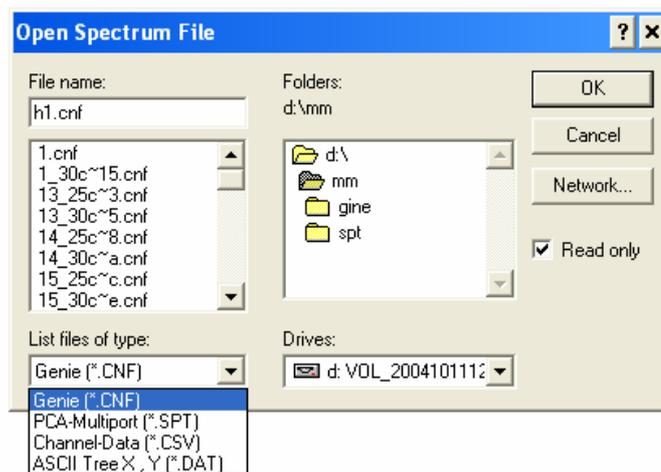


Figure 3. A dialog window in GWTM program for reading spectra.

The fourth step is calculating net area under peaks. GWTM has used two modified Gaussian models. The first model is a Gauss supported by exponential tail in the low energy side. The second model is a Gauss supported by two exponential tails, one of them in the low energy side and the other in the high energy side. It is recommended to use the double tail model in the case of high counting rate. The two modified Gaussian peak models are drawn in the dialog window as shown in figure 5.

Finally, the program can save the results in either of two forms. If the user wants more analysis for the spectrum it should be saved in a binary form (\*.wgm). This format is suitable for the next program GIM to read it. But if the user will not do more analysis, the data can be saved in ASCII form.

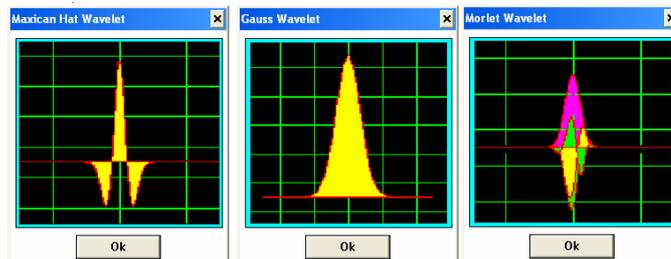


Figure 4. Dialog windows for all basis wavelets supported by GWTM program.

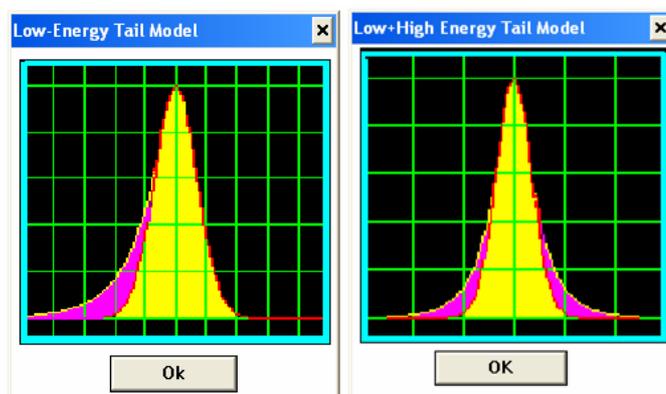


Figure 5. Dialog windows for peak area models supported by GWTM program.

### 3. Gamma identification model (GIM)

It was designed to identify peaks in the investigated spectrum. The nuclide identification procedure is started by comparing the energy of each spectrum peak with the energies of the gamma lines of all the nuclides in the gamma library. If a peak energy matches within a given tolerance with a gamma line energy of a library nuclide, it is possible that this nuclide is present and its other lines are checked. Note that only the spectrum peaks and library lines within the energy range analysed are considered. GIM program builds a matrix of possible identifications by comparing each nuclide in the analysis library against the observed peaks.

The library used in GIM code includes three data files. Every data file consists of a list of nuclei with their energies, intensities and half-lives. The first file is SHORT.LIB which is a library of isotopes produced when the sample is irradiated by a neutron beam for a short time (from seconds to hours). The second file is MEDIUM.LIB which is a library of isotopes produced when the sample is irradiated by a neutron beam for medium time (from hours to a few days). The third file is LONG.LIB which is a library of isotopes produced when the sample is irradiated by a neutron beam for a long time (more than few days).

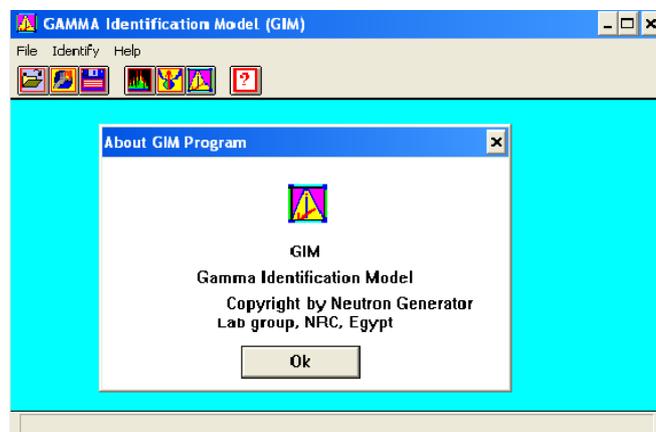


Figure 6. Main window of GIM program.

Index	Energy	Abund.	T1/2 (h)	Isotopes
1	77.60	17.10	18.60	PT197
2	94.70	3.58	2.30	DY165
3	320.00	93.00	0.10	TI51
4	388.50	83.00	2.80	SR87M
5	417.00	29.20	0.90	IN116M
6	442.70	16.00	0.40	I128
7	526.00	1.53	0.40	I128
8	617.70	6.63	0.30	BR80
9	640.40	0.23	0.30	BR80
10	665.70	1.10	0.30	BR80

Figure 7. Dialog window in GIM program for reading the library file SHORT.LIB.

The main window of GIM is shown in figure 6. The first step in the program is to read a file in binary form (\*.wgm) to get information about peaks under investigation such as energy, channel, width and net area. The second step is to read a library file for identification as shown in figure 7.

Finally the program can make identification for all peaks. It can save the results in two forms. If the user wants more analysis for the spectrum it should be saved in a binary form (\*.gim). This format is suitable for the next program CGM to read it. But if the user will not do more analysis, the data can be saved in ASCII form.

#### 4. Concentration gamma model (CGM)

Concentration gamma model (CGM) is designed for calculating the isotopic concentration of samples which are irradiated by neutron beam or natural radioactive samples. The code is used as the output file of GIM code. The elemental concentration of elements in a sample can be evaluated by using the activation analysis technique. The principle of activation analysis is to induce radioactivity in the element of interest. Decay products are then detected and identified by their energies while the decay rate is used to make a quantitative determination of the target element.

CGM code has the facility for calculating the elemental concentration of a sample by using absolute or comparator methods. The concentration of a certain element  $C$  within an irradiated sample can be obtained using absolute method from the activation equation:

$$C = \frac{P}{M_{SA} \left[ \frac{N_a \Omega}{M} \right] \Phi \sigma \varepsilon \Upsilon T_1 K_c K_w K_i}, \quad (11)$$

where  $P$  is the net peak area,  $M_{SA}$  is the mass of the foil,  $N_a$  is the Avogadro's number,  $\Omega$  is the isotopic abundance,  $M$  is the atomic weight of the foil element,  $\Phi$  is the neutron flux value,  $\sigma$  is the reaction cross-section,  $\varepsilon$  is the corrected detection efficiency at the peak energy,  $\Upsilon$  is the branching ratio of the peak energy,  $T_1$  is the live time of the collect in seconds,  $K_c$  is the counting correction factor for the nuclide decay,  $K_w$  is the waiting correction factor for the nuclide decay from the time the sample was obtained to the start of the measurement, and  $K_i$  is the irradiation correction factor. The correction time factors are calculated as

$$K_c = \frac{T_{1/2}}{\ln(2)t_c} \left[ 1 - \exp\left(-\frac{\ln(2)t_c}{T_{1/2}}\right) \right], \quad (12)$$

$$K_w = \exp\left(-\frac{\ln(2)t_w}{T_{1/2}}\right), \quad (13)$$

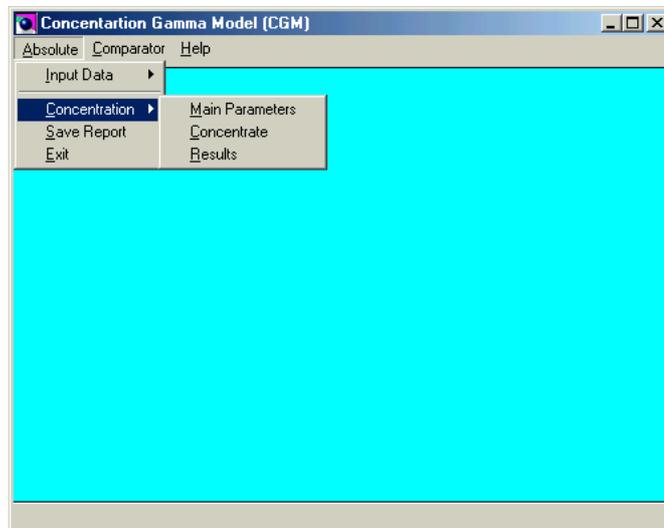
$$K_i = 1 - \exp\left(-\frac{\ln(2)t_i}{T_{1/2}}\right), \quad (14)$$

where  $T_{1/2}$  is the half-life of the nuclide,  $t_c$  is the elapsed real time during the measurement,  $t_w$  is the elapsed time to the beginning of the measurement, and  $t_i$  is the irradiation time.

In most applications, it is preferable to use a standard which contains the element which is to be determined. The elemental concentration ratio for standard and sample is

$$\frac{C_{ST}}{C_{SA}} = \frac{M_{SA} P_{ST}}{M_{ST} P_{SA}}. \quad (15)$$

This simple relationship is only valid if all the other factors are held constant. Obviously the cross-section, decay constants, atomic weights and isotopic abundances will be identical.



**Figure 8.** Main window of CGM program.

Even if the neutron flux is constant, the physical form of the standard must be the same as the unknown for the same flux to be seen by both the sample and standard.

Irradiation, decay and counting times must be constant too and the counting geometry should be identical if they are to have the same counting efficiency. It is more usual for some of the conditions to be the same but for others to be different and for corrections to be made to the appropriate factors.

When standards are used for comparison with unknown samples, there are very few corrections to be made. If the activation conditions are the same and they are counted on the same detector, then usually the only corrections are for different decay periods prior to counting and a flux correction due to irradiation position. Therefore, when the samples and standards are irradiated together, corrections are made for flux variation and decay time, but all other conditions remain constant.

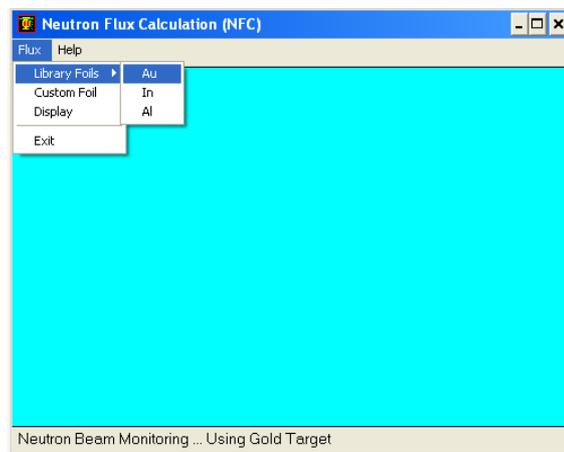
The program reads a file in binary form (\*.gim) to get information about peaks under investigation such as energy, channel, width, net area and isotope. Then the user has the choice to calculate the isotopic concentration by using absolute or comparator method. Finally the program can calculate the concentration for all isotopes in the list. It saves the results in ASCII form. The main window of CGM is shown in figure 8.

## **5. Neutron flux calculation code (NFC)**

It was designed for calculating the flux of a neutron beam. The program uses the activation method for calculating neutron flux. We supported our program with

**Table 1.** Nuclear data for three foils used in neutron flux measurement.

Foil	Au <sup>197</sup>	In <sup>115</sup>	Al <sup>27</sup>
Neutron reaction	Au <sup>197</sup> (n, γ)Au <sup>198</sup>	In <sup>115</sup> (n, γ) In <sup>116m</sup>	Al <sup>27</sup> (n, α)Na <sup>24</sup>
Mass number	100	114.8	27
Target abundance (%)	100	95.71	100
Cross-section (barn)	98.7	157	0.122
Energy (keV)	411.8	1293.5	1368.5
Line intensity (%)	95.5	84.4	1368.5
Half-life	2.69 D	54.41 M	15.1 H



**Figure 9.** Main window of NFC program.

database for three foils Au, In, and Al. The user can support the program with any custom foil. Then the program automatically calculates the flux of the neutron beam. The nuclear data of these foils are shown in table 1.

The main window of NFC is shown in figure 9. The first step in the operation of NFC code is choosing a foil from library foils or use a custom foil then fill its contents as shown in figure 10. From Flux Menu, click display to get the results as shown in figure 11.

## 6. Detector efficiency code (EFF)

It was designed for calculating detector efficiency at a certain energy. The peak efficiency  $\varepsilon(E)$  is defined as

$$\varepsilon(E) = \frac{S}{T_1 \Upsilon(E) A K_w K_c}, \quad (16)$$

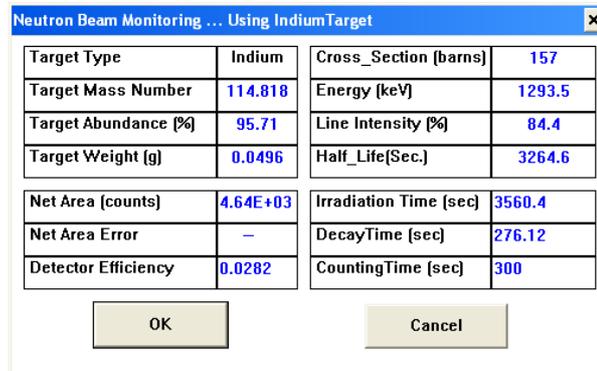


Figure 10. Dialog window for In foil.

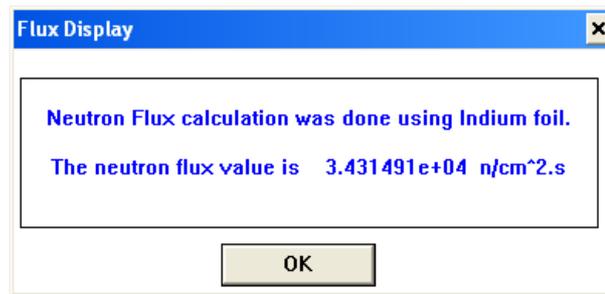


Figure 11. Dialog window for displaying neutron flux value.

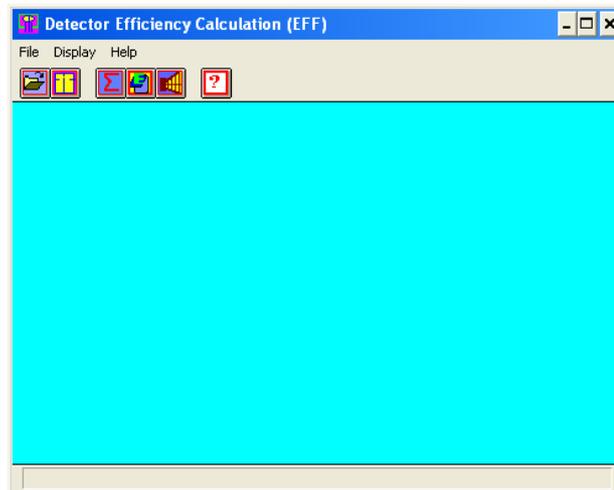


Figure 12. Main window of EFF program.

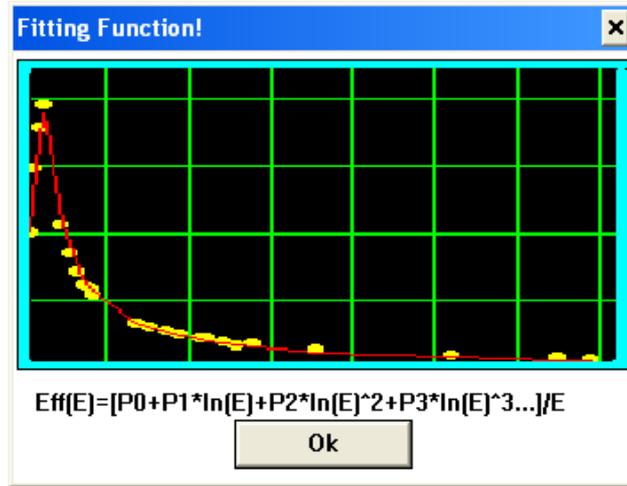


Figure 13. Dialog window for the used fitting function.

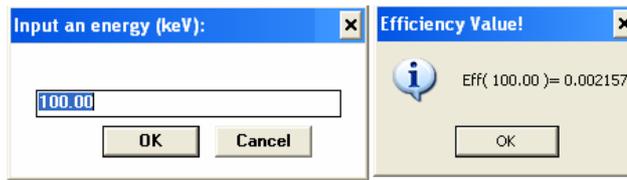


Figure 14. Dialog window for detector efficiency at a certain energy.

where  $S$  is the net peak area,  $T_1$  is the live time of measurement,  $\Upsilon(E)$  is the branching ratio of  $\gamma$ -line of energy  $E$ ,  $A$  is the activity at the source certificate time,  $C_{sa}$  is the correction factor for self-absorption,  $C_{se}$  is the correction factor for summing effect,  $K_w$  is the decay correction factor to correct the activity  $A$  at the starting time of measurement and  $K_c$  is the counting correction factor.

The peak efficiency must be calculated for a set of well-defined peaks. Only singlet peaks with good precision in conjunction with good quality nuclear data should be used to construct an efficiency calibration. EFF program is supported by different mathematical functions that might choose to fit the efficiency.

The main window of EFF is shown in figure 12. The first step is reading the data efficiency file, then choosing a fitting function as shown in figure 13, and choosing the efficiency value at a certain energy as shown in figure 14.

## 7. Conclusion

A package for gamma spectrum analysis has been developed using Borland C++ for windows. The use of this package allows the routine neutron activation analysis steps to be faster and more accurate.

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