k_0-based instrumental neutron activation analysis using MS-Excel and Canberra Genie-2000

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Resumen

Se describe una aplicación desarrollada en Microsoft Excel, para el procesamiento completo de datos y presentación automatizada de resultados de análisis por activación neutrónica instrumental paramétrico, según el método del k_0. La aplicación hace uso extensivo de la información generada por el sistema de espectroscopia gamma Genie-2000, de Canberra, minimizando el ingreso manual de datos por parte del usuario. Una característica especial de la aplicación es la determinación automática del número de cifras significativas de cada resultado, así como el redondeo y presentación automáticos, de los resultados y sus incertidumbres expandidas (k=2), en los formatos correctos. La aplicación ha sido validada mediante el análisis de materiales de referencia y se encuentra en etapa de producción y mantenimiento. El uso de la aplicación ha permitido incrementar la eficiencia en el trabajo analítico, en el Laboratorio de Técnicas Analíticas Nucleares del IPEN.

Abstract

We describe an application, developed in Microsoft Excel, for the complete processing of data and automated presentation of results, of k_0-based instrumental neutron activation analysis. The application makes extensive use of the data generated by the Canberra's Genie-2000 spectroscopy system, minimizing the manual input of data by the user. A special feature of the application is the automatic determination of significant figures for each result, as well as the automatic rounding and presentation of the results and their expanded uncertainties (k=2), in the right format. The application has been validated by the analysis of reference materials and it is on production and maintenance steps. The use of the application has allowed the improvement of the efficiency, of the analytical work, in the Laboratory of Nuclear Analytical Techniques of IPEN.

1.   Introduction

Despite that few commercial software packages are currently available, for the determination of elemental concentrations in k_0-based instrumental neutron activation analysis, several INAA laboratories prefer to develop their own in house packages [1]. Some reasons for this are that the commercial packages are expensive and not too friendly to the user [2]. In addition, a specific purpose software package, tailored according to the needs and instrumentation of a particular laboratory, is sometimes required.

In the last ten years, the Microsoft Excel Application has been used as a calculation tool in scientific laboratories [3, 4]. In 2005, Landsberger *et al.* [2] described an application based in Microsoft Excel and Canberra's Genie-2000, for the automatic

calculations of results of the traditional multi-comparator method of instrumental neutron activation analysis. Because the calculations involved are relatively simple, they were able to use a very simple approach, "placing the heart of the comparator standard method of NAA calculation in an Excel spreadsheet" [2]. The cited application was devised for educational purposes, allowing the students to modify the calculations by direct changing the formulas or data in the cells of the spreadsheet.

In the k_0-based INAA, the experimental work is relatively easier, at a cost of a quite more involved mathematical processing of the data. In addition, an application for routine analytical work has to be able to process

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large sets of samples, in an unattended way. In that situation, it is better to put the mathematical and presentation engine in a suitable high level computer code.

The present work describes and discuses, an application, developed in Microsoft Excel, for the complete processing of data and automated presentation of results, of k_0-based instrumental neutron activation analysis.

2.   Methodology

The application has been developed using the Microsoft Visual Basic for Applications, already included with the Microsoft Excel 2003. As well as in the case of [2], the Canberra software Genie-2000 is used for the detector calibrations, MCA settings, spectral acquisition and peak fitting routines.

2.1   Program structure: input data

The general structure of the application it is shown in figure 1. In few words, a block of data is read and processed by the main engine. The first 09 items of data have to be furnished by hand for each sample, in a row of a spreadsheet. This task is performed by the analyst before the irradiation, for a set of samples, using a simple spreadsheet form.
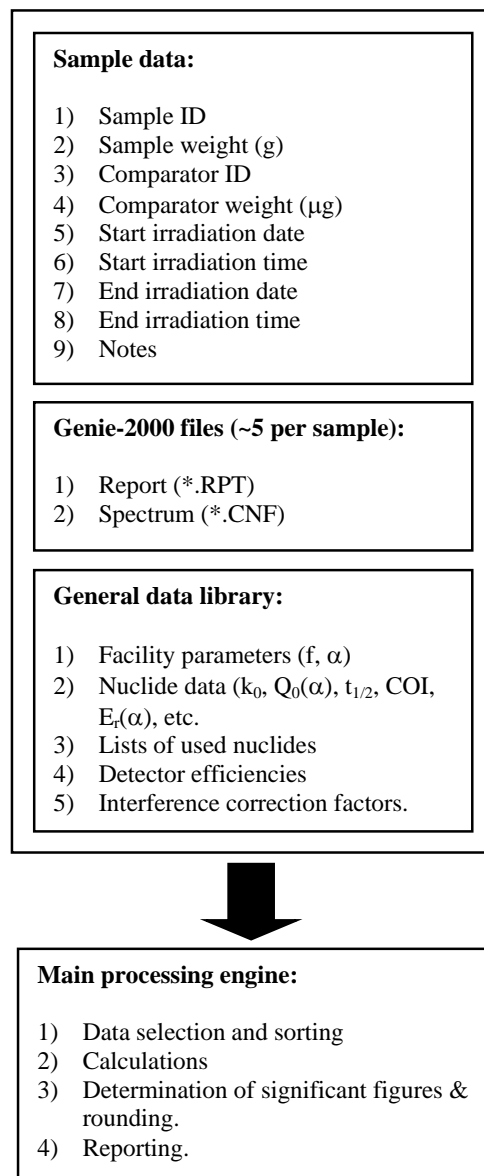
The biggest part of the analytical data per sample (about a hundred of gamma peak intensities + dates and times of counting + dead and live counting times) are found and read by the application, in an automatic way, from the data files produced by the Canberra's Genie-2000 software.

Another important set of data it is comprised by the parameters f and α [5 - 7] of the irradiation facility, a set of nuclear constants of the used nuclides, the efficiencies of the gamma ray detector and the correction factors for spectral interference, blanks, etc. These data are kept in a spreadsheet working as a data base which is consulted by the application.

2.2   Program structure: calculations

The main engine starts with a selection and sorting of the input data, which are necessary for the next step. The calculations proceed according to the cumbersome and well known mathematical equations of the k_0 method of neutron activation analysis, which

have been repeatedly appeared in literature [5 - 7].

Sample data:

1) Sample ID
2) Sample weight (g)
3) Comparator ID
4) Comparator weight (μg)
5) Start irradiation date
6) Start irradiation time
7) End irradiation date
8) End irradiation time
9) Notes

Genie-2000 files (~5 per sample):

1) Report (*.RPT)
2) Spectrum (*.CNF)

General data library:

1) Facility parameters (f, α)
2) Nuclide data (k_0, $Q_0(\alpha)$, $t_{1/2}$, COI, $E_r(\alpha)$), etc.
3) Lists of used nuclides
4) Detector efficiencies
5) Interference correction factors.

Main processing engine:

1) Data selection and sorting
2) Calculations
3) Determination of significant figures & rounding.
4) Reporting.

Figure 1. General program structure.

The next step is also a calculation. The number of significant figures of each analytical result is determined and each result is rounded to the corresponding number of significant figures. The expanded uncertainties associated to the analytical results are rounded to 01 significant figure. The details of these calculations have been described elsewhere [8].

2.3   Software validation

The validation of the application has been done using, as input, available sample data and Genie-2000 files, corresponding to neutron activation analysis of different reference materials, performed in the laboratory in the past two years. An example of the final report generated by the program it is shown in table 1.

Table 1. Example of report for the NIST-SRM-1633b-Coal Fly Ash.

The Element	Result (crude) (mg/kg)	Result (rounded) (mg/kg) ± U (k=2)	Certified Values (U), k=2
As	126,653229	130 ± 10	136,2 (2,6)
Ba	651,544219	650 ± 70	709 (27)
Ce	186,64804	190 ± 20	190
Co	49,0591127	50 ± 5	50
Cr	200,356786	200 ± 20	198,2 (4,7)
Cs	10,8073281	11 ± 1	11
Eu	3,58165087	3,6 ± 0,4	4,1
Fe	78693,3722	79000 ± 8000	77800 (2300)
Ga	49,5615	50 ± 5	
Hf	7,09383057	7,1 ± 0,7	6,8
K	19080,4977	19000 ± 2000	19500 (300)
La	83,0648507	86 ± 9	94
Lu	1,35586931	2,5 ± 0,2	1,2
Na	2089,4277	2100 ± 200	2010 (30)
Nd	82,2478388	82 ± 8	85
U	8,06732477	8,1 ± 0,8	8,79 (0,36)
Th	25,6278757	26 ± 3	25,7 (1,3)
Rb	132,454984	130 ± 10	140
Sb	5,93712971	5,9 ± 0,6	6
Sc	42,6348673	43 ± 4	41
Sm	8,16886663	8,6 ± 0,9	20
Sr	1199,62795	1200 ± 100	1041 (14)
Ta	1,80093457	1,8 ± 0,2	1,8
Tb	2,78837536	2,8 ± 0,3	2,6
W	5,48883751	5,5 ± 0,5	5,6
Yb	8,13789581	8,1 ± 0,8	7,6

3.   Results and discussion

The results in table 1 are one example to show that the developed application works in a right way, giving accurate results and expressing those in a proper format. It can be seen that the order of magnitude covers the range (10^0, 10^4). Table 1 has results for 26 elemental concentrations, determined by INAA using intermediate and long lived nuclides. Another about nine elements should be added if we consider the INAA using short lived nuclides (Al, Cl Cu, In, Mg, Mn, Ti, V, Dy). Having to round by hand 35 crude results and 35 crude uncertainties (not shown in table 1) per sample, for a batch of a hundred samples, would be a very uncomfortable task for any analyst.

It could be commented that having to input by hand a set of nine entry data per sample, for a batch of a hundred samples is still an unpleasant task. For the moment, that is the situation in our laboratory. Even so, the actual application had allowed a significant improvement of the efficiency of the analytical work in the laboratory, in comparison with the former situation, in which it was being necessary to input by hand about a hundred of numerical data for each sample. A comprehensive automation project, currently in an early step of progress [9], will allow the automatic feed of the numerical data required by the items 2, 4 to 8, in a near future.

A special feature of the developed application is the automatic determination of the number of significant figures and the automatic rounding and presentation of the final results in a proper format. It seems that, for the moment, this capabilities are only (or almost only) available in some commercial and expensive LIMS (laboratory integrated management system) software [10-12].

4.   References

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