Applied Radiation and Isotopes 87 (2014) 425–428

Contents lists available at ScienceDirect

Applied Radiation and Isotopes

journal homepage: www.elsevier.com/locate/apradiso

A dedicated LIMS for routine gamma-ray spectrometry

M. Bruggeman*, L. Verheyen, T. Vidmar

SCK · CEN, Belgian Nuclear Research Centre, Boeretang 200, Mol 2400, Belgium

HIGHLIGHTS

- We outline the automation methods and data management of a LIMS.
- We explain the interfacing with Genie2K™ and EFFTRAN.
- We discuss the automation of efficiency transfer and true summing correction.
- Potential for human error is strongly reduced by introducing a LIMS.

ARTICLE INFO

Available online 1 December 2013

Keywords:
LIMS
Gamma-ray spectrometry
Efficiency transfer
Summing corrections

ABSTRACT

We developed a Microsoft® Access-based LIMS (Laboratory Information and Management Systems), γ-LIMS, for the management of our gamma-spectrometry laboratory, in which thousands of routine, but high-quality analyses are performed each year. This paper explains the main features of the γ-LIMS and puts special attention on the interfacing methods and solutions for using the Genie™2000 spectrometry software in conjunction with the EFFTRAN package, which serves for efficiency transfer calculations, coincidence summing corrections and a procedure for uncertainty estimation.

1. Introduction

LIMS (Laboratory Information and Management Systems) are used in many laboratories with the aim to run processes with high efficiency and quality and to guarantee data integrity (ASTM E1578 (ASTM, 2013)). One of the challenges when opting for a LIMS is the interfacing between the hardware and the existing analysis software. In general there are three options available for selecting a LIMS. The laboratory can decide to program an in-house, proprietary system fulfilling all its needs. Alternatively, they may buy a commercial product and modify it to fulfil their specific requirements, a process known as customization. The last option is to buy a commercial off-the-shelf (COTS) solution covering most of the needs. In case of the gamma-ray spectrometry analysis process a key point is proper interfacing of a LIMS with the detectors (required for automation of the spectrum acquisition) and with the specific spectrometry analysis software in order to automate these processes and to guarantee sound data management.

We developed a Microsoft® Access-based LIMS, called γ-LIMS. The LIMS is used for the daily management of our gamma-spectrometry laboratory and covers all aspects of this analytical service. We selected Microsoft Office Access® because it is easy to use, has a worldwide community of users who often make their solutions publicly available on the internet. It is important for a LIMS to be both simple and intuitive, if we wish it to achieve user-acceptance and increase productivity. The γ-LIMS is a file-server application which consists of a back-end database stored on a network computer and a front-end Microsoft® Access database supplemented with VBA® (Visual Basic for Applications) modules (scripts) for interfacing to all the data. The front-end software typically is installed on different laboratory computers and is used by the laboratory personnel in their daily work. This paper focusses on the interfacing of our LIMS with the Genie™2000 spectroscopy software (Genie, 2009) and with the EFFTRAN package, which is used for the calculation of efficiency transfer and coincidence summing corrections.

The γ-LIMS completely covers all the steps involved in the routine analysis by gamma-ray spectrometry: registration of a request for the analysis, sample registration, data acquisition, spectrum analysis, approval, reporting and mailing, sample storage management, accountancy, QA-QC and many other aspects. We focus here on the automated use of efficiency transfer, coincidence summing correction, uncertainty estimation and final reporting. The introduction of the γ-LIMS in our laboratory has proven to substantially minimise errors resulting from human interactions related to e.g. the loading of calibrations and background files, to largely simplify reporting, to produce a high level of accuracy, to improve the laboratory-specific information exchange amongst its users, to optimise the workflow amongst the laboratory analysts and to facilitate training of personnel.

* Corresponding author. Tel.: +32 14 338886.
E-mail address: michel.bruggeman@sckcen.be (M. Bruggeman).

0969-8043/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.apradiso.2013.11.083

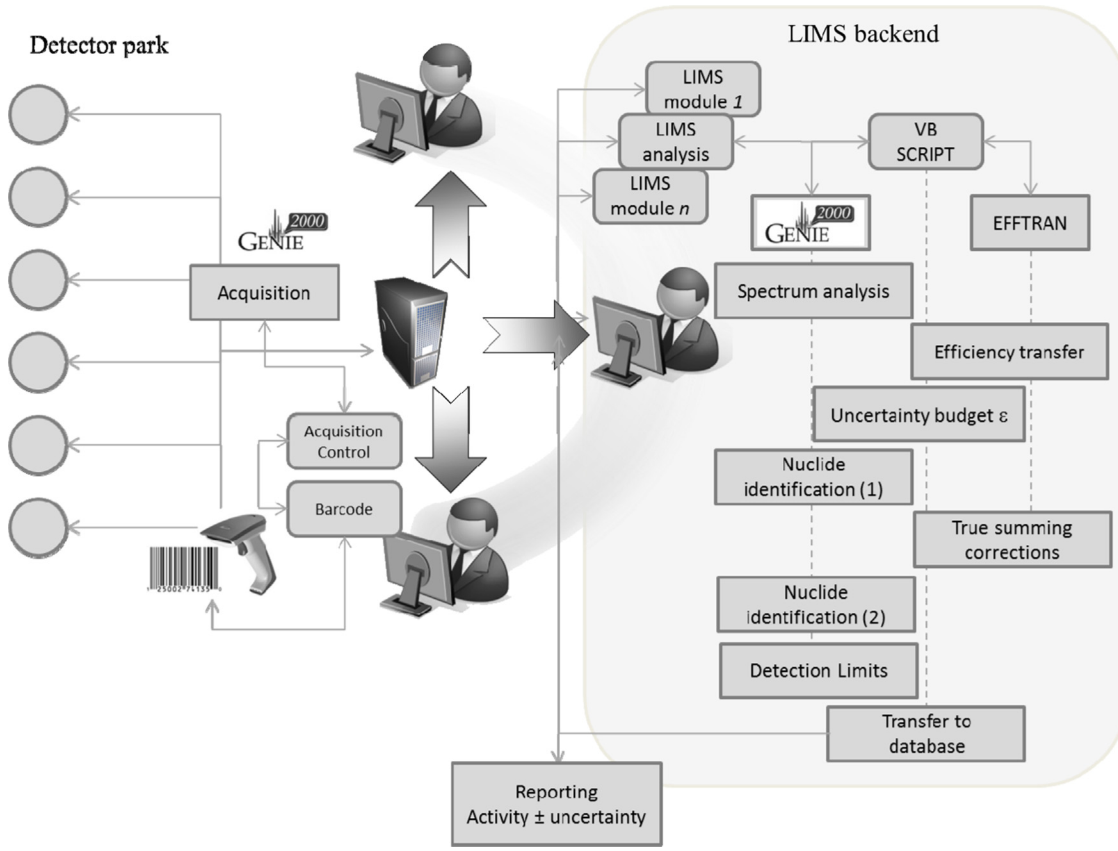

Fig. 1. Layout of the basic γ-LIMS architecture and the spectrum analysis process. Rectangles represent activities or external software; rectangles with rounded corners represent γ-LIMS modules. Only the analysis module is detailed here. For the reporting module only the generation of the report is shown.

2. Discussion

2.1. *Interfacing the analysis process to a database*

In order to automate and/or interface the LIMS to spectrum analysis methods involving third party software, it is necessary to have access to the specific software components e.g. dynamic link libraries, ActiveX® controls or executable code and to their data file structures. This may not always be possible or the options may just not be available and it is important to check this issue prior to the design of LIMS software. We use Genie™2000 as the gamma-ray spectrometry software for acquisition and analysis and complement this software with EFFTRAN (Vidmar, 2005, 2011) for efficiency transfer and coincidence summing correction. Both Genie™2000 (Genie2000 customisation tools manual) and EFFTRAN allow for a full control of their components and file structures, making them ideal for automation. Fig. 1 shows the basic layout of the γ-LIMS architecture and shows the main data flow and the activities executed during the analysis process that will be discussed in this paper.

The following paragraphs explain how routine gamma-ray spectrum acquisition and analysis is controlled and automated by the γ-LIMS.

2.2. *Sample registration with the γ-LIMS*

The first step in the spectrometry process is triggered by an incoming request for analysis from a client. This request is registered in the LIMS and for each sample belonging to the request all sample data are entered into the system. The sample registration involves the recording of all parameters of a subsample prepared in one of the counting vials. The sample information is subdivided into different information units: client-related, geometry-related, acquisition parameters, reporting-related and other sample data. The client-related information includes the sample data provided by the client. Registration of the geometry parameters involves the input of all parameters required for the computation of the detection efficiency via efficiency transfer with EFFTRAN. The geometry parameters are: the counting vial used, sample mass, sample volume, mass of additives or moisture content and the matrix material (selected from a predefined list of materials). Actually, only parameters different from those of the reference geometry should be entered. A measurement time can be set. The reporting parameters involve the units for reporting, the nuclides to report (selected from a predefined list of nuclide vectors), the reference date and the reporting due date. Other sample data that may be provided involves safety information and the date for sample disposal. All this information is stored in the γ-LIMS relational database. At the end of the registration process, unique barcode labels are printed and samples are labelled. The sample barcode plays an important role in the automation of spectrum acquisition and sample management.

2.3. *Spectrum acquisition with the γ-LIMS*

The spectrum acquisition involves starting the acquisition and automatically saving the spectrum file when the measurement life time is reached or when the acquisition is stopped by the operator. Starting and stopping spectrum acquisitions on one of the detectors is done by commands initiated by reading the barcodes of the sample and the detector with a barcode reader. Reading these barcodes in sequence, including a confirmation reading, starts the spectrum acquisition and generates a record in the database that couples the sample-ID and detector-ID. The start and stop