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GAMMACAL – A USEFUL COMPUTER PROGRAM FOR NEUTRON ACTIVATION ANALYSIS AND RADIOACTIVITY CALCULATIONS

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GAMMACAL is a computer program with graphical user interface for the calculation of radionuclide activity of gamma emitting radionuclides and elemental concentration using neutron activation analysis data. The software has been tested and is in use for the last ten years. It provides not only concentrations but also quality control data. The program is available for free of cost on writing request to the author.

Keywords: GAMMACAL, Neutron Activation Analysis (NAA), Relative method in NAA, Gamma spectrometry software

1. Introduction

Natural and anthropogenic radionuclides are measured in order to get the information about their amount, distribution and behaviour in the environment. Natural radionuclides, which are present in our environment and are readily detectable by γ-ray spectrometry, include primordial radionuclide ^{40}K, radionuclides of terrestrial origin such as ^{238}U and ^{232}Th and radionuclides in their decay chains. Moreover, γ-emitting anthropogenic radionuclides are also present in the environment such as ^{60}Co, ^{137}Cs and others which are from nuclear weapon tests and nuclear accidents. The determination of ^{40}K, ^{238}U, ^{232}Th, ^{60}Co and ^{137}Cs is very important in geological and biological materials [1] from dose management point of view.

Neutron activation analysis (NAA) was introduced by Georg Hevesy and Hilde Levi in 1936 as an analytical technique for the determination of elemental composition of a sample. The method is in use by a large number of laboratories due to its accuracy and precision for biological, geological, environmental and high purity materials [2]. The type of the NAA, which does not involve any kind of chemical or physical separation or pre-concentration, is known as instrumental neutron activation analysis (INAA). The classical and wide spread version of quantitative INAA utilizes relative approach, where a reference material having matrix similar to the sample are irradiated together and counted under identical geometries [3]. The unknown concentrations of the elements are measured by comparing normalized and decay corrected peak areas in samples and standards.

The software relating gamma-ray spectrometry can be divided into two main categories: (i) software for data acquisition with spectrum analysis routines such as GammaVision by Ortec [4] and Genie 2000 by Canberra [5] and others (ii) software with NAA utility programs such as ADVNAA [6], NADA92 [7] and others. Among these most of the software packages are equipped with a radionuclide library [8] for nuclide identification. Software giving an option for nuclide library does not necessarily has a complete and fully updated library. Considering this requirement IAEA developed a comprehensive database named "NUDAT", which is accessible through World Wide Web [9-11]. After retrieving data from NUDAT, a database called "NUCDATA" [12] was developed in Microsoft Access to provide data for our utility programs. GAMMACAL is one such program.

GAMMACAL, stands for "Gamma Calculations" and is a software with graphical user interface for the calculation of radionuclide activity using gamma-ray spectra and elemental concentration employing neutron activation analysis data. Although, it belongs to the second types of the software described above, but it is not equipped with the advanced routines for nuclide

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identification. GAMMACAL was developed in 1999 and its version 2.0 is available since the year 2000. This program is in continuous use and over the years has been evaluated by a large number of researchers and students [13-20]. It determines activity and concentration using "relative or comparator method". The main purpose of this paper is to provide information about GAMMACAL, its working and utilization to the scientific community involved in research using γ-ray spectrometry research.

2. Data Analysis

In relative NAA, it is assumed that (i) samples and standards are irradiated together (ii) both receive same flux (iii) both are counted under identical geometry (iv) both are having similar matrices and (v) samples are quantified against the same energy as in the standard. In this case, the activation equation for concentration calculation becomes:

$$c_{sam} = c_{std} \frac{w_{std}}{w_{sam}} \frac{N_{sam}}{N_{std}} \frac{\left(1-e^{-\lambda t_{m,std}}\right)}{\left(1-e^{-\lambda t_{m,sam}}\right)} e^{-\lambda\left(t_{d,std}-t_{d,sam}\right)}$$

where c is the concentration of an element, w is weight, N is full energy peak area corrected for background, λ is decay constant, t_m is measurement time and t_d is decay time. The subscript *sam* refers to sample and *std* refers to standard. For most measurements where measurement time is kept same for sample and standard, the Eq. (1) reduces to;

$$c_{sam} = c_{std} \frac{w_{std}}{w_{sam}} \frac{N_{sam}}{N_{std}} e^{-\lambda T_d}$$

where T_d is $(t_{d,std}-t_{d,sam})$.

In the calculations of concentration activity when no irradiation is involved, an expression similar to Eq. (2) is used, with T_d slightly different as $[(t_{m,std}-t_{m,sam})-(t_{ref,std}-t_{ref,sam})]$ where t_{ref} is reference date.

3. Software

The software was written and its graphical user interface was designed in Visual Basic Version 6 and tested on various computers, which includes computers with processors P-II and P-IV and on operating systems Windows 98 and Windows XP. The structure of the software is given in Fig. 1, where the communication of the main program is presented. The main program takes user data as input, retrieves a list of radionuclide and half-life data from the installed file HalfLifeData.txt and calculates results with quality control (QC) report as output. The file "HalfLifeData.txt" contains data in five fields: (i) element (ii) mass number (iii) product state (iv) half-life (v) half-life unit. The half-life units are "Y" for years, "H" for hours, "M" for minutes, "S" for seconds, "D" for days, "MS" for milliseconds, "US" for microseconds and "NS" for nanoseconds. Since the file "HalfLifeData.txt" has ASCII format the data therein can be modified or updated by the user.

The software is available free of cost on request. It comes in the form of installable package, with relevant components, mostly *.dll files, to be installed in the Window's system directory. The main program must be installed in the directory "C:\GammaCal".

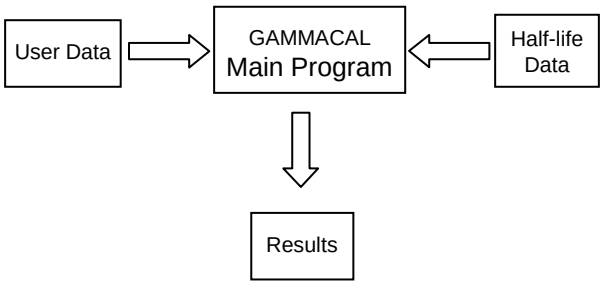

Figure 1. Structural diagram of GAMMACAL.

4. Results and Discussion

The main interface, as shown in Fig. 2, appears on running the executable file "GammaCal". This window provides four options for calculations; the first "Radionuclide Calculations" is used for the measurement of concentration activity of natural or anthropogenic radionuclides. Rest of the three options are related to NAA measurements. Fig. 3 shows the interface for the determination of activity concentration of various radionuclides. It can be observed in this window that "Reference Date" is required because activity always refers to some point in time. Similarly, Fig. 4 provides a view of the graphical user interface for sequential and re-counting calculations. In all data entry interfaces, a list of elements has been provided at the top of the window, which contains 91 elements sorted alphabetically. On selecting appropriate element from the list, the associated mass numbers appear in the adjacent list. Similarly, selecting a suitable mass number from the second list, the product states associated with the element and mass

number are filled in the next list. The list of product states includes “G” for ground, “M” for metastable, “M1” for first metastable and “M2” for second metastable state. If there is only one product state then half-life of the radionuclide appears automatically, otherwise half-life appears on selecting the relevant product state from the list. It is not important to provide acquisition date if all countings are performed on the same day, however, acquisition start time is important to be entered. Similarly, if decay time is same in sequential countings it is, then, not required. The program offers space for 6 samples and 6 standards. The entry of date requires US date format, which is “month/day/year”. The program assumes that all the data provided by the user is accurate and there is no need to correct for spectral interferences. However, background correction is performed by the GAMMACAL.

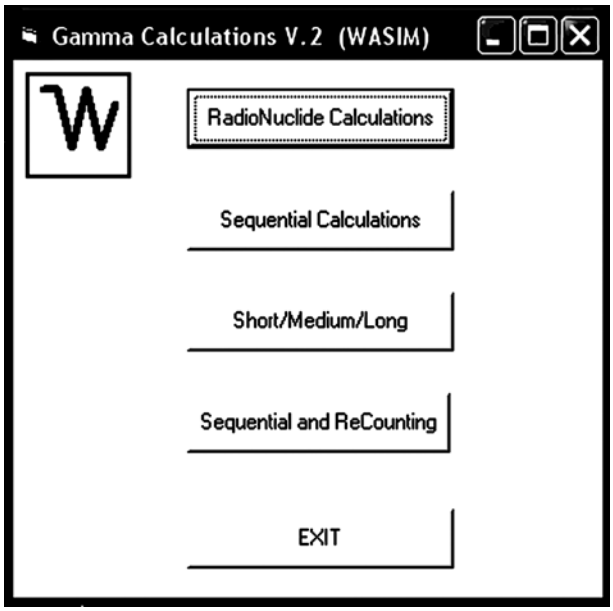

Figure 2. Main window of the GAMMACAL.

Finally, the results are provided in a separate window, as shown in Fig. 5, this window can either be saved by using a PDF printer or printed on the default printer. The result report provides information in three parts, in the first part date of analysis, sample ID (SID) and radionuclide used in calculations with energy is given. In the second part sample concentration or activity concentration, in the case of radiological measurements, is shown with mean, standard deviation and relative standard deviation (% RSD). The third part shows quality control analysis. This part calculates concentration of the element in one standard against the other standards used in the study. This information is important for quality assurance of the data. Fig. 5 presents results of Al found in two “Air Filters” 161F and 162F quantified against IAEA-S-7 (Soil) and IAEA-SL-1 (Lake Sediment). The QC results indicate about 10% relative deviation of one standard against the other. The results calculated by GAMMACAL have been checked by comparing with the results calculated either manually or by other means and found accurate.

GAMMACAL will be updated and new features will be introduced in the future version, considering the valuable feedback from the users. The future version will include more space for samples and standards, error analysis, options for save and recall and some other modes of calculations.

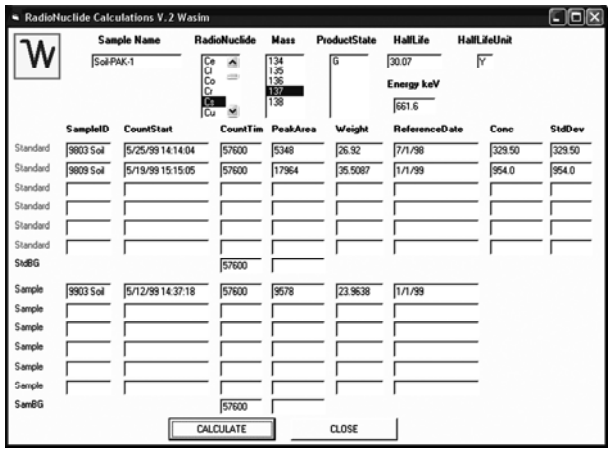

Figure 3. Window for activity concentration calculations.

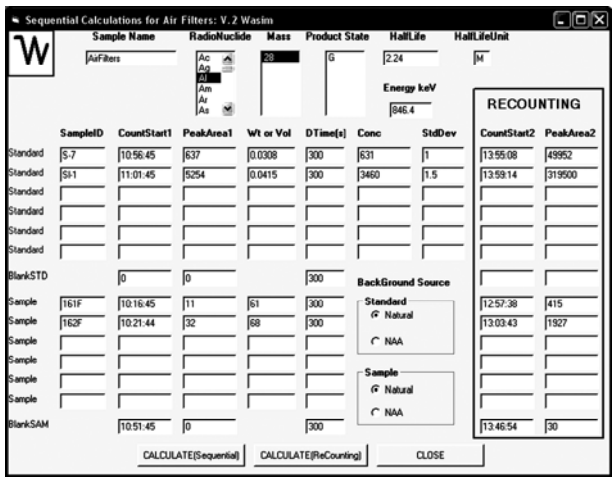

Figure 4. Interface for sequential and recounting calculations.

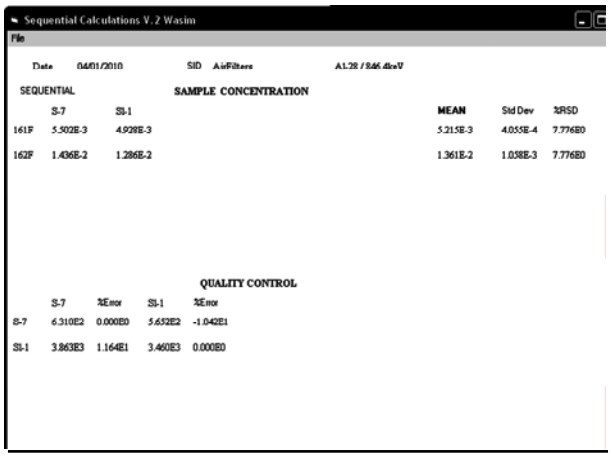

Figure 5. Results of concentration calculations for sequential counting with quality control data.

5. Conclusions

The software GAMMACAL has been used by a number of researchers for the calculation of elemental concentration using relative NAA and for activity concentration in radiological measurements. The program has been found easy to install, user-friendly and useful for quick calculations. It provides results of activity or elemental concentration using user input and reference data taken from IAEA NUDAT. The results calculated by GAMMACAL have been found accurate as checked by other means.

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References

[1] I. Fatima, J. H. Zaidi, M. Arif, M. Daud, S. A. Ahmad and S. N. A. Tahir, Rad. Prot. Dos. **128** (2008) 206.

[2] T. Weizhi, The Nucleus **46**, No. 4 (2009) 365.

[3] M. Wasim, J. H. Zaidi, M. Arif and I. Fatima, J. Radioanal. Nucl. Chem. **277** (2008) 525.

[4] ORTEC home page (2010): http://www.ortec-online.com/

[5] CANBERRA home page (2010): http:// www. canberra.com/

[6] N. Bangfa, W. Pingsheng, N. Huiling, L. Shuyuan, L. Xuefeng and T. Weizhi, J. Radioanal. Nucl. Chem. **244** (2000) 665.

[7] S. Landsberger, W. D. Cizek and R. H. Campbell, J. Radioanal. Nucl. Chem. **180** (1994) 55.

[8] International Atomic Energy Agency, TECDOC-1011, Intercomparison of gamma ray analysis software packages, Vienna, Austria, April (1998).

[9] R. R. Kinsey, C. L. Dunford, J. K. Tuli and T. W. Burrows, Ed. G. L. Molnar, T. Belgya and Zs. Revay, Proceedings of the 9th International Symposium on Capture gamma-ray spectroscopy and related topics, October 1996, Springer, Budapest, Hungary (1997).

[10] I. M. Iyer, P. Oblozinsky, D. W. Muir and O. Schwerer, J. Radioanal. Nucl. Chem. **239** (1999) 139.

[11] IAEA Nuclear Data Services (2010): http://www-nds.iaea.org/

[12] M. Wasim and J. H. Zaidi, Nucl. Instrum. Methods Phys. Res., Sect. A **481** (2002) 760.

[13] S. Waheed, A. Rahman, M. Daud, S. Rahman, Z. Islam and S. Ahmad, Radiochim. Acta **93** (2005) 487.

[14] S. Waheed, A. Rahman, N. Khalid and S. Ahmad, Radiochim. Acta **94** (2006) 161.

[15] M. Daud, N. Khalid, J. Iqbal, S. Ahmad and J. H. Zaidi, Radiochim. Acta **94** (2006) 871.

[16] M. Daud, N. Khalid, J. Iqbal and S. Ahmad, Radiochim. Acta **95** (2007) 423.

[17] S. Waheed and S. Ahmad, J. AOAC Int. **91** (2008) 392.

[18] S. Waheed, S. Rahman and K. P. Gill, J. Radioanal. Nucl. Chem. **279** (2009) 725.

[19] S. Rahman and S. Waheed, J. Radioanal. Nucl. Chem. **279** (2009) 915.

[20] M. Daud, M. Wasim, N. Khalid, J. H. Zaidi, J. Iqbal and S. Ahmad, Radiochim. Acta **97** (2009) 117.