Development of a Web Free Software for the Absolute Efficiency Calibration for HPGe Type Detectors

Thiago José Sampaio Kaiser[1], Renato Semmler[2], Gean Batista de Lima[3]

[1]Master's Student in the Nuclear Technology Program at the University of São Paulo, Brazil.
[2]Institute of Energy and Nuclear Research (IPEN / CNEN – SP), Brazil
[3]Master's Student in the Nuclear Technology Program at the University of São Paulo, Brazil.

Abstract— The IEA-R1, swimming pool research reactor, from the Institute of Energy and Nuclear Research (IPEN), among other uses, the instrumental neutron activation analysis technique is widely used, and successfully, by the Neutron Activation Laboratory (LAN), using the comparative method. In this method a sample is irradiated simultaneously with a standard. In order to overcome the difficulty of a multi-elementary analysis, because it was necessary to prepare several standards, the k0 method of neutron activation was developed. In method k, the concentration of sample elements is calculated in relation to a comparator element, generally gold. However, for the use of the k0 method, it is necessary to accurately determine the detection efficiency in the energy range of interest and the geometry of the experimental arrangement. In order to circumvent the manual processing of the data in spreadsheets, which could be affected by errors, a free code web software was developed for calibration in absolute efficiency of an HPGe type detector for neutron activation analysis based on the k0. We used the free, low learning curve standardized Python programming language in the eScience project, which is part of the software, and the Django web framework with a simple and intuitive interface. In the system it is possible to register the detectors, radioactive sources and their manufacturers, projects and spectra, attributes necessary to calculate the absolute efficiency of an HPGe type detector. In addition to calculating efficiency, the system plots the graph with the efficiency points, trend curve, with possibility of adjustments, and error bar representing the uncertainties. The system issues reports on spectra and efficiency data for each project. The reports make it possible to check the data as well as its use in other applications. Because it is a web software, its access is allowed from any device with an internet connection. Another result obtained with the system is the reduction of the possibility of errors with the manual treatment of the data in spreadsheets.

Keywords— django, free software, k0, neutron activation, python.

I. INTRODUCTION

The IEA-R1 is a pool type, moderate and water-cooled research reactor utilizing beryllium and graphite elements as reflectors. The core of the reactor is located 6.9 m from the pool surface, has the shape of a parallelepiped, and consists of 20 standard fuel elements, 4 fuel control elements, about 25 reflectors and 7 irradiation positions. Designed to operate at a maximum power of 5 MW, this reactor, in the first decades, operated the power of 2 MW. Its first criticality occurred on September 16, 1957 and, after the initial testing and commissioning phase, started to operate at 2 MW, in an 8-hour cycle, 5 days a week. From 1993, it began operating in cycles of 64 continuous hours per week at 3.5 MW of power. As of August 2011, it started to operate at 4.5 MW of power. The increase in power to 4.5 MW allows the irradiation of materials with thermal neutron fluxes of the order of $9.7.10^{13}$ n/cm².s and epithermal and fast neutrons of the order of 10^{13} n/cm².s. Currently, the IEA-R1 reactor is used for the following purposes: a) Production of radionuclides for use in nuclear medicine; b) Production of radionuclides used in industrial applications; c) Research in Nuclear Physics and Solid State; d) Neutronography services; e) Training of licensed personnel to operate reactors; f) Irradiation of samples for multielement analyzes using the Neutron Activation Analysis technique in geological materials, industrial products such as plastics and resins, catalysts, petroleum, metals and metal alloys, archaeological samples, animal and human tissues, plants, food and environmental samples.

Among the reactor uses described above, the instrumental neutron activation (INAA) technique, an

important and powerful technique that allows the knowledge of the concentration of chemical elements in samples, has been successfully used in numerous experiments carried out by the Laboratory of Neutron Activation (LAN) of IPEN (Institute of Energy and Nuclear Research). For more than 40 years the LAN has been analyzing different matrices such as geological, biological, archaeological and environmental, among others, using the comparative method (FUGA *et al.*, 2008, SAIKI, SOARES and ADACHI, 2008). In this comparative method, sample and standard (material with known concentration and mass of the element to be determined) are irradiated simultaneously with neutrons, under the same conditions, and both are measured under the same experimental conditions. In this way, all parameters associated with irradiation and detection are the same for both the sample and the standard, making it possible to determine the concentration of a given element in the sample through a simple comparison between the activities induced in the sample and in the standard. However, for multi-element analysis this procedure requires the preparation or acquisition of standards for each of the elements to be analyzed, which makes the method very laborious, expensive and time consuming, and requires high purity reagents, which are usually expensive. The time spent in the analysis also increases due to the measurement time of the patterns. In addition, some elements present in the sample cannot be analyzed due to the absence of a corresponding standard or because of their nuclear characteristics.

To overcome these difficulties, the k_0 method of neutron activation was developed by the Institute for Nuclear Sciences, Gent, Belgium (DE CORTE, 1986). This is a "quasi-absolute" neutron activation analysis technique which, because of its excellent accuracy, has emerged as an alternative to the comparative method, eliminating some of its disadvantages. The factors k0 are independent of the reactor spectrum and detector characteristics and have been experimentally determined for several target nuclei (DE CORTE and SIMONITS, 2003). The concentration of the elements is calculated relative to a comparator element, generally gold, eliminating the need for standards. The method k_0, because it allows the determination of the elemental concentration with great accuracy, has been widely accepted by users in several laboratories of the world, including Brazil (BACCHI, FERNANDES, DE OLIVEIRA, 2000).

A new pneumatic transfer system for irradiation of samples in the core of the IEA-R1 reactor was implemented to carry out multielement analyzes using the Neutron Activation Analysis technique (FERNANDO, 2011). This pneumatic station has a transfer time of

approximately 12 s and is suitable for short-term irradiation (up to 30 minutes) Long-term irradiation is performed on the Water-cooled Irradiation Element (EIRA). For the use of the neutron activation method k0, a precise characterization of the irradiation position is required as well as a characterization of the detection system. The precise characterization of the irradiation facility requires the determination of the ratio between the thermal and epithermal neutron fluxes (f) and the parameter (α) related to the epithermal neutron flux distribution, approximately given by $1/E^{1+\alpha}$ (it is a measure of how far the epithermal neutron flux from ideal behavior 1/E) (DE CORTE, 1986). These 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 in the energy range of interest and in the geometry of the experimental arrangement.

There are some softwares available that allow the determination of the efficiency curve, such as the k_0-IAEA program, KayWin, Gespecor, Hyperlab, Hypermet. The k0-IAEA program is provided free of charge by the International Atomic Energy Agency (IAEA) to neutron activation laboratories. However, its structure of operation, insertion of data in the permanent database and the analysis of the spectra are not friendly to be realized. The software KayWin, Gespecor, Hyperlab has a high cost for acquisition, over three thousand euros, and the latest version of Hypermet is 2008, which makes it incompatible with current computer systems.

The objective of this work was the development and implementation of a free code web software for the calibration of the absolute efficiency of an HPGe type detector for neutron activation analysis. In a complementary way, the aim was to integrate the software to the e-Science project to obtain gamma ray data from the cataloged projects, with a view to performing the absolute efficiency calibration efficiency curve determination.

It should be noted that the development was aimed at meeting the specific needs of CERPq (Center of the Research Reactor of IPEN), applying the concepts of software usability, at an extremely low cost when compared to the acquisition of proprietary software. It is also worth mentioning that it is a web-based software, access to information is available regardless of geographical location, and only Internet access is required.

II. MATERIALS AND METHODS

The present work was developed within the scope of the Cooperation Agreement signed between the Institute of Energy and Nuclear Research - IPEN and the Federal

Institute of Education, Science and Technology of Rondônia - IFRO and, therefore, the activities related to the development of the project happened in the dependencies of IFRO with esporadics visits to IPEN.

2.1 Software Engineering

Software Engineering emerged in the mid-1970s in an attempt to circumvent the software crisis and provide an engineering (more systematic and controlled) treatment to the development of complex software systems. 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 each other, composing the software architecture, which must be executed in computational systems. A formal definition of Software Engineering is the creation and use of sound engineering principles in order to obtain economical software that is reliable and that works efficiently on real machines (PRESSMAN, 2006).

2.1.1 Determination of requirements

Through the Engineering of Requirements one can define what really must be built in a software. The initial set of requirements must be to represent what the user wants and needs, given that software full of options and functionalities, since the customer needs a "lean" and simple system, is unnecessary. According to GUEDES (2011, p. 22), "the requirements survey and analysis steps work with the problem domain and try to determine 'what' the software should do and if it is actually possible to develop the requested software." In this sense, in order to actually understand the problem to be solved, it is necessary to understand the user's wishes regarding the system now being projected. In this paper, Guies (2011, p. 22) states that "in the stage of requirements gathering, the engineer seeks to understand the needs of the user and what he wants the system to be developed." It is then verified the real need to raise the requirements of a software in the initial stage of its development.

2.2 Database

A database is understood to mean any system of data storage on the subject (KORTH; SILBERSCHATZ; SUDARSHAN, 2006). A phone book, a book record, a collection of stamps in an album, each of the data series is a database.

Among the advantages of using a database can be found security, data storage in an orderly manner and data independence in relation to applications.

2.2.1 SQL

Structured Query Language, SQL, was originally developed in the early 1970s at IBM's San Jose labs, within the w: System R project, which aimed to demonstrate the feasibility of implementing the relational model proposed by E. F. Codd. The SQL language is the most used and is a standard in databases, and this stems from its simplicity and ease of use. It differs from other database query languages in the sense that a SQL query specifies the form of the result and not the path to get there. ROB and CORONEL (2011) state that: "Its basic set of commands has a vocabulary of less than 100 words. And, what is better, SQL is a non-procedural language: just enter the command on what should be done. There is no need to worry about how it should be done." (ROB and CORONEL, 2011, p.224). SQL presents a series of commands that allow the definition of data, called DDL (Data Definition Language), composed among others by the Create commands, which is intended to create the Database, the tables that compose it, in addition to the relationships between the tables. As an example of the DDL class we have the Create, Alter, Drop and Rename commands (DATE, 2004). Data Manipulation Language (DML) commands, intended for queries, insertions, deletions, and changes to one or more records of one or more tables simultaneously. As an example of DML class commands we have the Select, Insert, Update, Delete, Commit and Rollback commands.

2.3 Absolute efficiency calibration

In gamma spectroscopy, in the characterization of a detection system, the parameters of great importance to be determined are: calibration in energy, calibration of the resolution in energy and calibration of the detection efficiency in function of the energy, in the interval of energy of interest and in the geometry of the experimental arrangement. Gamma spectrum analysis involves, firstly, the assignment of the energy values to the spectrum peaks and, subsequently, the determination of the number of counts of each peak. The determination of the energy of the spectral peaks is performed by calibrating the detector with standard radioactive sources that emit gamma rays with known energies and intensities. In this way the relation between the gamma radiation energy and the channel number must be established. The performance quality of a detection system employed in the use of measurements of energy values is characterized by the pulse width of the distribution obtained with particles of the same energy. Even in the case where each particle deposits exactly the same energy in the detector, the pulse height distribution will not be a single line. Instead, there will always be a finite width which will be due to statistical fluctuation in the number of charge carriers

produced in the detector; due to the electronic noise produced in the detector itself, the preamplifier and the amplifier; and the incomplete collection of loads produced in the detector. The detector (Canberra 8) semiconductor of the hyperpure germanium type (HPGe), Canberra brand model GX3018, with cylindrical geometry and relative efficiency of 30% for the energy of 1332.5 keV of ^{60}Co was used. For this energy, the resolution is 1.8 kV. The associated electronics is the conventional one for simple spectroscopy. The detector is connected to a Canberra DSA-LX multichannel analyzer on a microcomputer available from IPEN's neutron activation laboratory. Gamma ray spectra were collected and processed using the Genie 2000 v.3.3 software. The efficiency curve for the HPGe spectrometer was determined using the standard sources of 241Am, 243Am, 133Ba, 166mHo, 60Co, 57Co, 54Mn, 137Cs, 152Eu and 22Na, with energies ranging from 43 keV to 1500 keV. The efficiency was adjusted according to the energy by means of appropriate parameterization. The parameterization used in this work is the Least Squares Method using the covariance matrix methodology that provides information about the existence of the level of correlation between the uncertainties in the parameters of the adjusted function and calculated efficiencies for different energy values (DE CORTE et al, 1993). All the described experimental analysis was applied to experimental data obtained at the IPEN Research Reactor Center (CERPq).

III. SOFTWARE MODELING
3.1 Unified Modeling Language

The Unified Modeling Language (UML) is the most widely used language for the specification and design of software in the object-oriented approach. The UML is the instrument that allows the modeling of the software "visually", making it easy to start from the requirements of the system to the implementation in a friendly way (BRAHA and RUMBAUGH, 2006). GUEDES (2011) states that: "The UML - Unified Modeling Language - is a visual language used to model software based on the object orientation paradigm. It is a general-purpose modeling language that can be applied to all the fields of application. " (GUEDES, 2011, p.19). The UML covers all stages of software production but is mainly used to translate system requirements (at a high level and closer to the user) into coded components (closer to the application). Even among these two layers, the UML aims to be easy to understand for all involved (BRAHA and RUMBAUGH, 2006). In this sense, GUEDES (2011) states that: "It should be made clear, however, that UML is not a programming language, but a modeling language, a notation, whose purpose is to help software engineers define the characteristics of the system (...). Such characteristics can be defined through UML before the software actually begins to be developed. " (GUEDES, 2011, p.19). UML is a language, and as such, it is a means of communication. PENDER (2004) states that through graphic diagrams it is easier to discuss and visualize the ideas and solutions between the team, or the user. Much simpler than with code programs.
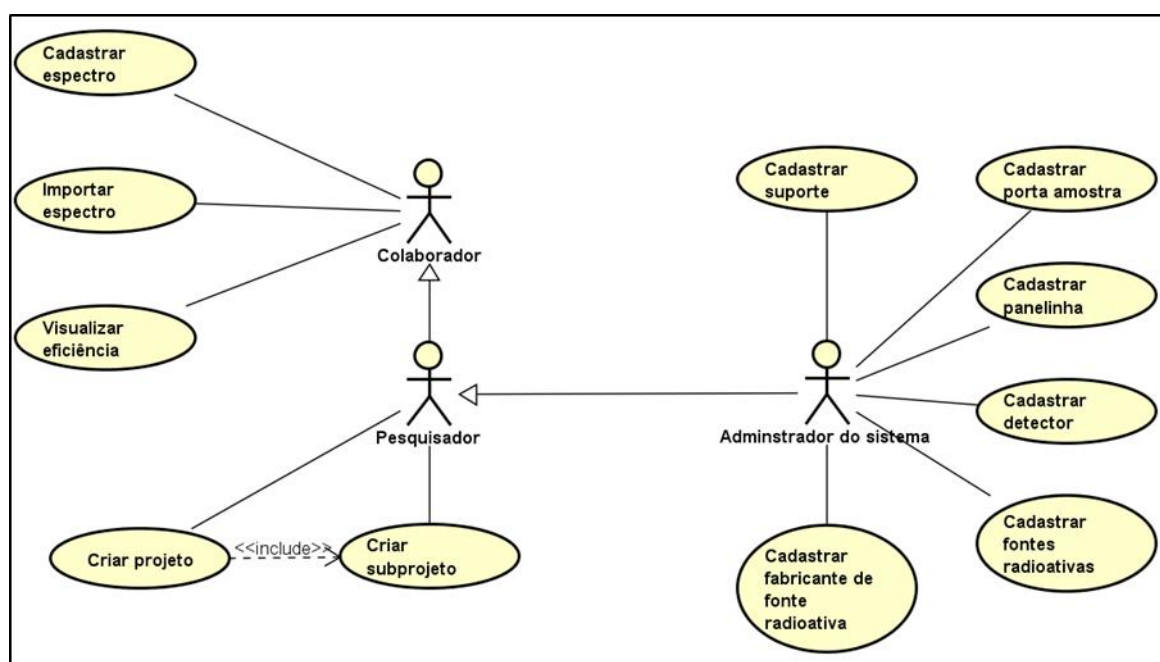

Fig. 1: Use-case diagram

Source: Elaborated by the authors

3.2 Use-case diagram

In order to provide the user with a simple presentation on the functionalities of the system, the use case diagram is presented as a viable alternative, since, according to GUEDES (2011, page 52), "the case diagram of use seeks, through a simple language, to enable the understanding of the external behavior of the system (...) by any person (...) ". It can be said that the use case diagram provides an external view of the system, delimiting its scope and indicating the services it has and the services it provides (PENDER, 2004). The use-case diagram is also used to demonstrate user interaction, through actors, with the system. Figure 1 shows the use cases of the developed system.

3.3 Class diagram

The class diagram provides a view of all the "structures" that are manipulated and/or managed by the system. The fundamental element of this type of diagram is the classes. GUEDES, 2018 states that: "Its main focus is on allowing the visualization of the classes that will compose the system with their respective attributes and methods, as well as on how the diagram classes relate, complement and transmit information among themselves. This diagram presents a static view of how classes are organized, worrying about how to define their logical structure. " (Guedes, 2018, p 112). Figure 2 presents the classes, and how they relate, of the developed system.
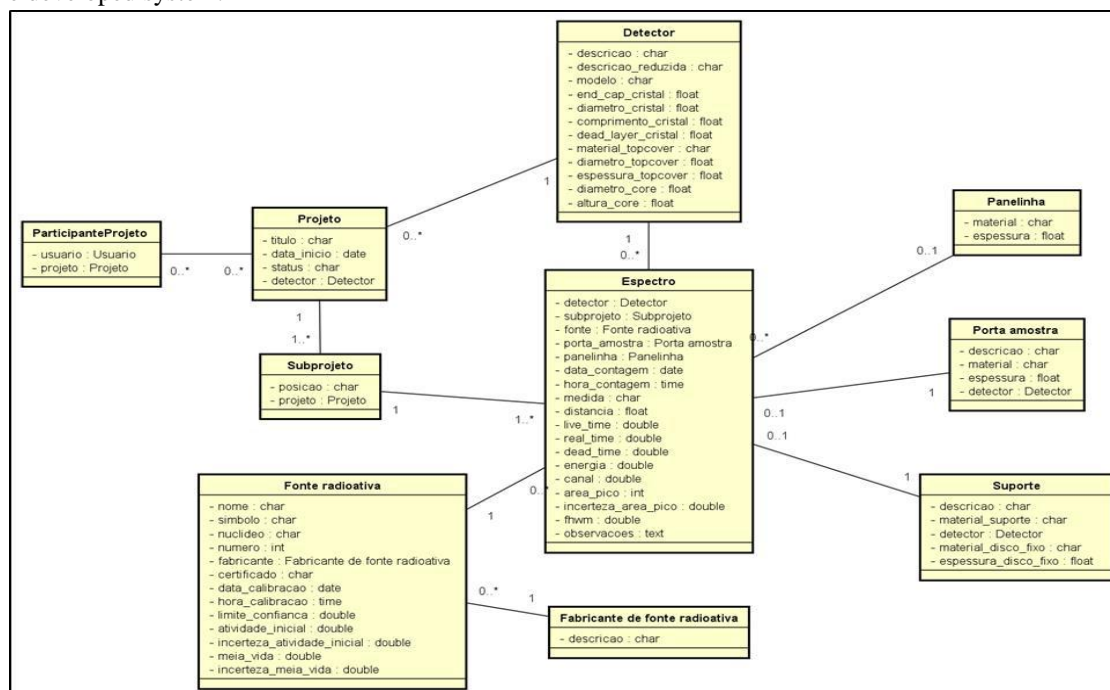
Fig. 2: Class diagram

Source: Elaborated by the authors

IV. SOFTWARE IMPLEMENTATION

4.1 Python

Language created in the 1990s by Guido van Rossum focusing on users as physicists and engineers. Because it is a language of the highest level, it has an easy understanding "and that supports multiple programming paradigms: imperative, object oriented and functional" (CRUZ, 2015, p.3).

With a clear and somewhat summarized language, the readability of the written code is favored, making it a more productive language. (BORGES, 2010). Among the main features of the Python language are: a) Low learning curve; b) Simplicity of the code; c) Library of functions; d) Multiplatform; e) Free software.

4.2 PyCharm

PyCharm is an integrated development environment, that is, a programming environment that is able to provide the developer with a single, comprehensive and tool-based environment that speeds up the process of building software used specifically for the Python programming language. Owned by the JetBrains company, it has paid version (Professional) and free (Community). In this work, due to the condition of Professor of the Federal Institute of Rondônia, had been used the professional version, since teachers are contemplated with a JetBrains program of unrestricted use of its tool for free.

V. RESULTS AND DISCUSSION

5.1 Comparison between spreadsheets and developed software

The current method of calculating absolute efficiency is done using spreadsheets, with manual data entry. This type of control presents a greater possibility of human errors being committed, which can compromise the result

and all the processes that are associated with it. Figure 3 shows how the data is manipulated in the spreadsheet that is currently used.
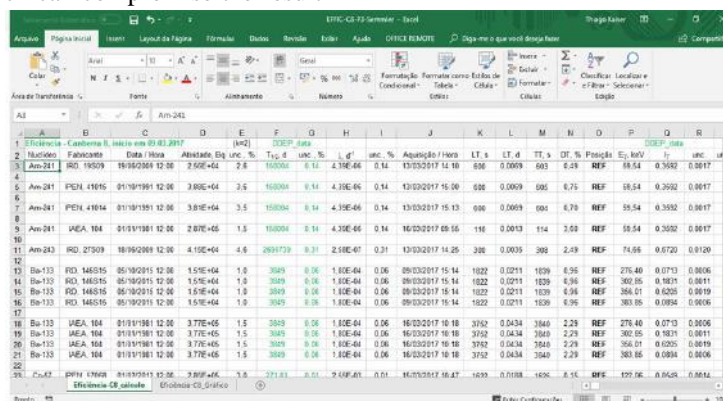
Fig. 3: Spreadsheet with data

Source: Elaborated by the authors

In addition to calculating the efficiency values for each energy, the efficiency curve and its adjustment are also obtained using the spreadsheet, as shown in figure 4.
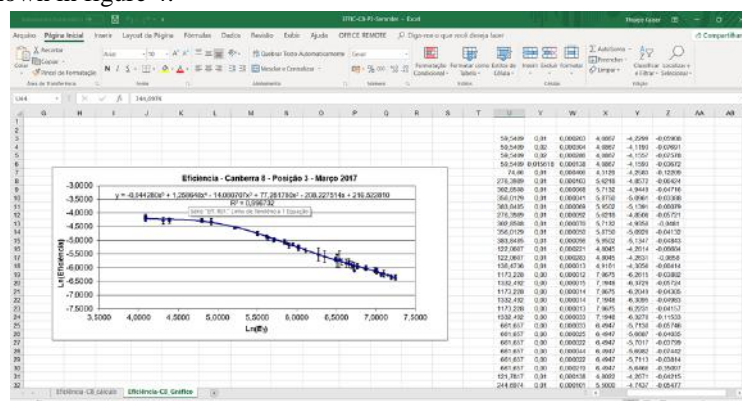
Fig. 4: Spreadsheet with efficiency chart

Source: Elaborated by the authors

The use of an information system, developed specifically for this purpose, provides the reduction in the incidence of errors during the handling of the data. It also provides the structuring and organization of all data artifacts that make up the scope of the activation analysis.

The system, developed in the Python language using the Django web framework, makes it possible to register the detectors, radioactive sources, projects and subprojects. All these registrations follow simple and

intuitive interface in the system, based on the user experience.

The efficiency calibration curve is obtained for each subproject, that is, for each counting position of a given detector in a specific project, therefore, it is necessary to create the projects in the system. The interface for project registration can be seen in figure 5 and the subproject visualization interface in figure 6.

Fig. 5: Project registration
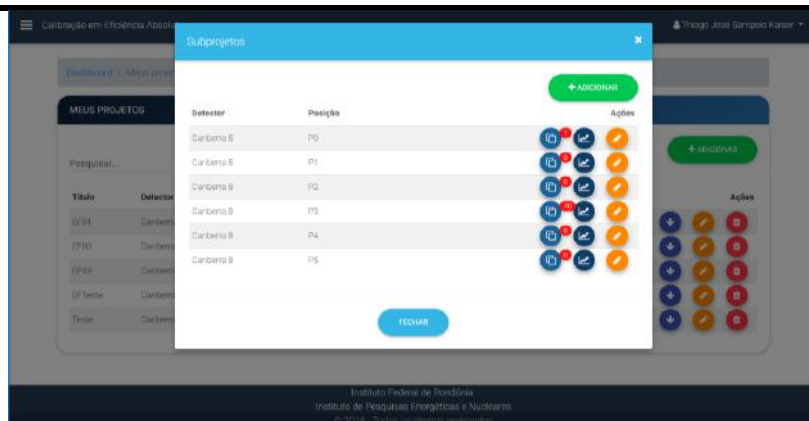
Source: Elaborated by the authors

Fig. 6: List of subprojects

Source: Elaborated by the authors

Figure 7 shows the list of gamma spectra associated with a given subproject of absolute efficiency calibration. It is the systematized representation of the spreadsheet data presented previously in figure 3.

Fig. 7: List of spectra

Source: Elaborated by the authors

In addition to the evident improvement in the organization of data, a clear and intuitive interface for insertion of new data into the project is observed. In the spreadsheet, you need to navigate between cells, using the keyboard or mouse, until you find the desired cell and enter the values manually. That's when mistakes can happen. When you enter the value in an incorrect cell, the entire calculation will be based on incorrect data, causing an error in the efficiency calculation.

It should be noted that, even with the manual insertion of the data, the system, when saving, performs the validation of this data. This way you can minimize the possibility of entering incorrect data.

5.2 Efficiency calculation results

With the data of the spectra duly inserted in the software, the efficiency was calculated for each energy of interest and, for purposes of validation of the software, the values of the obtained efficiencies were compared with those obtained by the use of the spreadsheet. Table 1 shows the results of the efficiency calculations for position 03 (three) of the Canberra 8 detector. Column A has the calculation made by the use of the spreadsheet and in column B that obtained by the system for a standard radioactive source of ^{133}Ba, (IRD, 146S15 certificate). The uncertainties for the values of the efficiencies were obtained by simple propagation of the uncertainties of the quantities involved in the calculation: number of counts in the photopic, probability of gamma emission by decay of the line considered, initial activity of the standard source and half-life of radionuclide.

Table.1 - Comparison of efficiency: ^{133}Ba / IRD 146S15

Energy (keV)	Efficiency A	Uncertainty A (%)	Efficiency B	Uncertainty B (%)	Difference (%)
276,40	7,6632E-03	1,40	7,6842E-03	1,37	0,27
302,85	7,0227E-03	0,88	7,0184E-03	0,96	-0,06
356,01	6,0427E-03	0,66	6,0452E-03	0,67	-0,04
383,85	5,7906E-03	1,30	5,8011E-03	1,21	0,18

Source: Elaborated by the authors

The difference obtained by comparing the values of the efficiencies is due to the way of obtaining the area of the peak. In the case of the spreadsheet the software used in the deconvolution of the spectra was the Hypermet, in the 2008 version, and for the use of the developed system, the software was Genie 2000 v.3.3. Area differences are shown in Table 2 and may be considered negligible.

Table.2 - Area comparison and uncertainty: ^{133}Ba / IRD 146S15

Energy (keV)	Area A	Area B	Uncertainty area A (%)	Uncertainty area B (%)	Difference area (%)
276,40	13702	13741	1,00	0,96	0,28
302,85	32246	32230	0,40	0,56	-0,05
356,01	94028	94078	0,30	0,33	-0,05
383,85	12982	13007	1,00	0,88	0,19

Source: Elaborated by the authors

5.3 Efficiency chart

Figure 8 shows the logarithmic efficiency graph generated from the developed system. A grade 5 polynomial fit was obtained.

Eficiência: $- 0,04750x^5 + 1,36896x^4 - 15,52965x^3 + 86,49699x^2 - 236,76939x^1 + 251,06350$
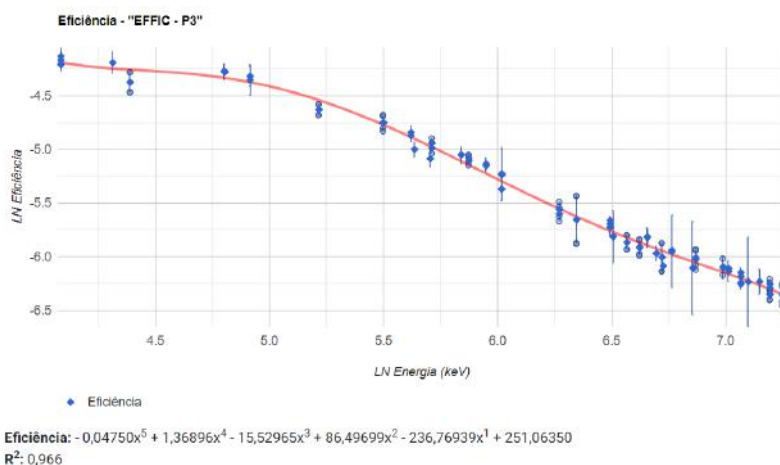R^2: 0,966

Fig. 8 Graph obtained in the developed system Source: Elaborated by the authors

For comparison purposes, the efficiency graph, calculated with the same data using the Excel worksheet is shown in Figure 9.
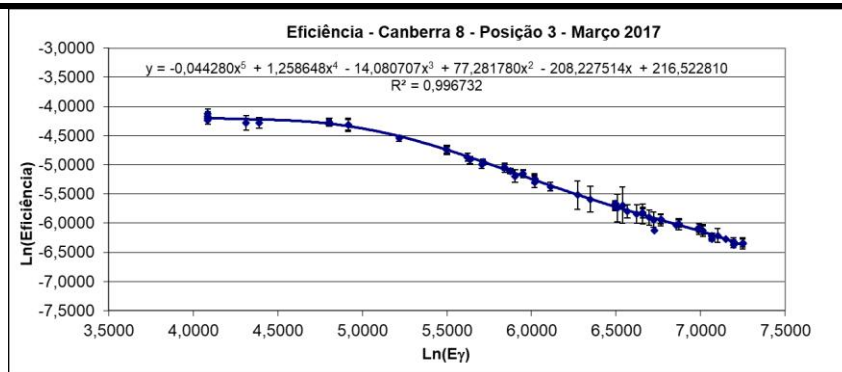
Fig. 9: Chart obtained in spreadsheet

Source: Elaborated by the authors

5.4 Issuance of reports

In addition to performing calculations and managing stored data, the system is able to issue several reports, in Portable Document Format (PDF) and Comma-separated values (CSV) formats, so that they can be used in other platforms, at the discretion of the researcher. Figure 10 shows the spectra report, its efficiencies and uncertainties, in PDF format, for a given subproject. Figure 11 shows the report, with the same data, in the CSV format.

Fig. 10: Reporting efficiency data in PDF
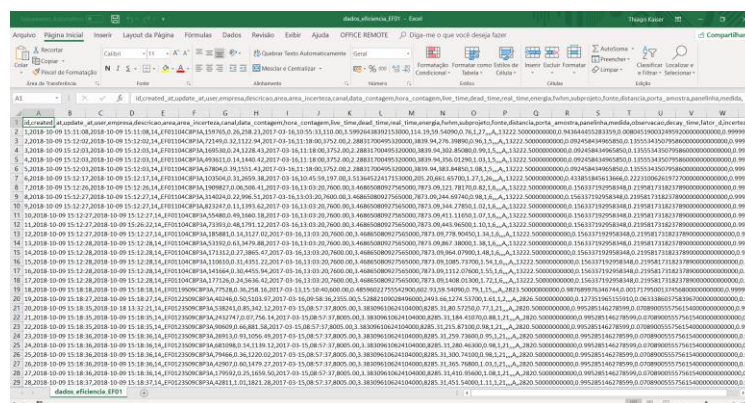
Source: Elaborated by the authors

Fig. 11: Reporting efficiency data in CSV

Source: Elaborated by the authors

VI.   CONCLUSION

The purpose of this work was to develop a free code web software to calculate the efficiency of HPGe type detectors from the Neutron Activation Analysis Laboratory (LAN) of the Energy and Nuclear Research Institute (IPEN).

The use of the software aims to avoid errors in efficiency calculations, as well as agility in performing these calculations and chart plotting. It is also mentioned the standardization of information in an intuitive and friendly environment. The use of the activation k_0 method requires an accurate characterization of the detection

system and thus the detection efficiency in the energy range of interest and the geometry of the experimental arrangement must be known with precision.

The validation of the results was obtained by obtaining several spectra in the LAN, which had the efficiency calculated in the system and the results compared with the procedures currently used in IPEN, thus proving the efficiency of the developed system, reaching the initially proposed objective.

As future work we have developed a specific software for the k0 method: analysis of gamma spectra, calibration of efficiency, determination of the parameters related to the characterization of the irradiation position (alpha ef) and correction factors (self-shielding, sum cascade) and efficiency calculation for thick fountains.

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