AN ELEMENTAL CONCENTRATION OPEN SOURCE DATABASE FOR HØGDAHL-CONVENTION AND WESTCOTT-FORMALISM BASED ON K_0-INAA METHOD IN MALAYSIA

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ABSTRACT

An electronic database has been developed and implemented for k_0-INAA method in Malaysia. Databases are often developed according to national requirements. This database contains constant nuclear data for k_0-INAA method; Høgdahl-convention and Westcott-formalism as 3 separate command user interfaces. It has been created using Microsoft Access 2007 under a Windows operating system. This database saves time and the quality of results can be assured when the calculation of neutron flux parameters and concentration of elements by k_0-INAA method are utilised. An evaluation of the database was conducted by IAEA Soil7 where the results published which showed a high level of consistency.

Abstrak

Satu pangkalan data elektronik telah dimajukan dan melaksanakankerana kaedah k0-INAA di Malaysia. Pangkalan data selalunyadibangunkan mengikut keperluan-keperluan negara. Pangkalan dataini mengandungi data nuklear malar kerana kaedah k0-INAA; Høgdahl-convention and Westcott-formalism apabila 3 berasinganantara muka pengguna perintah. Ia telah diwujudkan menggunakanMicrosoft Access 2007 di bawah sistem pengendalian Windows.Pangkalan data ini menjimatkan masa dan kualiti hasil-hasil boleh dipastikan apabila pengiraan parameter fluks neutron dan tumpuanunsur-unsur oleh kaedah k0-INAA menggunakan. Satu penilaianpangkalan data menjalankan oleh IAEA Soil7 di mana keputusanmenerbitkan yang menunjukkan satu tahap yang tinggi ketekalan.

Keywords: Database, Høgdahl-convention, Westcott-formalism, k_0-INAA method

INTRODUCTION

The development of database for neutron activation analysis (NAA) has increased in its utilisation in all NAA laboratories. It is common for a data analyst to write scientific programs. The acquisition of the data is the first move in gaining insight into a system. In all probability, it can be said that without an effective data analytical tool, the information will remain hidden behind the numbers. Nowadays, the scientific computing in a modern analytical laboratory plays a very important role (Wasim 2010; Wasim & Zaidi 2002).

The k_0-INAA (Instrumental Neutron Activation Analysis) was introduced in early 1970's (Simonits et al. 1975). The implementation of k_0-INAA requires careful determination of full peak efficiency calibration coefficients of the detector for different counting geometries and characterization of neutron flux for irradiation channels. The

k_0-INAA method has been formulated according to the Høgdahl convention and the Westcott formalism. To use the k_0-INAA method, two formalisms were regulated according to 1/v and non-1/v (n, γ) reaction nuclides. The reactor neutron spectrum parameters, the thermal to epithermal neutron flux ratio (f) the epithermal neutron flux shape factor (α) were measured using the bare bi-isotopic monitor and bare triple monitor methods, respectively, utilising the Høgdahl convention. In addition, modified reduced resonance integral $S_0(\alpha)$, the modified spectral index $r(\alpha)\sqrt{T_n/T_0}$, the Westcott $g_{Lu}(T_n)$ factor and the absolute neutron temperature T_n parameters were determined using the Westcott formalism (Acharya & Chatt 2003; Akaho & Nyarko 2002; Alghem & Ramdhane 2008; De Corte 2001; De Corte & Simonits 2003; De Corte et al. 1993; Dung & Hien 2003; Lin & Li 1997; Simonits et al. 1975; Yavar et al. 2011a, 2011b).

After the launching of the k_0-INAA in 1970 and due to intensive investigations of an international group of scientists, the method has been significantly developed in both the methodology and nuclear data used for computations. Currently, the method is in active use in a number of laboratories across the globe. Using a commercial computer program would be an easier and faster solution; the software development could result in a more effective contact with the k_0-INAA, which is a new method for most of the laboratory staff. Also, considering the small market for INAA software, companies are not expected to develop the ultimate product (Wasim 2010; Wasim & Zaidi 2002).

There are a few requirements the software should be able to do. Firstly, it should solve all the basic calculations involved in the k_0-INAA. Also, this database should contain nuclear constants, k_0-INAA parameters, and information related to analytical conditions involving samples, irradiations and detections. Finally, it should run within this environment due to the fact that Microsoft Windows is largely used between most Scientifics and research groups, (Wasim 2010; Wasim & Zaidi 2002).

Many NAA laboratories were provided databases for applications of NAA, however, most of the databases based on their national requirements like BANDRRI (Los Arcos et al. 2000). Moreover, all database programs in other laboratories only have utilised Høgdahl convention for determination of elemental concentration, but utilizing the Westcott formalism is important for the calculation of Westcott elements such as ^{103}Rh, ^{113}Cd, ^{115}In, ^{135}Xe, ^{148}Pm, ^{149}Sm, ^{151}Sm, ^{151}Eu, ^{152}Eu, ^{153}Eu, ^{154}Eu, ^{155}Eu, ^{155}Gd, ^{157}Gd, ^{164}Dy, ^{175}Lu, ^{176}Lu, ^{177}Hf, ^{182}Ta, ^{185}Re, ^{187}Re, ^{197}Au, ^{231}Pa, ^{235}U, and ^{238}U (Holden 1999). Therefore, our NAA laboratory at the National University of Malaysia (UKM) made the important decision to create a database for constant nuclear relevant to k_0-INAA; Høgdahl-convention and Westcott-formalism.

MATERIALS AND METHOD

A database was created with the intention to meet the particular work conditions of our laboratory. This database was prepared by Microsoft Access (MS Access). The advantages of using MS Access are its extended capabilities for transferring data in various different formats.

As a first step, constant nuclear data were collected from published literatures and used in our database (see Figure 1).Subsequently, k_0-INAA parameters were determined in this program. Finally, elemental concentrations in samples by Høgdahl-convention and Westcott-formalism were calculated (shown in Figures 2 and 3).

The k_0-INAA parameters relates to ε_p (efficiency of detector), α, $Q_0(\alpha)$, f, $S_0(\alpha)$, $r(\alpha)\sqrt{T_n/T_0}$, $g_{Lu}(T_n)$. After calibration the HPGe detector, ε_p was obtained that its equation was also used for other computations.

After irradiation of samples and monitors Au, Zr, and Lu in Malaysian nuclear agency research reactor, samples and monitors were counted by HPGe detector. The values of net peak area, irradiation time, decay time, counting time, and mass of monitors and samples were determined. Subsequently, the parameters such as, specific count rate, $A_{SP}=\frac{N_P/t_C}{SDCW}$; Saturation factor; $=1-e^{-\lambda t_i}$, with t_i irradiation time; and $\lambda=\frac{\ln 2}{T_{1/2}}$ with $T_{1/2}$ half life;

Decay factor; $=e^{-\lambda t_d}$, with t_d decay time (s); Counting factor; $=(1-e^{-\lambda t_c})/\lambda t_c$, with t_c counting time (s) were calculated by this database. Later on, α was calculated by Mathematica software because of its high accuracy, simplicity and fast use. Also α can be obtained by Excel software, but it is time consuming and inaccurate. After obtaining the α, the parameters of $Q_0(\alpha)$, f, $S_0(\alpha)$, $r(\alpha)\sqrt{T_n/T_0}$, $g_{Lu}(T_n)$ were determined by this database. Finally, these parameters were utilised for the calculation of elemental concentration of samples by the database program.

Figure 1. The nuclear constants window for K_0-NAA method

Figure 2. Calculation of elemental concentration by Høgdahl-convention window

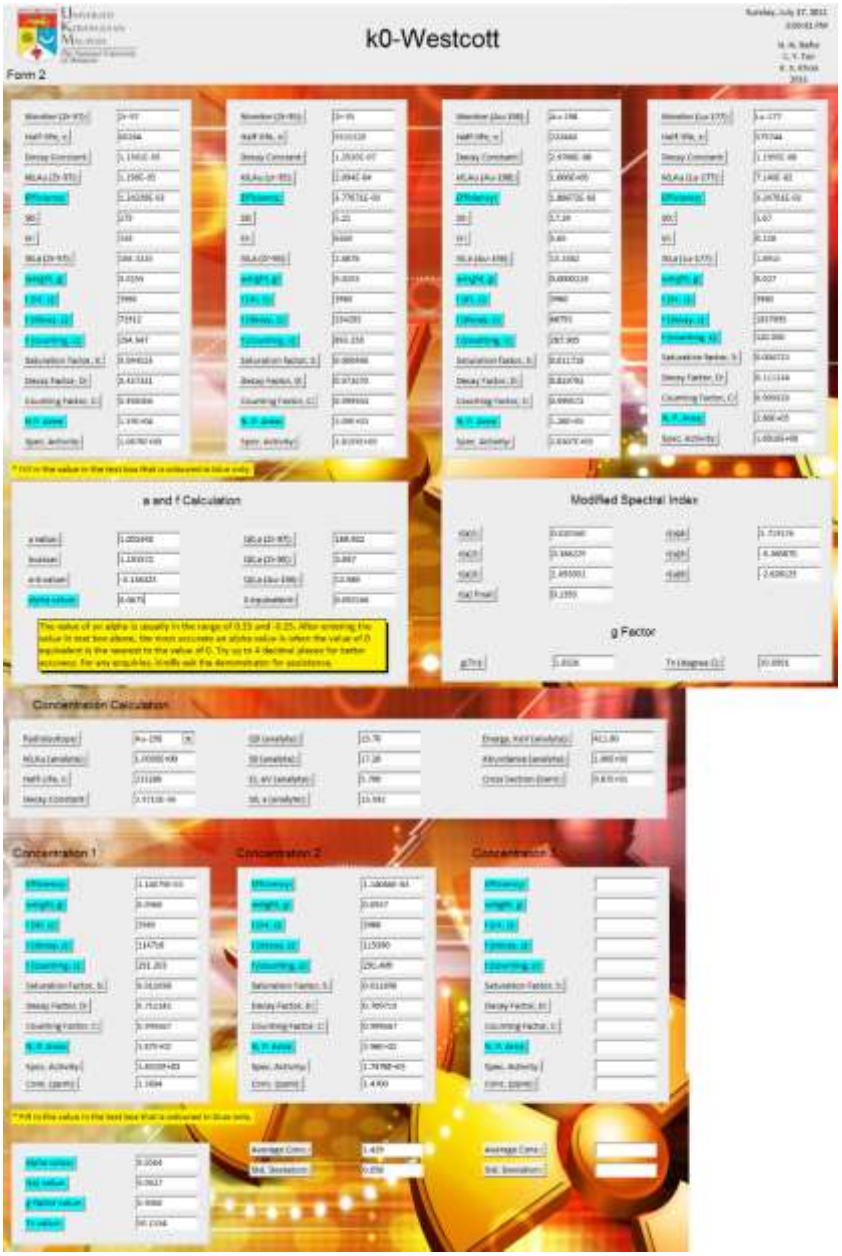

Figure 3. Calculation of elemental concentration by Westcott formalism window

RESULT AND DISCUSSION

The database was evaluated using certified reference materials IAEA Soil7 utilised by Yavar et al. 2011b. The observed average values of f and α were 13.90 with RSD (Relative Standard Deviation) of 3.02%, and 0.0615 with RSD of 8.62%. The average values of $r(\alpha)\sqrt{T_n/T_0}$, $g_{Lu}(T_n)$ and T_n were determined to be 0.1795±0.0044, 1.9729±0.0234 and 50.12±3.21°C, ℃ respectively. The average value of T_n was 50.12±3.21 °C in satisfactory agreement with the comparable reported value from the MNA research reactor (45°C). The results signify a high level of consistency between our database and results presented by Yavar et al. 2011b. The computation of experimental work by Yavar et al. 2011b was utilised by Excel software and Mathematica software. The way the database operates is quite simple and user friendly especially with its self-explanatory features.

CONCLUSION

This paper present a database for Høgdahl-convention and Westcott-formalism base on k_0-INAA method in Malaysia. This database was carried out for first time in Malaysia. The utilisation of Westcott formalism in this database makes it unique therefore this database can benefit all other NAA laboratories. The current version of the database is for PC and is available upon request.

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