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Development of web software for determining element concentrations based on the k_0 standardization method of neutron activation analysis

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***Abstract*—** *This work presents the development and validation of the K0-WEB software, dedicated to the determination of elemental concentrations based on the k_0-standardization method of Neutron Activation Analysis (NAA). This method, recognized for its high accuracy, enables multielement analyses of samples without the need for standards, relying on the precise characterization of facilities and the use of nuclear parameters such as k_0-factors, Q_0, and decay constants. The system stands out for its innovative web-based architecture and the automation of nuclear data import, providing originality and operational autonomy. The software integrates essential corrections—such as cascade summing, geometry factor, and allows step-by-step monitoring of calculations, interactive visualization, and report generation. The validation of K0-WEB was carried out by comparing its results with those of the K0-IPEN program, previously submitted to an international intercomparison exercise of the International Atomic Energy Agency (IAEA), ensuring the reliability of the new system. The experimental part employed standardized data from IAEA-TECDOC-2026. Concentration, efficiency, and thermal and epithermal flux parameter calculations were performed according to methodologies established in the literature, with emphasis on the bare triple monitor method and the cadmium ratio method. Additionally, an uncertainty analysis based on error propagation and covariance matrix was applied. The results demonstrated the validation of K0-WEB, and it can be concluded that K0-WEB represents an innovative, accurate, and efficient solution for application in NAA laboratories.*

I. INTRODUCTION

The knowledge of the concentration of chemical elements in samples is of great interest in several fields of study. In this context, Neutron Activation Analysis (NAA) stands out as an important and powerful technique. In this method, the stable nucleus of the chemical element to be identified is irradiated in a neutron flux, its induced activity is subsequently determined, and from the value of this activity, it is possible to obtain the concentration of that element in the irradiated sample. This is an analytical

technique of high sensitivity, excellent precision, and accuracy, suitable for multielement quantitative analyses of elements that may be present in high, medium, or even trace concentrations in samples from the most diverse fields of application.

The k_0 method of neutron activation [1] is a neutron activation analysis technique considered "quasi-absolute" (uncertainties must be considered), which, due to its excellent accuracy, emerged as an alternative to the comparative method, eliminating some of its disadvantages. This method requires precise characterization of irradiation and detection facilities, the use of nuclear constants from the literature (k_0 factors, Q_0, and decay constants), as well as the determination of parameters necessary for calculating the activity of irradiated samples (detection efficiencies and gamma intensities). The k_0 factors are independent of the reactor spectrum and detector characteristics and have been experimentally determined for several target nuclei [2]. The concentration of the elements is calculated in relation to a comparator element, usually gold, eliminating the need for standards. The k_0 method, because it enables the determination of elemental concentrations with high accuracy, has been widely accepted by users in several laboratories worldwide, including Brazil [3] [4] [5] [6].

II. THEORETICAL FOUNDATIONS

This chapter brings together the theoretical foundations that support the development and application of K0-WEB. It first addresses concepts of software engineering, which provide the methodological basis for the construction of the system, and aspects related to databases. Subsequently, it presents the principles of the k0 method and its associated steps, including the determination of concentration.

2.1 Software Engineering

The concept of software engineering dates to the late 1960s and early 1970s, when the software crisis demanded a solution due to the growing demand for new software, considering their development timelines and costs [7].

A complex software system is characterized by a set of abstract software components (data structures and algorithms) encapsulated in the form of procedures, functions, modules, objects, or agents interconnected with one another, forming the software architecture, which must be executed in computer systems. With this systematic approach, commonly referred to as the software process, software engineering presents a "sequence of activities that leads to the production of a software product" [8].

2.2 Database

A database is understood as any system intended for the storage of organized information about a given subject [9]. Simple examples include a telephone directory, the record of employees in a book, or even a stamp collection gathered in an album, all characterized as series of data that constitute databases.

Among the main advantages of using a database system are secure access and manipulation of information, the possibility of structured and ordered storage, as well as the independence of the data in relation to the applications that use them. These aspects ensure greater reliability, consistency, and efficiency in handling information, making them fundamental elements for the development of modern computational systems.

2.3 The k_0 method

The k_0 factor of the isotope of an element to be analyzed can be defined, with reference to the gold comparator, as [10]:

$$\left(k_{0,Au}\right)_a = \frac{M_{Au}\theta_a I_{\gamma a}\sigma_{0,a}}{M_a\theta_{Au}I_{\gamma Au}\sigma_{0,Au}}$$

Fig. 1: The k_0 factor equation

Source: Simonits, De Corte, Hoste, 1975

where:

M is the atomic mass of the irradiated elements;

θ is the isotopic abundance of the isotopes of interest in the irradiated elements;

Iγ is the probability of gamma emission per decay for the considered transition;

σ0 is the neutron absorption cross section at thermal energy (2,200 m/s); with the index "a" referring to the analyte (the element of the sample to be analyzed) and the index "Au" referring to gold (and to the reaction $^{197}Au(n,\gamma)^{198}Au$, Eγ = 411.8 keV and $k_{0,Au} = 1$);

The k_0 factors, for most of the elements that can be analyzed by neutron activation analysis, have been experimentally determined with good accuracy and are found in the literature [11] [12]. The k_0 method was developed using the Högdahl convention [13], which assumes that the (n,γ) cross section varies according to the 1/v law in the thermal region, that is, up to approximately 1.5 eV, for which the Westcott factor is equal to 1 (g = 1). For nuclides that do not follow the 1/v law, the Westcott formalism [14] is adopted and requires the determination of the modified spectral index $r(\alpha)\sqrt{(T_n/T_0)}$ and the Westcott

factor g(T_n), with T_0 = 293.6 K corresponding to the neutron velocity of 2200 m/s, and T_n being the neutron temperature for a Maxwellian distribution.

This method requires precise characterization of the irradiation and detection facilities, the use of nuclear constants from the literature (k_0 factors, Q_0, and decay constants), as well as the determination of parameters necessary for calculating the activity of irradiated samples (detection efficiencies and gamma intensities).

The precise characterization of the irradiation facility requires the determination of the flux ratio (f)—the ratio between thermal and epithermal neutron fluxes—and the parameter α related to the distribution of the epithermal neutron flux, described by the energy function 1/E^(1+α). This is a measure of how far the actual epithermal neutron flux deviates from the ideal 1/E behavior. These two parameters are characteristic of the irradiation position in the nuclear reactor.

In the characterization of the detection system, a parameter of great importance to be determined is the detection efficiency within the energy range of interest and in the geometry of the experimental setup for measuring the induced activity in the sample.

In addition, the nuclear constants k_0 and $Q_0 = I_0/\sigma_0$, where I_0 is the resonance integral for the (n,γ) reaction, must be known to determine the concentration of a given element in the sample.

2.4 Determination of concentration

Within the scope of Neutron Activation Analysis with k0 standardization, the determination of the concentration of an element constitutes one of the fundamental steps of the analytical process, as it translates the measured radiation intensity into quantitative values associated with the sample. This relationship is established based on previously known nuclear parameters and corrections applied to the experimental conditions. In this context, the concentration (ρ) could be calculated according to the formulation presented by [10]:

$$\rho_a = \frac{A_{sp,a}}{A_{sp,Au}} \cdot \frac{\varepsilon_{p,Au}}{\varepsilon_{p,a}} \cdot \frac{1}{(k_{0,Au})_a} \cdot \frac{G_{th,Au} \cdot f + G_{e,Au} \cdot Q_{0,Au}(\alpha)}{G_{th,a} \cdot f + G_{e,a} \cdot Q_{0,a}(\alpha)}$$

$$A_{sp} = \frac{N_p}{m \cdot t_m \cdot S \cdot D \cdot C}$$

$$Q_0(\alpha) = \frac{I_0(\alpha)}{\sigma_0} = \left[\frac{Q_0 - 0{,}429}{(E_r)^\alpha} + \frac{0{,}429}{(2\alpha+1)(0{,}55)^\alpha}\right]$$

Fig. 2: Concentrarion equation

Source: Simonits, De Corte, Hoste, 1975

where:

Asp – specific count rate;

Np – net number of counts under the full absorption peak for the considered gamma energy during the measurement time tm;

m – mass of the element in the sample or of the irradiated monitor;

tm – measurement time;

S – saturation factor: S = (1 − e^(−λti));

D – decay factor: D = e^(−λtd);

C – counting factor: C = ((1 − e^(−λtm)))/(λtm);

tm – measurement time, in seconds;

ε – peak detection efficiency for energy Eγ;

k_0, Au(a) – i0 factor for the analyzed isotope, referenced to the gold comparator;

Gth – self-shielding correction factor for thermal neutrons;

Ge – self-shielding correction factor for epithermal neutrons;

f – ratio between thermal and epithermal neutron fluxes;

Q_0 – ratio between the resonance integral (I_0) and the thermal neutron cross section (σ_0), that is, $Q_0 = I_0/\sigma_0$, where σ_0 (n,γ) is the thermal neutron cross section;

α – parameter related to the distribution of the epithermal neutron flux, approximately given by 1/E^(1+α);

$\bar{E}_r$ – effective resonance energy.

III. MATERIALS AND METHODS

This chapter presents the materials and methods employed in the development and evaluation of K0-WEB. It first describes the experimental part, with emphasis on the standardized data used and the procedures for obtaining and organizing the information. Next, it addresses the software validation process, a fundamental step to ensure the reliability and accuracy of the results produced by the system. Finally, it details the calculation of uncertainties, covering the statistical methods and corrections applied to guarantee the scientific robustness of the analysis.

3.1 Experimental part

The experimental part was based on the use of standardized data from the intercomparison exercise organized by the International Atomic Energy Agency, as described in the technical document IAEA-TECDOC-2026 [15]. These data were selected primarily for their recognized reliability and for their use with other software, particularly K0-IPEN, which enables the validation of K0-WEB. They constitute a set of validated and traceable data, obtained under strict quality control by accredited laboratories, ensuring the legitimacy of the reference values.

3.2 Software validation

For the validation of the data generated by K0-WEB, the K0-IPEN program was used as a reference, as described by [16]. The choice of this system was based on its participation in an international intercomparison exercise conducted by the International Atomic Energy Agency [15] and published by [17]. Such participation granted K0-IPEN international recognition regarding its reliability, which legitimized its adoption as a benchmark for evaluating the effectiveness and accuracy of the newly proposed system. Figure 3 presents the table that compares the results obtained by K0-IPEN in relation to the certified values [16].

Element	Assigned value			k0-IPEN					E_n	Bias (%)
	X_{CRM}	±	U_{ref}	U_{ref} (%)	X_{lab}	±	U_{lab}	U_{lab} (%)		
As	21.7	±	2.0	9.2	21.8	±	3.3	14.9	0.03	0.5
Co	9.7	±	0.6	6.2	10.1	±	0.5	4.9	0.52	4.2
Cr	59	±	4	6.8	60	±	4	6.6	0.26	2.4
Fe	25,700	±	1,300	5.1	25,726	±	1,281	5.0	0.01	0.1
Hg	0.85	±	0.09	11	0.85	±	0.12	13.9	−0.01	−0.1
Mn	910	±	50	5.5	907	±	56	6.2	−0.04	−0.4
Sc	5.2	±	0.4	7.7	5.4	±	0.3	6.2	0.44	4.4
Th	5.3	±	0.4	7.5	5.7	±	0.3	4.8	0.76	6.9
U	1.56	±	0.20	13	1.56	±	0.11	7.2	−0.01	−0.1
V	46.5	±	2.8	6.0	45.4	±	4.4	9.6	−0.22	−2.5
Zn	319	±	20	6.3	329	±	19	5.9	0.35	3.1

Fig. 3: Mass fractions of some elements contained in the irradiated sample (IRMM BCR–320R)

Source: DIAS et al., 2023

3.3 Calculation of uncertainties

For the calculation of uncertainties, error propagations among the variables were carried out, considering the correlations between them. In other words, Covariance Analysis was applied [18]. This approach proved to be essential, since the assumption of completely independent variables could lead to an inadequate estimate of the uncertainties. Considering the correlations made it possible to more realistically represent the joint contribution of the variables to the result, ensuring greater scientific rigor and reliability in the values obtained.

IV. SOFTWARE MODELING

This chapter presents the modeling of K0-WEB through the Unified Modeling Language (UML). The use case diagrams are described, representing the main user interactions with the system, including operations such as project creation, sample registration, data import, and recording of nuclear parameters. Finally, the class diagram is presented, which highlights the internal structure of the software and the relationships among its components.

4.1 Unified modeling language

The Unified Modeling Language (UML) is currently the most widely used language for software specification and design within the object-oriented approach. UML is the tool that enables software modeling "visually," making it easier to move from system requirements to implementation in a user-friendly manner [19].

UML covers all stages of software development but is mainly used to translate system requirements (at a high level and closer to the user) into codifiable components (closer to the application). Even though it lies between these two layers, UML aims to be easy to understand for all stakeholders [19]. UML is a language, and as such, it is a means of communication. Through graphical diagrams, it is easier to discuss and visualize ideas and solutions within the team or with the user—much simpler than using code programs [20]. UML is defined as a language; it can be used to describe things [21]. These things can be understood as the functioning of an information system.

It is important to emphasize that not all diagrams are used during the software development process. Part of the analysis process is to verify which diagrams are truly necessary to build, so that they can effectively assist in development, rather than fostering delays and excessive documentation without concrete utility.

In this regard, for the development of K0-WEB, use case and class diagrams were created, which will be defined and presented in the following subsections.

4.2 Use case diagram

With the aim of providing the user with a simple presentation of the system's functionalities, the use case diagram presents itself as a viable alternative. It can be said that the use case diagram provides an external view of the system, defining its scope and indicating the services it contains and the services it provides [20]. The use case diagram is also used to demonstrate the interaction between the user and the system. The role of the user in a use case diagram is described by the term actor. An actor, that is, the representation of a system user, is responsible for carrying out or executing the use case, considering its flows and conditions.

In short, a use case diagram can be defined as a graphical summary of all the functionalities expected from the software under development [21]. Figure 4 shows the use case diagram of the K0-WEB system.

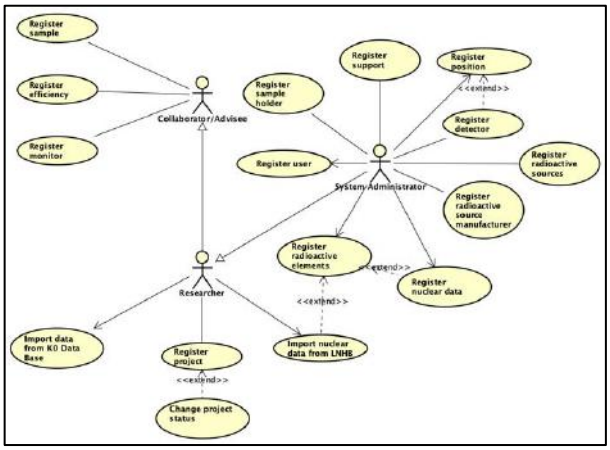

Fig. 4: Use case diagram

Source: Elaborated by the authors

4.3 Class diagram

The class diagram provides a comprehensive view of the structures that are manipulated or managed by the system. In this type of diagram, the central element consists of classes. As its name suggests, a class diagram is composed of classes that are related to one another. Each class, represented by a rectangle in the diagram, is organized into three sections, which respectively indicate the class name, its attributes, and its operations. Attributes describe the properties of the class, that is, characteristics that must be present in any object instantiated from it. Operations, also called methods, define the behavior that the instantiated object can perform [22].

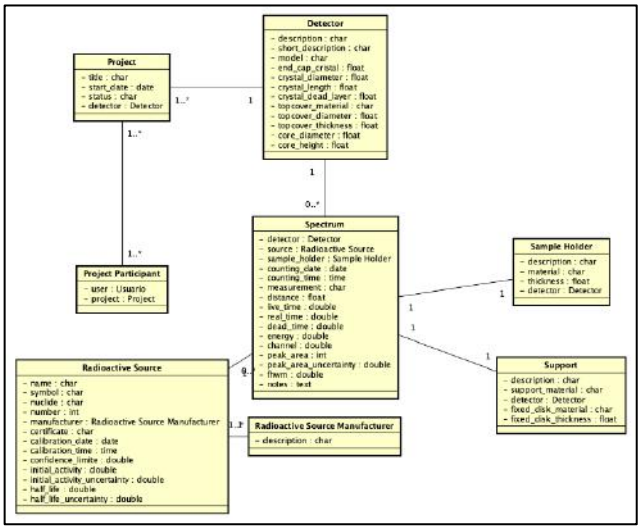

Fig. 5: Class diagram

Source: Elaborated by the authors

For explanatory purposes, the following scenario is proposed: the class Dog, understood as a representation of a real-world element, has attributes (characteristics) and methods that define the membership of an object in that class. An object of the Dog class presents, for example, two ears, four legs, and a tail (attributes), in addition to performing functions such as barking and hunting (methods). Figure 5 shows the class diagram of the K0-WEB system, highlighting the way these classes are related.

V. SOFTWARE IMPLEMENTATION

In this chapter, the results to be obtained from the development of the system for determining element concentrations based on the k_0 standardization method of neutron activation analysis will be presented.

5.1 Python programming language

Language created in the 1990s by Guido Van Rossum, with a focus on users such as physicists and engineers. Being a very high-level language, it is easy to understand "and supports multiple programming paradigms: imperative, object-oriented, and functional" [23].

With a clear and somewhat concise syntax, the readability of the written code is enhanced, making it a language with greater productivity [24].

Python has become a highly popular programming language due to the characteristics mentioned, particularly its efficiency. It is possible to achieve significant results in terms of execution, whether for automation, data analysis, or web programming, among others, with very few lines of code. It is also important to highlight its simplicity of syntax when compared to other programming languages, such as Java or C++ [25].

Alongside the features presented, the Python language has a rich library consisting of modules with pre-created processes/functions, making it possible to build sophisticated applications using code with a relatively simple appearance and without the need for rewriting [26].

5.2 Django framework

Alongside the Python programming language, there is the Django framework, which is used for developing Python-based web software. A framework is "a set of classes implemented in a given programming language, designed to facilitate the creation of applications" [25].

Django is based on the DRY (Don't Repeat Yourself) principle, that is, "do not repeat yourself." This principle aims to avoid code redundancy, preventing multiple parts of the code from being copied and pasted into other parts of the application, which would make the maintenance process highly complex. Moreover, it is a mature framework, with years of development, and is used by major companies in the technology market, such as Instagram, Spotify, YouTube, and Dropbox [25].

Thus, the Django framework proves to be a good choice for working together with the Python language in the development of web software.

VI. RESULTS AND DISCUSSION

In this chapter, the results obtained with K0-WEB in determining elemental concentrations using the k0 standardization method of Neutron Activation Analysis are presented. The presentation of these results aims not only to demonstrate the practical applicability of the developed system but also to highlight its ability to reliably and accurately reproduce established reference values.

6.1 Import of nuclear data

As an integral part of the variables involved in calculating elemental concentrations based on the k0 standardization method of neutron activation analysis, the nuclear data of radioactive elements are important and must be kept up to date to provide the highest possible accuracy to the results obtained.

These data are commonly made available by the *Laboratoire National Henri Becquerel* (LNHB) on its official website. Obtaining these data manually proves to be laborious and error-prone, since manual actions are inherently subject to such risks.

In this context, the combined use of web scraping techniques for file retrieval and file-reading techniques allows K0-WEB to automatically import the nuclear data provided by LNHB, without the need for human intervention. This approach reduces the occurrence of errors, speeds up the process, and enables the maintenance of a data history, when applicable. It is also worth emphasizing the originality of this procedure in comparison with other software designed for calculating elemental concentrations based on the k0 method of Neutron Activation Analysis, thereby conferring an innovative character to the system.

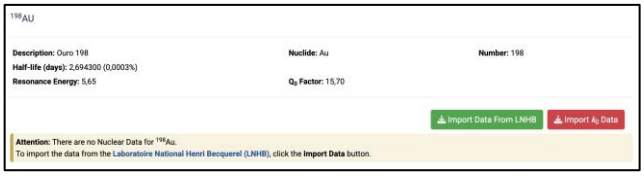

Fig. 6: Interface for importing nuclear data

Source: Elaborated by the authors

These data are imported directly from the LNHB official website into the system and stored in the database. Thus, in addition to maintaining a historical record should the data be updated by LNHB, this automated process minimizes the incidence of errors arising from manual handling. Figures 6, 7, and 8 below respectively show the interface for importing nuclear data, the result of this import, and the source data from the website, for comparison purposes, of the radioactive element ^{198}Au.

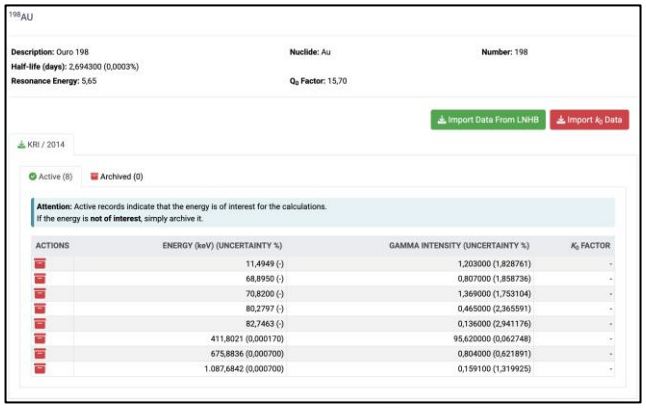

Fig. 7: Result of nuclear data import

Source: Elaborated by the authors

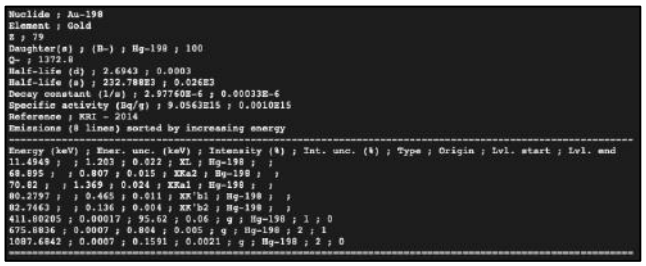

Fig. 8: Original nuclear data on the LNHB website

Source: LNHB (2014)

6.2 Import of k_0, Q_0, and Er data

Just as nuclear data are an integral part of the variables involved in calculating elemental concentrations based on the k_0 standardization method of neutron activation analysis, the k_0 factor, for each energy of interest of the radioactive element, is required.

These data are commonly made available by the Kayzero Data Base on its official website. A spreadsheet file containing the data is provided for manipulation. Obtaining these data manually proves to be laborious and error-prone, since manual actions are inherently subject to such risks.

In this context, the developed platform includes a function that reads the file obtained from the website and, through file-handling techniques, can automatically extract the k_0 factor for each energy of interest, for use in calculating elemental concentrations based on the k0 standardization method of neutron activation analysis.

In this sense, the use of file-reading techniques allows K0-WEB to automatically import the data required for the calculation, such as the k_0 factor for each energy of interest, without the need for human intervention. This approach reduces the occurrence of errors, streamlines the process, and enables the maintenance of a historical record of the data, when applicable. It is also worth emphasizing the originality of this procedure in comparison with other software designed for calculating elemental concentrations based on the k_0 method of Neutron Activation Analysis, thereby conferring an innovative character to the system. Figures 9 and 10 below respectively show the interface for importing k_0 data and the result of this import, for the radioactive element ^{198}Au.

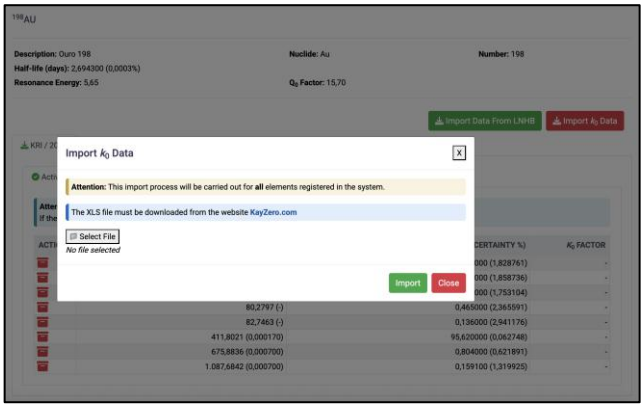

Fig. 9: Interface for importing k₀ data

Source: Elaborated by the authors

Fig. 10: Result of k₀ data import

Source: Elaborated by the authors

6.3 Result of the concentration

The values obtained demonstrate the effectiveness of K0-WEB in the identification and quantification of trace elements. The consistency of the results reinforces and validates the use of K0-WEB. It should be noted that any differences observed in the last decimal places arise from particularities related to the type of numerical data employed by each programming language used.

Table 1 presents the comparison of the concentration results obtained with K0-IPEN and K0-WEB.

Table 1 - Comparison of concentration results

Radionuclide	Energy (keV)	K0-IPEN (unc. %)	K0-WEB (unc. %)
^{28}Al	1778.90	5.9635E+06 (2.94)	5.9673E+06 (2.94)
^{27}Mg	170.70	3.6304E+04 (38.89)	3.5851E+04 (38.81)
	843.80	5.4194E+05 (5.84)	5.4159E+05 (5.84)
	1014.80	5.2921E+05 (11.37)	5.2917E+05 (11.36)
^{38}Cl	1642.70	7.0859E+04 (5.24)	7.0904E+04 (5.24)
	2167.40	7.2008E+04 (4.60)	7.2046E+04 (4.61)
^{52}V	1434.10	5.2249E+03 (4.71)	5.2276E+03 (4.70)
^{56}Mn	846.80	2.9402E+03 (3.84)	2.9384E+03 (3.83)
	1810.70	2.7475E+03 (3.41)	2.7494E+03 (3.41)
	2113.10	2.7342E+03 (4.10)	2.7357E+03 (4.10)

Source: Elaborated by the authors

VII. CONCLUSION

This work proposed the development of K0-WEB, aimed at determining elemental concentrations based on the k_0 standardization method applied to neutron activation analysis, in accordance with the practices adopted at the Nuclear Metrology Laboratory (LMN) of the Institute for Energy and Nuclear Research (IPEN). The main objective was to automate and enhance the calculation process, reducing human interference in critical stages and, consequently, mitigating errors associated with manual data handling.

The use of K0-WEB provides significant agility in performing analyses, while ensuring greater reliability and reproducibility of the results. By delegating the most sensitive computational steps to the software, the user can focus efforts on the scientific interpretation and validation

of the obtained data, promoting a more efficient and safer approach in the context of nuclear analyses.

The results presented throughout this study highlight the high efficiency and accuracy of K0-WEB. The comparison with the K0-IPEN software revealed a remarkable similarity in the values obtained, demonstrating the robustness of the implemented algorithm and the adequacy of the methods employed. Such performance reinforces the potential of K0-WEB as a useful tool for high-precision laboratory applications.

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