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VALIDATION OF THE CANBERRA G2KNAA SOFTWARE FOR MASS FRACTION DETERMINATION BY NEUTRON ACTIVATION ANALYSIS

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ABSTRACT

Users of the comparative method at Neutron Activation Analysis laboratories apply gamma ray spectrometry to obtain sample and comparator spectra using the software provided by the hygh-purity Ge spectrometer producer, such as the Genie 2000 software family of Canberra Industries. Later they apply separate software to compare sample and comparator peak areas and calculate sample mass fractions. This calculation is time consuming and subject to human error as usually information is transferred by hand from one system to the other. This study aimed to validate the Canberra G2kNAA software. The software directly extracts spectra information from Genie 2000 software to calculate element mass fractions in NAA applications. It was used for the determination of Ag, As, Co, Rb, Se and Zn, taken randomly among analyzed elements in a sample set used for the homogeneity study of a mussel candidate reference material. The sample set consisted of six bottles of the reference material with eight replicate analyses performed for each bottle resulting in 48 measurement results for each element. Student's *t*-test and correlation analysis were applied in order to compare obtained results with those obtained with an in-house software and hence to validate the G2kNAA software and allow its utilization at a routine basis.

Key-words: software validation, INAA; reference material, mussel

1. INTRODUCTION

The use of Neutron Activation Analysis comparative method to quantify element mass fractions is widely known by its large pool of detectable elements, fast results and also by not destroying samples [1]. Another benefit of this method is the accuracy of the technique. The requirement for this type of analysis is a source of neutrons, which will bombard the sample and activate its nucleus, and a detector. The detector used is a germanium semiconductor, cooled by liquid nitrogen.

This paper aims on optimizing the process of gathering the activity information and transforming its values into mass fraction in the unknown sample. That mechanism is actually done by transferring the data gathered by the detector manually to another system able to quantify the elements in the sample, comparing activities to standards prepared with known mass fractions. To optimize this procedure, the validation of the software G2kNAA is needed, as it lessens the time consumed to get the result. It gets the data directly from the main

software Genie 2000 and calculates, based on neutron irradiation time, sample mass, element mass in the standard, cooling time and the elemental half life [2, 3].

For the validation to take place, *Perna perna* (Linnaeus, 1758) mussel reference material already irradiated and analyzed by the NAA method had their information saved, then calculated by G2kNAA. For each element, results were compared with those results achieved by transferring manually the data from Genie 2000 and calculating by other means.

This comparison may result in a more comfortable work pace for all researchers who might have contact with the G2kNAA software, as it will optimize their time, and ease their everyday load.

2. EXPERIMENTAL

By using data acquired from mussel tissue analyses, it is possible to compare, adopting Student's *t*-test, manual and automatically calculated results by using G2kNAA.

Mussel information was gathered when the samples and elemental standards were irradiated simultaneously for 8 h at 10^{12} cm^{-2} s^{-1} thermal neutron flux of the IEA-R1 Nuclear Research Reactor at IPEN – CNEN/SP, applied on vials number 19, 40 75, 112, 143 and 156 of the mussel reference material [4, 5]. After convenient decay times, the samples and standards were ready to be analyzed using a GC2018 Canberra HPGe detector coupled to a Canberra DSA–1000 multi–channel analyzer, with which we could get the gamma decay information needed to calculate the elemental mass fraction in the mussel reference material. With this data, a comparison between two methods of calculation: one with the help of Microsoft Office program Excel, and another one, more automated with G2kNAA, software already on the same computer used to analyze data from the detector, was performed. The comparison of results will be tested with Student's *t*-test to validate the use of the G2kNAA software.

3. RESULTS AND DISCUSSION

3.1 Mass fraction calculations

Table 1 presents the mass fraction results obtained using the G2kNAA software as well the comparison to results obtained with Excel spreadsheet, using the Sudent's *t* test.

As shown below, the standard deviations on both Excel and G2kNAA results are compatible. The main information to be concerned with is the comparison of *t* stat and *t* crit bi-caudal, as in Statistics, if *t* stat < *t* crit then both methods are compatible and able to be used, which means that the values gathered by Excel as well as the ones gathered by G2kNAA are equally close representatives of a truthful quantitative analysis results. This affirmation can be backed for every element compared but As, as was confirmed also in 3.2 item.

Table 1: Mass fraction (µg g^{-1}) means, standard deviations and *t*-test's.

Element	Method	Vial						mean	standard deviation	*t* stat.	*t* crit.[a]
		19	40	75	112	143	156				
Ag	Excel	2.28	2.30	2.23	2.26	2.48	2.22	2.25	0.12	1.73	2.00
	G2kNAA	2.30	2.34	2.27	2.32	2.35	2.25	2.30	0.12		
As	Excel	14.3	13.9	14.0	14.0	13.9	13.8	14.0	0.37	14.17	1.99
	G2kNAA	12.3	10.4	11.1	12.0	10.1	12.4	12.2	0.29		
Co	Excel	0.84	0.83	0.82	0.84	0.83	0.83	0.83	0.0011	0.43	2.00
	G2kNAA	0.82	0.84	0.82	0.85	0.83	0.82	0.83	0.0012		
Rb	Excel	4.59	4.31	4.51	4.64	4.58	4.50	4.52	0.074	0.35	2.00
	G2kNAA	4.59	4.48	3.95	4.21	4.03	4.46	4.54	0.052		
Se	Excel	4.29	4.22	4.26	4.37	4.38	4.23	4.29	0.038	1.63	2.00
	G2kNAA	4.34	4.40	4.22	4.36	4.26	4.23	4.37	0.035		
Zn	Excel	115	115	118	116	114	117	115	19	-1.22	2.00
	G2kNAA	116	117	118	116	111	118	117	19		

a. Bi-caudal

3.2. Graphical Data Comparison

With the values gathered, there were a means of 35 pairs to work with, and so they were tested graphically, as presented in Figures 1 to 6.

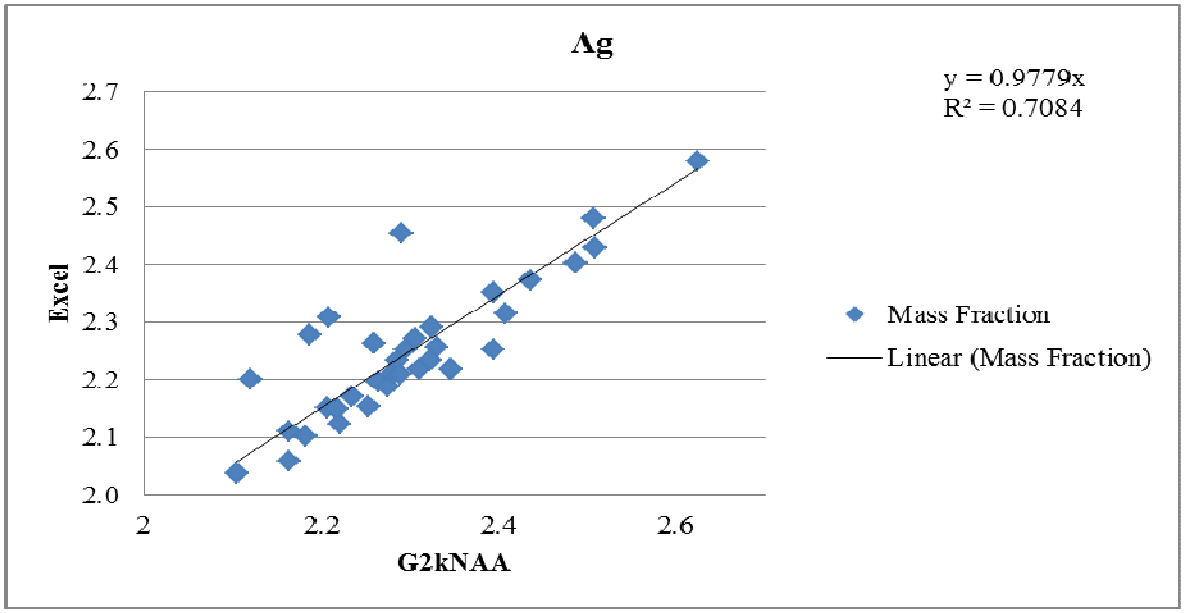

Figure 1: Ag mass fraction (µg g^{-1}) comparison

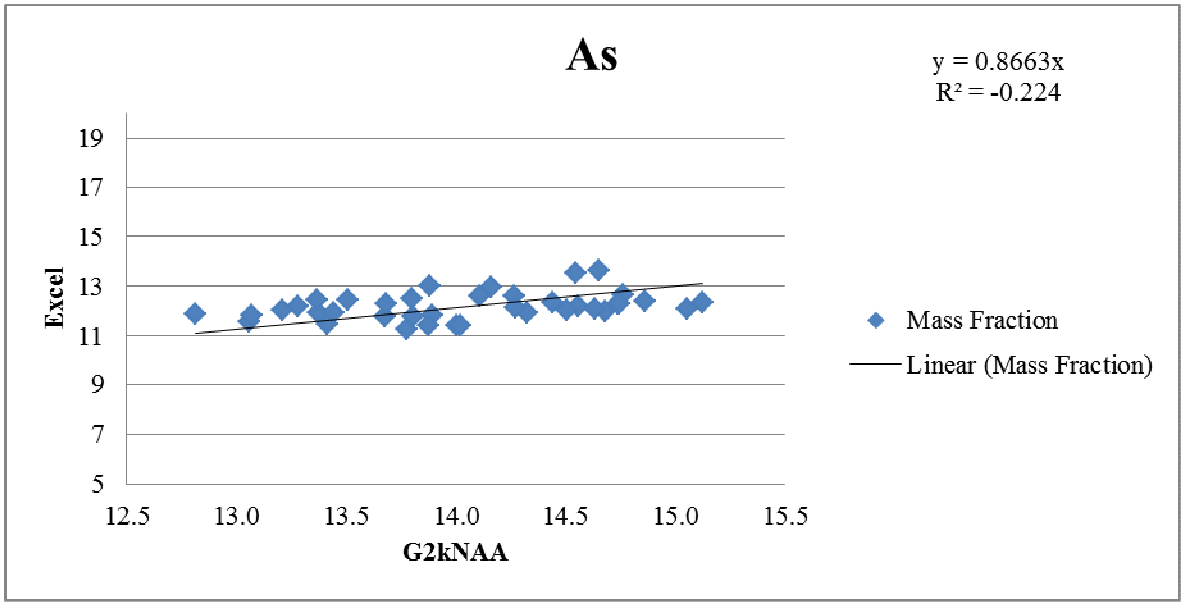

Figure 2: As mass fraction (µg g^{-1}) comparison

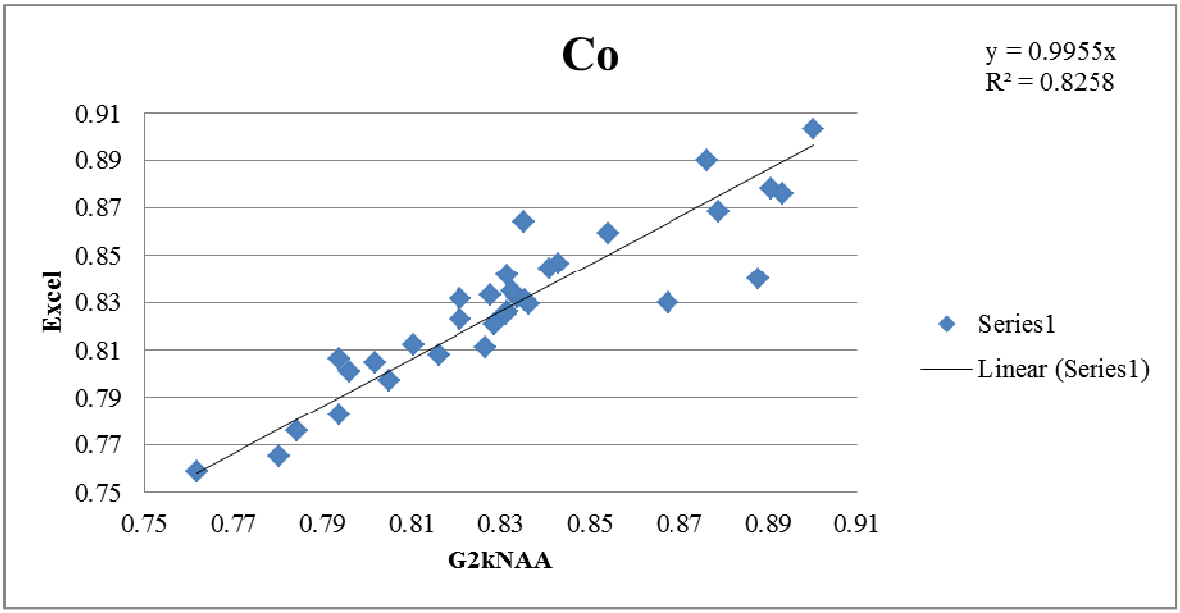

Figure 3: Co mass fraction (µg g^{-1}) comparison

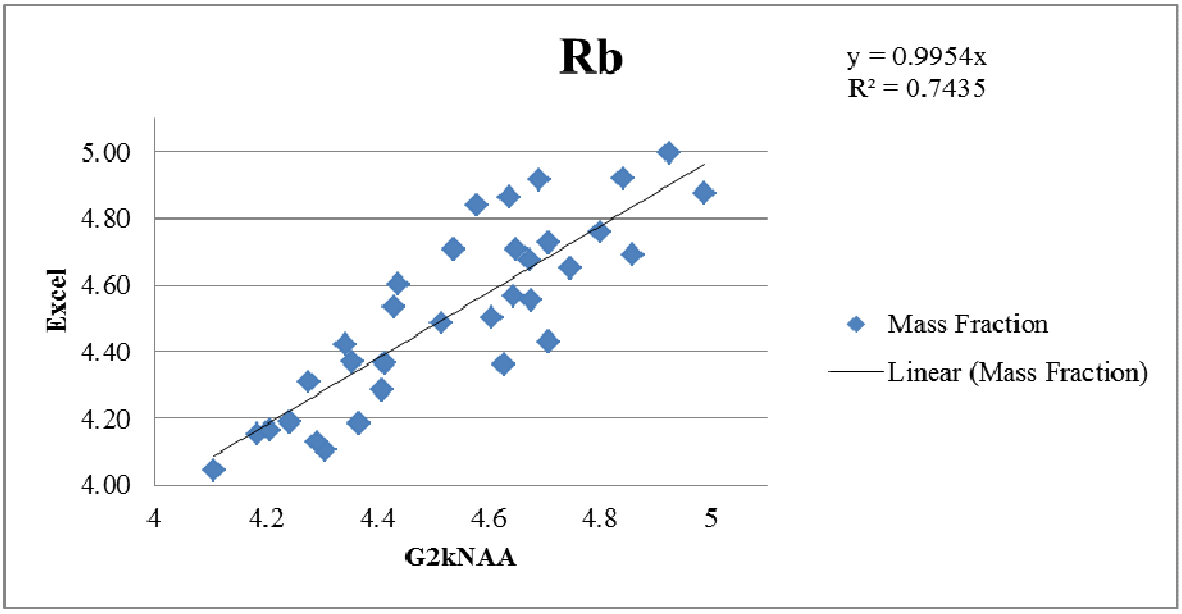

Figure 4: Rb mass fraction (µg g^{-1}) comparison

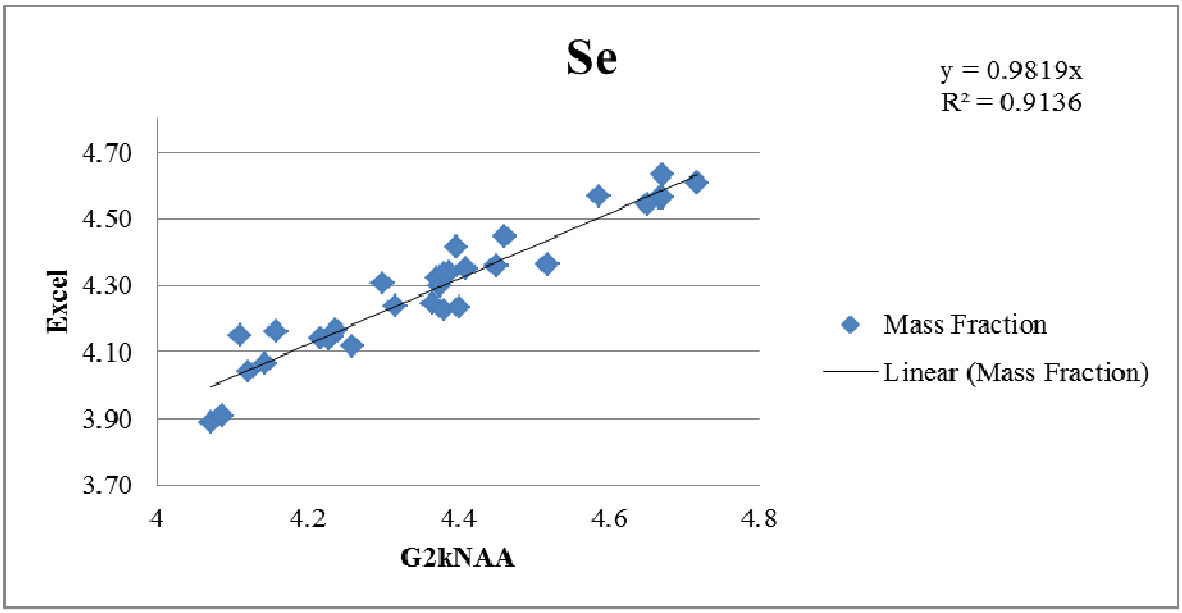

Figure 5: Se mass fraction (µg g^{-1}) comparison

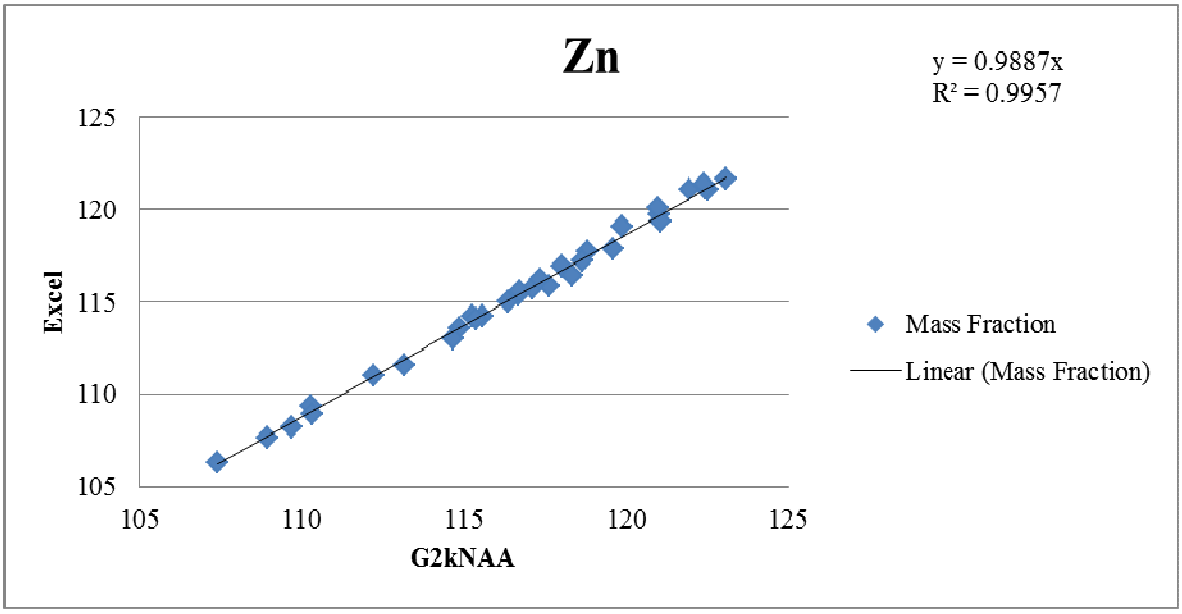

Figure 6: Zn mass fraction (µg g^{-1}) comparison

Figures 1 to 6 express the values from both calculation methods graphically. It is evident that the majority have a good comparative function but As. This deviation was not expected, and requires further investigation as to be clear what caused such difference.

These elements were selected randomly, as a trial to investigate the G2kNAA software performance. So the other elements left out need to be compared as well, as to further increase this software's approval rate.

4. CONCLUSIONS

Although there were systematic errors bound to the comparisons, which demands further investigation, the proximity in results between the two calculation methods, the analysis using Student's *t*-test and the graphical data together express in a luculent way the possibility to validate G2kNAA as a calculation technique able to express values in a coherent and trustworthy manner, as to help researchers lessen the time used to reach mass fraction results.

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