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Original Article

Development of quantification program for neutron activation analysis

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ABSTRACT

This work describes the use of C++ Builder to develop an INAA (Instrumental Neutron Activation Analysis) application for the quantification of trace elements mass fractions in samples from different origins using the relative method. Previously, our NAA laboratory relied on classic method, which caused delays in obtaining results, computational mistakes, and reduced productivity. The new application offers an improved interface with standardized actions, decreasing human error accumulation and provides users with rapid results. To evaluate the application, an INAA experiment using a high-resolution gamma-ray spectrophotometer was used to assess the air quality at Draria site in Algiers, by using an active bio-monitoring air pollution method. Therefore; tree barks, mosses, and lichens were used in this study. Samples and standards irradiations were carried out in NUR research reactor with thermal neutrons flux 10^{13} n $cm^{-2}s^{-1}$, and analyzed by gamma spectrometry using HPGe detector. We used the new developed application as well as the old method to calculate concentrations and determined several heavy metals and trace elements (Ba, Br, Co, Cr, Fe, Hf, La, Rb, Sr, Zn, and Ce). Comparison of the obtained preliminary results between the two methods has showed good agreement.

1. Introduction

1.1 Context and Importance of INAA

Instrumental Neutron Activation Analysis (INAA) is a highly sensitive and non-destructive analysis method developed in 1936, and it remains widely used in research, industry, and environmental studies [1]. INAA relies on the interaction between neutrons and sample nuclei, leading to the emission of characteristic gamma radiation from the elements present, making it a crucial technique for the quantitative multi-element analysis of major, minor, and trace elements [1, 2, 3].INAA excels at detecting trace elements in a variety of materials, offering precise measurements across a wide range of elements, including heavy metals [1, 7]. Its practical and technical foundation doesn't depend on the chemical properties of the elements but rather on the nuclear properties of the isotopes, a distinctive property that allows for the qualitative and quantitative analysis of elements with similar chemical properties that are challenging to separate and distinguish through traditional chemical methods [1].The ability to perform quantitative measurements of up to about 35 elements in small samples of 5 to 100mg showcases the versatility of INAA, with detection limits typically in parts per million or parts per billion, depending on the element [7,8]. Notably, INAA boasts several advantages, including the absence of the need for sample preparation, non-destructiveness, the measurement of multiple elements in a single analysis, and higher precision compared to other methods [1, 8].The role of trace elements in various fields such as environmental science, geochemistry, medicine, archaeology, and materials science is essential, as these elements are central to biological, environmental, and industrial processes. Accurate detection using INAA is paramount for assessing human health, mitigating environmental risks, and gaining insights into complex

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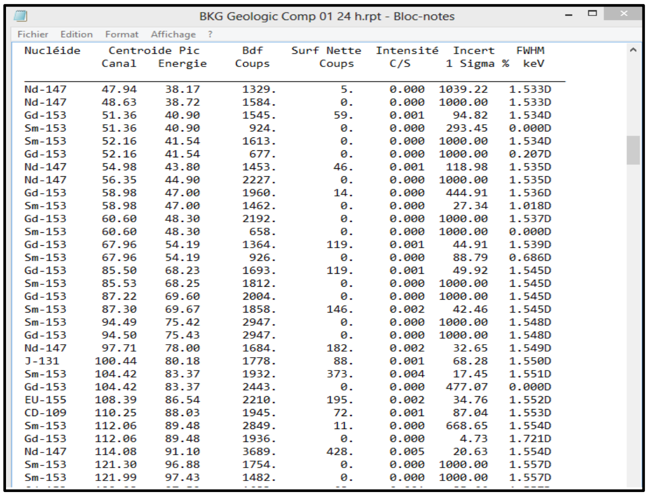
geochemical and biological phenomena [1, 3].Previously, our laboratory employed an Excel application for INAA calculations with limitations in speed, precision, and efficiency. This method involved manual steps prone to calculation errors, result delays, and human errors, hampering productivity and meeting industry and research demands In response to these challenges, an innovative INAA application was developed using C++ Builder, streamlining and standardizing INAA calculation, reducing human errors, and enhancing laboratory efficiency. The primary objective of this study is to present the development and evaluation of this application, with a specific focus on its ability to accurately quantify trace elements' mass fractions using the relative method of INAA.

1.2 Issues with the Previous Method

The previous method, which relied on Excel (as showed in figure 1), involved the programming of the neutron activation analysis equation on four distinct spreadsheets, each designated for a specific purpose: the sample packaging envelope, the standard, the standard reference, and the samples. In the course of calculations, each spreadsheet necessitated careful manual data entry derived from the neutron activation analysis equation, extracted from the report generated by the Gammavision spectrometry software(as showed in figure 2). To be specific:

- The spreadsheet of the envelope used for packaging samples and standards, contained data such as the irradiation date, the date and time of spectrum acquisition, mass measurements, gamma counts for each radioisotope at each energy .
- The spreadsheet of the standard used for quantification, contained information including the irradiation date, start time and date of spectrum acquisition, mass values, gamma counts for each radioelement and energy, as well as the concentration of each element contained in the standard provided by the manufacturer.
- The spreadsheet of the standard reference used for quantification, this page contained information regarding the irradiation date, the start date of spectrum acquisition, mass, gamma counts for each radioelement and energy, and the concentration of each element, provided by the manufacturer.
- The spreadsheet of the sample ,included information regarding the irradiation date, date of spectrum acquisition, mass values, gamma counts for each radioelement and energy,



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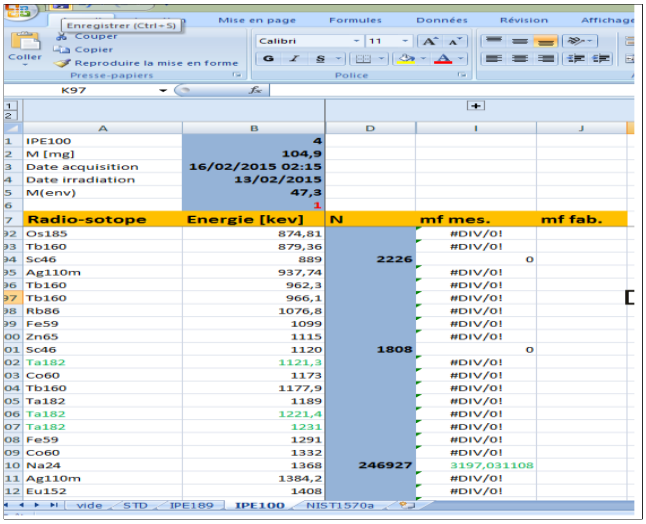
Nucléide     Centroide Pic      Bdf     Surf Nette  Intensité  Incert    FWHM
             Canal    Energie   Coups      Coups       C/S    1 Sigma %  keV

Nd-147       47.94    38.17     1329.         5.     0.000  1039.22   1.533D
Nd-147       48.63    38.72     1584.         0.     0.000  1000.00   1.533D
Gd-153       51.36    40.90     1545.        59.     0.001    94.82   1.534D
Sm-153       51.36    40.90      924.         0.     0.000   293.45   0.000D
Sm-153       52.16    41.54     1613.         0.     0.000  1000.00   1.534D
Gd-153       52.16    41.54      677.         0.     0.000  1000.00   0.207D
Nd-147       54.98    43.80     1453.        46.     0.001   118.98   1.535D
Nd-147       56.35    44.90     2227.         0.     0.000  1000.00   1.535D
Gd-153       58.98    47.00     1960.        14.     0.000   444.91   1.536D
Sm-153       58.98    47.00     1462.         0.     0.000    27.34   1.018D
Gd-153       60.60    48.30     2192.         0.     0.000  1000.00   1.537D
Sm-153       60.60    48.30      658.         0.     0.000  1000.00   0.000D
Gd-153       67.96    54.19     1364.       119.     0.001    44.91   1.539D
Sm-153       67.96    54.19      926.         0.     0.000    88.79   0.686D
Gd-153       85.50    68.23     1693.       119.     0.001    49.92   1.545D
Sm-153       85.53    68.25     1812.         0.     0.000  1000.00   1.545D
Gd-153       87.22    69.60     2004.         0.     0.000  1000.00   1.545D
Sm-153       87.30    69.67     1858.       146.     0.002    42.46   1.545D
Sm-153       94.49    75.42     2947.         0.     0.000  1000.00   1.548D
Gd-153       94.50    75.43     2947.         0.     0.000  1000.00   1.548D
Nd-147       97.71    78.00     1684.       182.     0.002    32.65   1.549D
J-131       100.44    80.18     1778.        88.     0.001    68.28   1.550D
Sm-153      104.42    83.37     1932.       373.     0.004    17.45   1.551D
Gd-153      104.42    83.37     2443.         0.     0.000   477.07   0.000D
EU-155      108.39    86.54     2210.       195.     0.002    34.76   1.552D
CD-109      110.25    88.03     1945.        72.     0.001    87.04   1.553D
Sm-153      112.06    89.48     2849.        11.     0.000   668.65   1.554D
Gd-153      112.06    89.48     1936.         0.     0.000     4.73   1.721D
Nd-147      114.08    91.10     3689.       428.     0.005    20.63   1.554D
Sm-153      121.30    96.88     1754.         0.     0.000  1000.00   1.557D
Sm-153      121.99    97.43     1482.         0.     0.000  1000.00   1.557D
```

Fig 1. Report generated by the Gammavision spectrometry software



	A	B	D	I	J
1	IPE100	4			
2	M [mg]	104,9			
3	Date acquisition	16/02/2015 02:15			
4	Date irradiation	13/02/2015			
5	M(env)	47,3			
6		1			
7	**Radio-sotope**	**Energie [kev]**	**N**	**mf mes.**	**mf fab.**
92	Os185	874,81		#DIV/0!	
93	Tb160	879,36		#DIV/0!	
94	Sc46	889	2226	0	
95	Ag110m	937,74		#DIV/0!	
96	Tb160	962,3		#DIV/0!	
97	Tb160	966,1		#DIV/0!	
98	Rb86	1076,8		#DIV/0!	
99	Fe59	1099		#DIV/0!	
00	Zn65	1115		#DIV/0!	
01	Sc46	1120	1808	0	
02	Ta182	1121,3		#DIV/0!	
03	Co60	1173		#DIV/0!	
04	Tb160	1177,9		#DIV/0!	
05	Ta182	1189		#DIV/0!	
06	Ta182	1221,4		#DIV/0!	
07	Ta182	1231		#DIV/0!	
08	Fe59	1291		#DIV/0!	
09	Co60	1332		#DIV/0!	
10	Na24	1368	246927	3197,031108	
11	Ag110m	1384,2		#DIV/0!	
12	Eu152	1408		#DIV/0!	

Fig 2. INAA excel application interface

The manual operation of transferring data from the spectrometry reports generated by Gammavision to the Excel application for INAA calculation involved multiple steps, and Human errors that led to result inaccuracies and delays. Standardization was also a challenge as different operators followed slightly different procedures, causing variations in results and hindering data reliability. The low efficiency of the manual method resulted in time-consuming analyses, delaying responses to urgent requests and large-scale studies. Additionally, the lack of a dedicated computer interface made data management and tracking cumbersome, relying on paper files or spreadsheets. To address these issues, we developed an innovative INAA application using C++ Builder, aiming to streamline procedures, reduce errors, and provide faster, more reliable results and this is achieved by automating the process of data transfer from the spectrometry reports generated by Gammavision, where the new application can automatically read the reports and apply them for INAA calculations.This article details the application's development and its evaluation against the previous method.

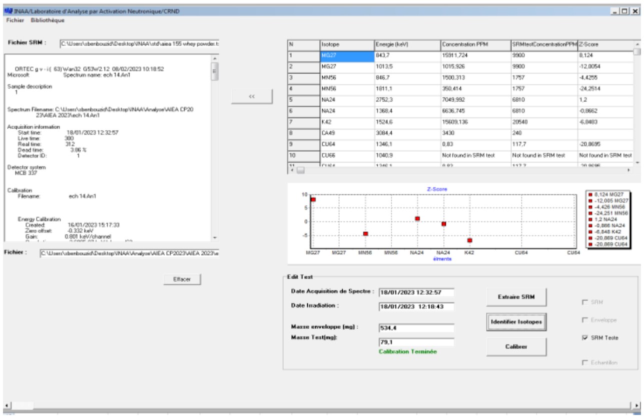
1.3 *Objective and Content Overview*

This work focuses on the development and evaluation of an INAA application using C++ Builder for precise trace element quantification through the relative method. The primary goal is to demonstrate how this application improves accuracy, reliability, and efficiency in comparison to our Excel method. This paper begins by detailing the methodology employed for developing the INAA application, emphasizing its user-friendly interface, automated data management, standardized procedures, and simplified element concentration calculations. Next, it explores the relative method used for trace element quantification, highlighting its precision, reliability, and ability to minimize analysis errors. The article proceeds to showcase the results of an INAA experiment, comparing outcomes obtained from the developed application with the previous manual method for quantification of and trace elements from an air pollution bio-monitoring study in Draria.

2. Materials and Methods

2.1 *Using C++ Builder to Develop the INAA Application*

To develop the INAA application (using C++ Builder) we used IDE (integrated development environment) to create Windows applications with intuitive graphical interfaces. The choice of C++Builder was motivated by its many advantages for scientific and technical applications. C++ Builder's support for object-oriented programming (OOP) made it possible to create well-structured, modular code, enhancing the readability and maintainability of the code. The extensive Graphical User Interface (GUI) library has accelerated application user interface development, offering components such as buttons, drop-down menus, tables, and charts for smooth user interaction. The IDE's compatibility with third-party libraries, such as Boost and Armadillo, made it easier to perform complex scientific calculations such as transfer data operations and statistical calculations necessary for the relative INAA quantification. As showed in figure 3, in addition, C++ Builder's database connectivity capabilities allow for efficient data management, automate the process of data transfer from the spectrometry reports generated by Gammavision, and allowing analysis results to be stored and retrieved in a database, which made it easier for us to program the equation of the relative INAA.



Fichier SRM : C:\Users\sbenbouzid\Desktop\INAA\std\aiea 155 whey powder.t

```
    ORTEC g v - i ( 63) Wan32  G53W2.12  08/02/2023 10:18:52
Microsoft                    Spectrum name: ech 14.An1

Sample description
    1


Spectrum Filename: C:\Users\sbenbouzid\Desktop\INAA\Analyse\AIEA CP20
                23\AIEA 2023\ech 14.An1

Acquisition information
      Start time:            18/01/2023 12:32:57
      Live time:             300
      Real time:             312
      Dead time:             3.86 %
      Detector ID:              1

Detector system
    MCB 337


Calibration
      Filename:              ech 14.An1



      Energy Calibration
          Created:           16/01/2023 15:17:33
          Zero offset:       -0.332 keV
          Gain:              0.801 keV/channel
```

Fichier : C:\Users\sbenbouzid\Desktop\INAA\Analyse\AIEA CP2023\AIEA 2023\e

N	Isotope	Energie (keV)	Concentration PPM	SRMtestConcentrationPPM	Z-Score
1	MG27	843,7	15911,724	9900	8,124
2	MG27	1013,5	1015,926	9900	-12,0054
3	MN56	846,7	1500,313	1757	-4,4255
4	MN56	1811,1	350,414	1757	-24,2514
5	NA24	2752,3	7049,992	6810	1,2
6	NA24	1368,4	6636,745	6810	-0,8662
7	K42	1524,6	15609,136	20540	-6,8483
8	CA49	3084,4	3430	240	
9	CU64	1346,1	0,83	117,7	-20,8695
10	CU66	1040,9	Not found in SRM test	Not found in SRM test	Not found in SRM test

Date Acquisition de Spectre : 18/01/2023 12:32:57
Date Irradiation : 18/01/2023 12:18:43
Masse enveloppe (mg) : 534,4
Masse Test(mg): 79,1
Calibration Terminée

☐ SRM
☐ Enveloppe
☑ SRM Teste
☐ Echantillon

Fig 3. INAA application interface

2.2 *Explanation of the INAA Relative Method*

The relative method is a widely used approach in Instrumental Neutron Activation Analysis (INAA) for quantifying trace elements in samples. This method compares gamma counting rates between samples and reference standards, making it suitable for complex or unknown samples. It doesn't require knowing the exact sample composition. The method involves calculating the ratio of the gamma counting rate of the element in the sample to that in a reference standard of known composition. Correction factors, accounting for experimental variations, are applied to these ratios to determine the element concentration [2,3]. In an INAA analysis using the relative method, reference standards with known element concentrations are irradiated alongside the samples. After irradiation, gamma counting rates are measured using a high-resolution gamma spectrophotometer [4].

The equation used in the calculation of the composite concentration by the relative INAA is as follows [3]:

$$C(s) = \left[\frac{CR(s)}{CR(s)}\right] \times C(std) \qquad (1$$

Where:
C(s) represents the concentration of the element in the sample.
CR(s) is the gamma counting rate of the sample.
CR(std) is the gamma counting rate of the standard.
C(std) is the known concentration of the element in the standard.

The next section will detail an INAA experiment conducted using a high-resolution gamma spectrophotometer to assess air quality in Draria, Algeria, using the air pollution bio-monitoring method. Results obtained with the developed INAA application will be compared to those from the Excel method.

2.3 Samples used in the air pollution bio-monitoring study

As part of the air pollution bio-monitoring study in Draria, various biological samples, including tree barks, mosses, and lichens, were collected due to their ability to accumulate trace elements from the air, serving as pollution indicators. Stringent collection procedures were followed to ensure sample integrity and prevent contamination [5]. These samples were ground into a fine powder, then in stringent cleanliness conditions, they were weighed and packaged in 5N purity (99.999%) aluminum foils and assembled together in a single package with the following standards: SRM-NIST 1573a, Lichen-336-IAEA reference material. Among these standards, one was used for internal quality control of the results, and the other for calculating trace element concentrations. The samples to be analyzed were prepared and placed in an aluminum capsule ready for irradiation at the NUR reactor with a power of 1 megawatt.

2.4 Description of the INAA Experiment with high-resolution gamma spectrophotometer

The experimental procedure involved exposing these samples to irradiation using a thermal neutron flux of 10^{13} n $cm^{-2}s^{-1}$ for 4 hours. Subsequently, gamma spectra were acquired using a modular electronic system in conjunction with a high-purity germanium detector, specifically the GR3019 model, boasting a resolution of 1.9 keV. The software utilized for the deconvolution of gamma spectra was GAMMA VISION, developed by ORTEC. For the quantification of medium half-life elements, the measurement of gamma spectra commenced five days after irradiation, employing a specific geometry (sample-to-detector distance) of six rings equivalent to 12 cm, with a measurement duration of 3600 seconds. In the case of long half-life elements, the second phase of spectral measurements began 20 days post-irradiation, utilizing a different geometry with two rings equivalent to 4 cm, and these measurements were conducted for 5200 seconds [2,6].

3. Results and Discussion

This section presents the results of the instrumental neutron activation analysis (INAA) experiment conducted using the newly developed application with C++ Builder and the classical method. The data collected includes gamma counting rates measured for each sample using a high-resolution gamma spectrophotometer in both. Applications.The gamma counting rates were used to calculate ratios between the gamma counting rates of each element of interest in the samples and in the reference standards. These ratios, were employed to determine the concentrations of heavy metals and trace elements in the samples.The results we obtained are shown in the following table:

Table 1: Example of the results of trace elements concentrations ((µg/g) obtained by the two methods on a lichen sample

Elements	**Using the new application**	**Using the excel**
Ba	500	500
Br	20	20
Ce	46	46
Co	9.35	9.35
Cr	55	55
Fe	25888	25888
Hf	6.2	6.2
La	18.22	18.22
Rb	22.85	22.85
Sr	44	44
Zn	133.1	133.1

As illustrated in the table 1, the results of the concentration obtained by the two methods are identical confirming the efficiency and reliability of the INAA new application developed . It's important to accentuate that the results obtained through the Excel application were the outcome of significant effort involving three individuals working over an extended two-day period. This process also entailed the correction of numerous data entry errors, unlike the new application, with its remarkable efficiency, managed to yield identical results within a short timeframe of just four hours and with the work of a single person. Moreover, the new application completely eliminated data transfer errors. This comparison underscores the efficiency and reliability of the INAA application as a method for obtaining results akin to those derived from the classical approach. The advantages offered by this innovative application, including its speed, standardization, and error-reduction capabilities, became exceedingly apparent when handling a substantial volume.

4. Conclusion

In conclusion, this study demonstrated the advantages and effectiveness of the developed INAA application in simplifying calculations, reducing human errors, and improving the reliability of results compared to the Excel method. Looking to the future, this innovative INAA app holds promising prospects. It can be adapted and expanded to include different areas of neutron activation analysis, such as water quality assessment and soil monitoring, which will enhance our ability to understand pollution and its health effects on populations by providing accurate and reliable data on concentrations of heavy metals and trace elements.

Conflict of Interest

We declare that we have no conflict of interest.

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