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Machine Learning Techniques for Simultaneous Determination of Parameters Associated with the k0 Method of Neutron Activation Analysis

Rafael Vanhoz[1], Maurício Moralles[1], Mauro da Silva Dias[1]

[1] *Instituto de Pesquisas Energéticas e Nucleares, IPEN-CNEN/SP, Av. Prof. Lineu Prestes 2242, 05508-000 São Paulo, SP, Brazil*

1. Introduction

One of the Neutron Activation Analysis (NAA) methods currently used in laboratories around the world is known as the k_0 Method [1-10]. Considering the standardization methods, the advantage of this technique is the ability to use a single comparator, usually gold, in different samples and matrices. This methodology makes it easier when you need to analyze a lot of samples.

The determination of the analyzed element concentration by the k_0 method involves many parameters and, therefore, it is necessary to consider the uncertainties of each one. In particular, the parameters α, f, k_0 and Q_0 are obtained by other expression involving parameters not explained in the concentration calculation, and which also have source of uncertainty [11-17]. The statistical analysis of the methodologies involved in the determination of theses parameters is the motivation for the present study.

With the literature review, it was possible to verify some studies that sought to develop methodologies for the treatment of uncertainties in the determination of theses parameters [13-17]. However, the methodologies presented do not describe the treatment completely, considering the complexity of the correlations existing between the adjustment parameters. IPEN's Nuclear Metrology Laboratory (LMN) has experience in field of radionuclide activity standardization, neutron fields, Monte Carlo modeling and statistical data processing [18-23]. Recently, the LMN implemented the methodology that use the Covariance Matrix analysis, applied to equations involved in k_0 Method [21-23].

The objective of this study was to develop a methodology to obtain parameters α, k_0 and Q_0 for several elements irradiated simultaneously in different years. This approach reduces the need of use data from literature. The development of a simultaneous adjustment for all the main parameters that make up the k_0 method using statistical analysis and machine learning is not similar in the literature, which makes it an unprecedented technique.

2. Methodology

In this study, the code called AKQFIT was developed, which performs a simultaneous adjustment of the parameters α, k_0 and Q_0 with the experimental data. The machine learning fit method was based on the Levenberg-Marquardt Algorithm [24,25] and written using the R [26] programming language. Irradiated samples performed at the LMN in 2010 were used for code analysis.

3. Results and Discussion

Table I shows the results obtained by the code AKQFIT for the 2010 irradiation data:

Table I: Results obtained with AKQFIT

	a	α	χ^2	χ^2_{red}		
AKQFIT	25.551(4)	-0.003(4)	44.0	2.2		
Product	**Energy (keV)**	**k_0 (AKQFIT)**	**k_0 (Literature) [27]**	**Q_0 (AKQFIT)**	**Q_0 (Literature) [27]**
^{95}Zr	724.2	8.89(7)×10^{-05}	8.90(12)×10^{-5}	4.98(5)	5.31(2)
	756.7	1.09(1)×10^{-04}	1.10(1)×10^{-4}		
^{65}Zn	1115.5	5.64(5)×10^{-03}	5.72(23)×10^{-3}	1.8(6)	1.9(1)
^{69m}Zn	438.6	3.94(2)×10^{-04}	3.98(4)×10^{-4}	2.65(6)	2.56(4)
^{140}La	328.7	2.83(2)×10^{-02}	2.87(3)×10^{-2}	1.21(6)	1,24(-)
	487	6.32(3)×10^{-02}	6.37(6)×10^{-2}		
	815.8	3.34(2)×10^{-02}	3.32(2)×10^{-2}		
	1596.2	1.33(7)×10^{-01}	1.34(1)×10^{-1}		
^{60}Co	1173.2	1.30(2)	1.32(5)	2.16(12)	1.99(10)
	1332.5	1.33(2)	1.32(7)		
^{46}Sc	889	1.210(7)	1.220(5)	0.50(4)	0.43(-)
	1120	1.214(9)	1.220(13)		

The AKQFIT obtained the value for the α parameter of -0.003±0.004, a value compatible with zero and in accordance with the Dias *et*. Al. [20,21]. The reduced chi-square was 2.2.
Figure 1 shows the correlation matrix of the parameters analyzed in the AKQFIT, in a qualitative way. Colors represent correlations: shades of red represents negative correlation, and shades of blue represents positive correlation.

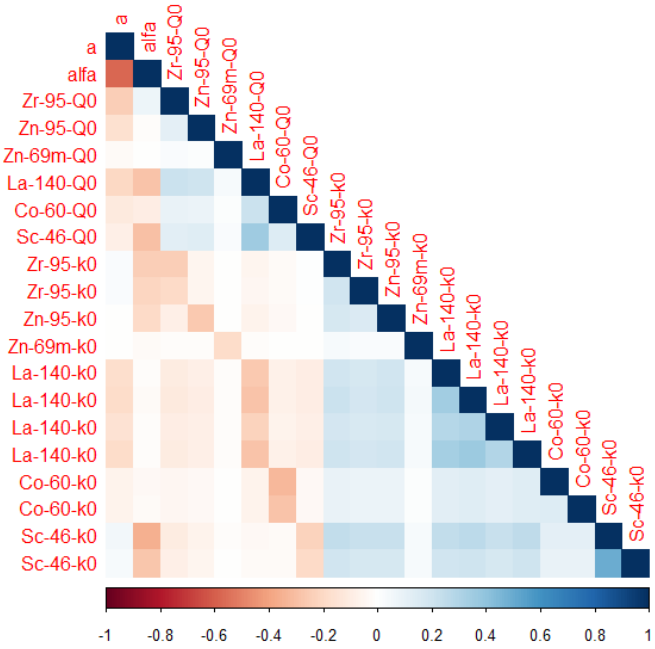

Figure 1: Correlation Matrix of parameters calculated by AKQFIT.

4. Conclusions

Based on the results obtained, the AKQFIT code, built in R, was in accordance with the theory and all results were within expectations, according to the information contained in the input data file. It was possible to calculate the parameters α, k_0 e Q_0 simultaneously in a single fit. The correlation matrix created in this study was important to verify the behavior of the data, helping in any analysis or measurement errors. Through it, it was possible evaluate the correlations of each parameter involved in the NAA that was analyzed in this study, and which was shown to be in accordance with the theory.

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