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DEVELOPMENT OF A SYSTEM USING THE LIBRARY OF THE GENIE SPECTROSCOPY SOFTWARE AND EXCHANGE OF SAMPLES

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ABSTRACT

One the great difficulties in using the NAA method is in regards to the time that the operator spends exchanging the samples after each measurement. It becomes a big problem in routine analyses when various chemical elements are determined and then each sample must be measured at different decay times. The application of the automatic sample exchanger reduces the time analysis by several hours and reduces the tedious manual operation. Then, the effective use of NAA depends on the availability of a suitable automatic sample changer. There are some systems that are sold commercially, however many laboratories can't acquire them because they are costly. This paper presents altered programs the G2KNAA.REX, which created a screen making possible automatic or manual acquisitions by calling the old program NAAACQ.rex for the procurement manual and the new program NAAACQ2.rex for automatic requisitions. In conclusion, as can be seen in the program lines, the synchronization to automation, which unites the three systems, (the computer, the Camberra Set, the sample exchanger) is done in a timely manner. The system was tested and is functioning in a satisfactory manner.

1. INTRODUCTION

In recent years, automation in analytical labs using sophisticated methods of analysis, in particular those that handle radioactive material, has evolved in order to increasingly obtain more accurate and exact results [1]. The automation system reduces operator interference preventing errors that result from routine analysis processes.

Automating an analytical process is not an easy task because it involves many factors. In the specific case of radioactive material, the method known as neutron activation analysis involves the measurement equipment and the spectrum analysis program.

In comparison with other analytical techniques, Instrumental Neutron Activation Analysis (INAA) involves relatively little handling of samples but requires sophisticated high resolution detectors so that individual gamma rays can be distinguished and identified. INAA has developed rapidly since the advent of large high resolution Ge(Li) detectors, multichannel analyzers with large memories and computers to reduce the vast amount of data produced [2-5]. Within this evolution, data acquisition is no longer performed for a single sample or in one single physical condition.

The data acquisition procedures are well known and developed; however, the processes involved in the measurements and in the exchange of samples work through interference, albeit remote, of the operator. This is one of the greatest difficulties faced by the labs, since

the projects are totally dissociated and are not adapted to work in synchrony due to the technological difficulties of such enterprises. However, most of the systems in operation at labs have serial or parallel interfaces and can be connected to a computer, enabling synchronization simply through the use of sophisticated software [6].

Synchronizing different systems is not easy and requires a detailed study and the development of a specific project to prevent interference in any of the systems in operation. As such, the need arose to develop systems linked to the spectrometer which contains the samples during the performance of the experiment [7,8].

In view of the above, this study was aimed at developing software that will enable the integration of the sample exchanging system in operation in the Radiochemical Supervision of IPEN-CNEN/SP and the spectrum analysis program, Genie-2000 NAA Processing Procedure of Canberra.

2. SYSTEMS INVOLVED

The automation process for the acquisition of data at IPEN's Radiochemistry Supervision lab took into consideration the project in operation avoiding any interferences that could significantly change the operator's routine. For such, a detailed study of the systems involved was undertaken as described below.

2.1. System Genie-2000 NAA Processing Procedure

The Genie-2000 NAA Processing Procedure software includes the following characteristics: "Running under WIN/95,98®[1] or WIN/NT®[1] or greater and requiring the S561 Batch Programming Option (Enterprise/REXX), as well as a Genie-2000 Basic Spectroscopy Package (S500, S502 or S504) and the Gamma Analysis Option (S501). Its system has the file REXX procedure: G2kNAA.REX (main procedures), NAAACQ.REX (Procedure for controlling 4 detectors, EDITBAT.REX (for creating and editing experimental RDF files), STDEDIT.REX (for creating and editing standard connections), WAITACQ.REX (a child process started by NAAACQ.REX).

A brief description of the procedures of Genie-2000 NAA Processing Procedure [4] is shown below.

The main program, **G2kNAA**, aimed at managing the entire system through five core tasks, is shown in Fig. 1:

1. Create/Edit Experiment: Allows the operator to include in the system new experiments based on a set of samples prepared for data acquisition. In this case, the **EDITBAT** procedure is used and its function is to create a Run Description File (RDF), where the specific data of the sample is recorded, including the status that indicates the stage of the process.

[1] It is registered mark of Microsoft®.

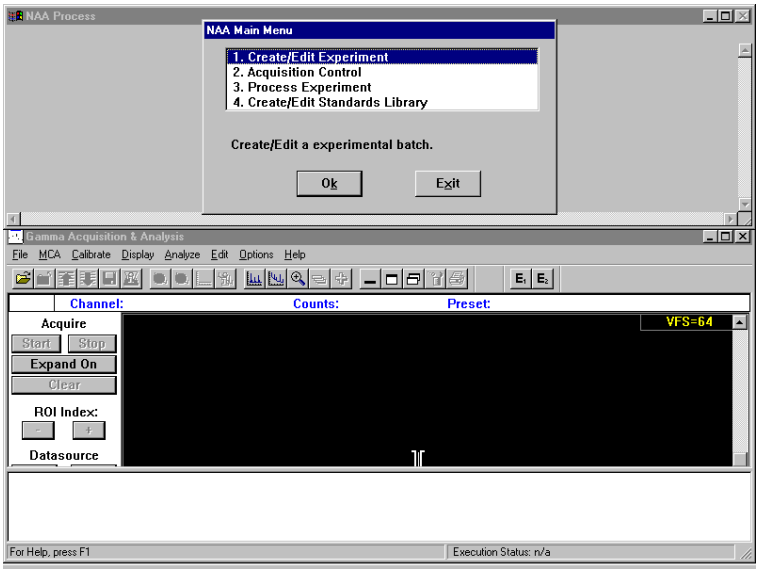

Figure 1. NAA Screen main menu

Fig 2 shows the details of the edition process (to the left) as well as the description of each sample analyzed (to the right).

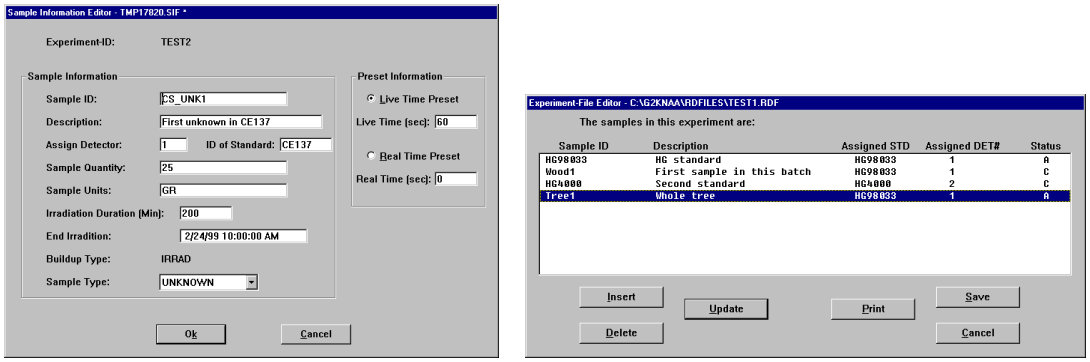

Figure 2. Sample information editor (left) and Edit Experiment Screen (right)

2. Acquisition Control: This is performed through the **NAAACQ** procedure which sends it to the general file where the predefined samples are found, choice of the sample.

   Despite this system permitting the parallel acquisition of up to 4 detectors, there is only one detector in operation in the Radiochemical Supervision lab of IPEN.

3. Process Experiment: This constitutes the process for analysis of spectrum photopeaks that can be automatically performed through five phases: peak search (using analysis sequence file NAAPEAK,ASF), Interactive peak fit (if S506 Genie-2000 Interactive Peak Fit is installed), nuclide identification (using analysis sequence file NAANID.ASF, Calculations using algorithms explained Genie-2000 NAA Processing Procedure, Reporting [4].

4. Create/Edit Standards Library: Used for create Standards library Genie-2000 Nuclide Library Editor program and also to edit into that library the known concentration for standards. Once a standards library is created its concentrations can be added by using the edit standard concentration option in the program.

In this study, no changes were made in the 3 and 4 tasks of the Genie-2000 program. The tasks changed in the Genie-2000 program were 1 and 2, which correspond to the main procedure (**G2kNAA**), procedures **NAAACQ** and **WAITACQ**.

2.2. System Automatic Sample Changer

The changer in operation at the Radiochemical Supervision lab of IPEN is basically comprised of two systems:

1. Mechanical: The transportation of capsule to and from the counting station is done pneumatically and is controlled electronically. Careful design of the counting station has reduced the counting errors considerably and the sample changer permits maximum utilization of the detector system.

   The terminal coupled to the spectrometer is shown in Fig. 3.

Figure 3. Terminal of sample changer connected to spectrometer

2. Electronic: Comprised of the Sample Changer Control module (Fig. 4) which can be controlled manually or automatically. The manual control is done using a two-way switch, Fig. 4. The IN, OUT, COUNT lights indicate respectively the status of the transfer of the sample to the spectrometer, the return to the shield and data acquisition. The cables, which control the positions of the valve and the electrovalve coupled to the connector for I/O auxiliary signals of the Multiport II Multichannel Analyzer [9], are located at the rear of the changer.

Figure 4. Electronic control of the sample changer

Multiport II is the module, double NIN [9], to the left of the BIN in Fig 5, that is connected to a microcomputer through an Universal Serial BUS (USB) interface controlled by the library of Genie-2000 [4].

Figure 5. Electronic data acquisition system connected to the spectrometer.

In these conditions, despite the existing connections of the system (spectrometer and sample changer) working separately, there is sometimes a need for interconnection in the automatic acquisition of several samples.

3. SOFTWARE IMPLEMENTED

The entire changing process was carried out in compliance with the Genie-2000 library and the programs developed in REXX for the execution of processes in sequence [4]. As such, we interfered as little as possible in the original procedures of the Genie-2000 program.

Changed Procedures

- G2kNAA.REX for G2kNAA2.REX: Changed block shown in Table 1

  Opening of a screen that enables respectively automatic or manual acquisition with a prompt for the former NAAACQ program for manual acquisition and the new NAAACQ2 program for automatic acquisition. According to item 2.1, task 2 Acquisition Control permits, after the change made, manual or automatic operation, as shown in Fig. 6.

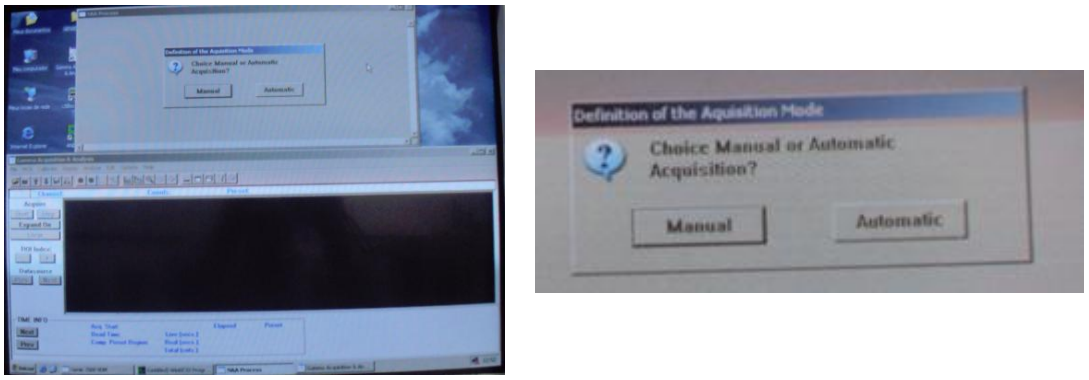

Figure 5. Choice mode acquisition of data.

  In the automatic mode, the acquisition process is executed for all samples corresponding to the experiment shown in Fig. 2.

- NAAACQ.REX for NAAACQ2.REX:

  Many changes were made in the NAAACQ.REX procedure, given that it allows the parallel processing of acquisition and/or analyses.

Since the system is only available for one detector and the acquisition process is specific for a set of samples, we chose to dedicate the computer only to data acquisition during the experiment.

As such, many changes were made in line 151 (NAAACQ2.REX), 141 (NAAACQ.REX) where the main change was made in line 316 (NAAACQ2.REX), 323 (NAAACQ.REX). The library was eliminated for the execution of acquisition in parallel (command SPAWN Table 1). The NAAWAIT.REX procedure, which is in charge of recording the data, logs and status changes of the run description files (RDF), is prompted in this line.

Table 1. Changing blocks of procedures

Before	After
G2KNAA	
G2KNAA.REX	G2KNAA2.REX

RC = NAAACQ()
IF RC <> 0 THEN DO
Err_Msg = "Error "RC" returned from NAAACQ.REX!."
CALL Disp_Err
END
SIGNAL Select_Menu
END /* start a count */
	/*HOME CHANGE*/
	Warn_Msg="Choice Manual or Automatic Acquisition?"
	Opt.Button1="~Manual"
	Opt.Button2="~Automatic"
	Opt.icon = "?"
	Show.Title="Definition of the Aquisition Mode"
	Show.Position="ICC"
	checksam=GBT_MESSAGE(Warn_Msg,'Opt','Show')
	Show.Position="ICC"
	IF checksam=">1" THEN DO
	RC = NAAACQ()
	IF RC <> 0 THEN DO
	Err_Msg = "Error "RC" returned from G2KNAA2.REX!."
	CALL Disp_Err
	END
	END
	IF checksam=">2" THEN DO
	RC = NAAACQ2()
	IF RC <> 0 THEN DO
	Err_Msg = "Error "RC" returned from G2KNAA2.REX!."
	CALL Disp_Err
	END
	END

NAAACQ	
NAAACQ.REX	NAAACQ2.REX
CALL GETPARAM Count_Workfile,Respo,0,'SURSTRING7', 'SURSTRING5', 'SURSTRING1';	/* was chenged the parameter Respo of GETPARM to snum */ CALL GETPARAM Count_Workfile,snum,0,'SURSTRING7', 'SURSTRING5','SURSTRING1';
RC = SPAWN("rexx.exe", 'NAAWAIT 'Detname tempdir data_dir RDFname samrecord.opennum, "Hide")	RC = NAAWAIT(Detname tempdir data_dir RDFname snum) /*last change*/ 'WAIT /ELAPSED=45'

Fig. 6 shows a schematic arrangement that summarizes the current project, which can work manually as well as automatically.

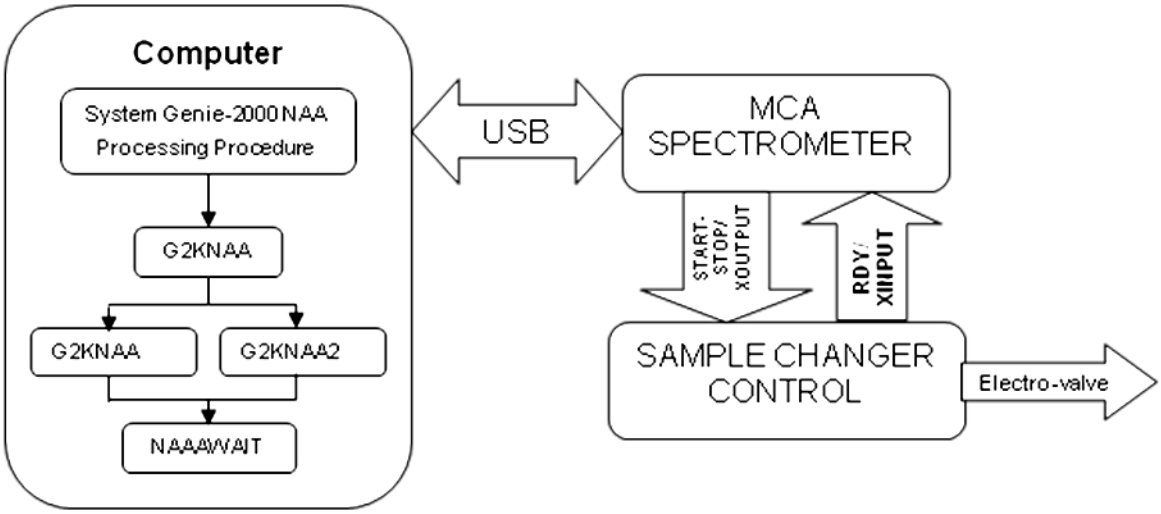

Figure 6. Functional diagram of the system deployed.

4. CONCLUSIONS

As shown above, this study was developed based on the need to implement an automatic sample changing system for data acquisition in neutron activation analysis.

To do so, we studied the project in operation at the lab in order to better situate the changing process. Subsequently, implementations were made in the routines of Genie-2000 to deploy the project in a way which allowed for the data to be acquired manually as well as automatically according to the need of the experiment in question.

The system as described herein has been operating successfully for more than two years and has handled many hundred of samples.

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