Annex C
Terms of Reference

Software for radionuclide analysis (SAINT3 Software)

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1 Summary

These are the Terms of Reference for the “Productizing of the SAINT software (radionuclide analysis)” Project comprising:

- Designing and developing software for gamma spectrum analysis (HPGe) for Particulate air filter and xenon gas samples including review of results from automatic processing, calibration and categorization.
- Assisting the Commission in testing the software and fixing bugs discovered during testing.

2 Background

The Preparatory Commission for the Comprehensive Nuclear-Test-Ban Treaty Organisation (hereafter referred to as the Commission), located in Vienna, Austria, is the international organisation establishing the global verification system under the provisions of the CTBT, which bans any nuclear weapon test explosion or any other nuclear explosion. The verification system includes the International Monitoring System (IMS), a global network of monitoring stations (radionuclide technologies: particulate and noble gases; waveform technologies: seismic, hydro-acoustic and infrasound), a global communications infrastructure, (hereinafter referred to as the GCI) an International Data Centre (hereinafter referred to as the IDC) and the capability to carry out on-site inspections.

IDC supports the verification responsibilities of the Commission by providing objective products and services for effective global monitoring. IDC collects data from the IMS network to detect, locate and analyse possible nuclear events. At the IDC, data are automatically processed and interactively analysed, and data and products are distributed in near real time to the State Signatories.

The radionuclide component has noble gas and particulate stations, all the particulate stations and part of the noble gas stations are equipped with HPGe detectors for high resolution gamma ray spectroscopy analysis of the samples. The spectra are measured and transmitted to the International Data Centre (IDC, Vienna) for analysis. The analysis software is used to calculate concentrations of the isotopes in the air.

3 Current Status

The current radionuclide analysis system is based on the SAINT (Simulation Assisted Interactive Nuclide Review Tool) software that comprises two parts: the automatic analysis tool autoSaint and the interactive MATLAB based review/analysis tool Saint2. Saint2 is built using Matlab and different versions of this tool have been in production use more than 5 years. Because of the use of Matlab, some of the features built into the software have performance
limitations, porting of the software to new operating systems is complicated and the distribution of the software is limited by Matlab licensing regulations. To overcome this and to assure that radionuclide processing tools have a sustainable platform in the future, the core functionality of Saint2 must be ported to run under the Linux environment. Furthermore, the layout and workflow of the tool must be re-engineered to better assist the analysts in performing error free reviews.

![Figure 1: Saint interface built with Matlab](image)

### 4 Description of the work assignment

The objective of the Work under this contract shall be:

- **Task 1**: To undertake a study under which the technical feasibility of the interface is investigated
  - **Task 1.1**: Document workflow for Xenon and particulate spectrum review and propose design for both Xe and particulate spectra analysis software.
  - **Task 1.2**: Refine design for both Xe and particulate spectra analysis software.

- **Task 2**: Deliver software to view spectra, analysis results and calibrations (Features common to Xe and particulate spectrum review) in accordance with the results of design study (Task 1).
- **Task 2.1.** Spectrum display with analysis results
  - **Task 2.2.** Calibration review and recalculation tool

- **Task 3:** Add functionality to perform Xe sample analysis and review in accordance with the results of design study (Task 1).
  - Xenon review and analysis tool including documentation
  - Tentative categorization with flags, testing of the Xe software

- **Task 4:** Add functionality of particulate sample analysis and review in accordance with the results of design study (Task 1). This includes:
  - The review of man-made and natural radionuclides.
  - Handling of missed peaks and explanation of peaks.
  - The review of special analysis like background subtraction, Tc-99m/Ge-75m tool, and other features that are currently in the SAINT2 interface.

- **Optional tasks:** Following options may be proposed by the contractor as an additional service with fee
  - Training of PTS staff to use the software after the delivery of phase 4. We assume 5 days travelling including 2 days set-up and dismantling of the training setting and 3 days training for max 12 person. One or preferably two experts are needed from the contractor.
  - Support and possible upgrades to the software. We assume 2 years period under which 60 working days could be used to implement improvements and to provide support for users. Mostly the support is done remotely but there is need to have the experts on site for at twice (once a year) for 10 days in total.

4.1 **Organization of work:**

The work shall be organized as follows: Tasks 1 shall be a pre-requisite for tasks 2, 3 and 4. Task 2 has to be delivered before task 3 starts since they are using common tools for spectrum and peak review and calibration review tasks. As noble gas capability is highest priority, task 4 shall be delivered after the delivery of task 3.

The Contractor shall complete the work under task 1 within 3 calendar months, under task 2 within 4 calendar months, under and task 3 within 3 calendar months and under task 4 within 3 calendar months. The total time allocated for the whole project is 13 calendar months.

These issues are illustrated in figure 2.
4.1.1 Task 1: Feasibility study, the design of the new portable interface for HPGe spectra review

Purpose: The Contractor shall undertake a study on how the review tool for radionuclide analysis should appear and what functionalities need to be built in. The contractor should investigate the workflow for Xenon and particulate spectrum review based on interviews with analysts and IDC scientists. The outcome of this investigation shall be a report that describes, in a structured approach, all actions required to perform spectrum review, corrective actions, issuance of a station problem reports, and other optional items. Based on the results of the workflow analysis, a new GUI design representing the workflow concept shall be proposed. The suggested design shall be documented through user interface mock-ups and use cases. The report shall also propose efficient methods to update the energy and resolution calibration and perform baseline correction. The study shall also investigate options to display time series of spectra, spectral regions of interest, spectral parameters (peak position, peak area, peak resolution, MDC) and analysis results in order to improve the analyst’s understanding of the station and its characteristics as well as the plausibility of the data. The study is done in co-operation with the Commission and the proposed plan is discussed and elaborated in meetings to be held with the Commission. The feasibility study should use the functionality of the current software as a starting point but shall not limit the Contractor in exploring other
design options resulting from interviews with end users and IDC scientists. The current available prototype software “SAINT2” covers both the function of particulate and xenon gamma spectrum analysis and review. Particulate and xenon spectrum review comprise a number of common features as well as different features. It should be one of the outcomes of the study to recommend if both functions should be integrated into a single program or handled by two separate programs.

Location: At the Contractor’s office and meetings at the Commissions premises.

Time: This task shall take a maximum of 3 months, before tasks 2, 3 and 4.

Deliverables: Two reports shall be delivered describing the findings of the study and proposing a way forward for the implementation of the software in tasks 2, 3 and 4.

Sub-task 1.1: intermediate report that is used as working document towards the final design. The report shall include:
- The documented workflow to be followed when reviewing Xe and particulate spectra
- A description of the graphical user interface based on screen mock-ups and use-cases.
- Any requirements that cannot be formulated through use cases, like: performance and response time bounds, accuracy, etc.

Sub-task 1.2 has final design report that is used as a basis for tasks 2, 3 and 4.
- A report describing the modeling approach proposed in terms of its capabilities and limitations.
- A software requirements document that:
  a. Illustrates the proposed GUI through screen mock-ups.
  b. Documents requirements through use cases and functional-style requirements.
- A high-level design document that describes the main components of the software and the third-party libraries (if any) that the Contractors intends to use.
- Usability issues like keyboard short-cuts should be considered in this report.

Meetings: A kickoff meeting that gives the baseline for the work to be done in task 1 (3-5 days).

A meeting to consolidate the views of PTS and Contractor be held after intermediate report has been delivered (3-5 days).

A meeting to consider acceptance of the final design and, if applicable, to move to task 2 (3-5 days).

4.1.2 Task 2: Spectrum display and calibration tool

Purpose: The Contractor shall develop stand-alone software to display and manipulate Xe- and particulate spectra and to perform necessary corrections energy and resolution calibrations, validate or correct results of automated processing by validating or correction of peak detection and nuclide identification, issuing of
comments on peaks and the spectrum in general and eventually validate parameters used for spectrum categorization. The software will be used to review spectra in accordance with the design written in task 1.

Location: At the Contractor’s office with 2 follow up meeting at commissions premises.

Time: This task shall take a maximum of 4 months and will be based on results of task 1.

Deliverables:

a) Sub-task 2.1: A software written in C++/Qt that enables end users to review spectra and analysis results to replace Saint 2 review software.

The basic functionality of the software delivered in this stage is to show HPGe spectra, parameters and results (spectrum display). The GUI of the software shall implement the workflow structure defined as part of Task 1.

b) Sub-task 2.2: A Calibration modification and management tool (including source code) integrated into the software above.

The software delivered in this sub-task shall offer user friendly options to:

- correct the calibrations as necessary
- select peaks in the spectrum and assign them energy/isotope
- fit ECR and RER under user control.

The following functionality is required (not excluding additional functionalities):

- view energy, FWHM and efficiency calibrations
- optionally view and select the possible calibrations (station, MRP, QC, CAL_PHD)
- optionally modify calibrations based on user input.

c) The source code, a system design document, an installation guide and a user guide for the software delivered.

d) The system design document should include doxygen documentation for the main elements of the software.

Meetings:

In the end of sub-task 2.1 the contractor should present the results (3 days)

In the end of sub-task 2.2 the contractor should deliver the product and present its capability for the Commission (3 days). In this meeting the acceptance of task 2 is considered and, if applicable, to move to task 3.

4.1.3 Task 3: Functionality for xenon spectrum review

Purpose: The Contractor shall develop a stand-alone review tool for Xe spectra in accordance with the requirements document that has been written in task 1. The task is split into 2 sub-tasks: Task 3.1 is the delivery of the Xe spectra review tools and 3.2 is the final product with categorization tool and data release.
Location: At the Contractor’s office with 2 follow up meetings at the commission’s premises.

Time: This task shall take a maximum of 3 months after tasks 1 and 2

Deliverables:

a) A software written in C++/Qt that enables end users to review and analyze HPGe Xe data analysis (SPALAX) and to review and categorize Xe spectra according to the specifications. Software to provide the following functionality:

- review the Xe peaks and calculate the concentrations;
- display only necessary information for noble gas review;
- include a baseline correction tool: simplify and assist fast baseline correction. Configuration of detector specific default energy ranges of undisturbed spectrum intervals which are used to calculate the baseline below peaks.
- Reprocess spectra with controlled parameters.

The following functionality is required (not excluding additional functionalities):

- Versatile spectrum display;
- View to the fitted gamma peaks;
- Display of X-ray peaks and allocation of peak area to specific isotopes;
- Option to select baseline manually in the fitted view;
- Show calculated activities and detection limits for Xe-131m, Xe-133m, Xe-133 and Xe-135;
- Possibility to reprocess and release the results.
- Possibility to subtract X-ray fluorescence peaks from activity analysis.

The software to be delivered shall display the following automatic categorization results and categorization parameters:

- Thresholds for isotope concentrations vs. current station specific values and errors;
- Source receptor sensitivities (SRS) from major sources and compare to thresholds (SRS is calculated by another software and stored in the data base);
- Isotope ratios with error estimates (Bayesian confidence limits).

The software should also include:

- A tool for editing categorization comments, including options to change the categorization including a menu for commenting categorization. This menu should provide a set of configurable standard text blocks and an option for free text. Categorization commenting is stored in the database with appropriate tracking (author, date etc.);
- A categorization review tool;
- Options for display of a freely selectable number of spectra from previous measurements, peak parameters, xenon concentrations and activities, MDCs, SRS
- Perform Standard Spectra Method (SSM) analysis (Fitting standard isotope response functions to the spectrum).

a) The source code, a system design document, an installation guide and a user guide for the software delivered.
b) The system design document should include doxygen documentation for the main elements of the software.

Meetings:  
When the contractor has basic Xe analysis review tool ready it should present the results for the commission (2 days)

In the end of task 3 the contractor should deliver the product and present its capability for the Commission (3 days). In this meeting the acceptance of task 3 is considered and, if applicable, to move to task 4.

4.1.4 Task 4: Functionality for particulate review

Purpose:  
The Contractor shall develop a stand-alone review tool for particulate spectra in accordance with the requirements document that has been approved in task 1.

Location:  
At the Contractor’s office

Time:  
This task shall take a maximum of 3 months, after the completion of tasks 1, 2 and 3.

Deliverables:

a) A software written in C++/Qt that enables end users to review and analyze particulate data and to review and categorize spectra according to the specifications. This is fully functional particulate data analysis software with all the relevant functionality that is currently in the SAINT2 software and additional features as described in the requirements document produced in task 1.

This includes necessary graphical tools to
• review the association of the peaks to relevant nuclides and review unidentified peaks,
• review the critical limit for the peaks and minimum detectable concentrations (MDC),
• perform a special review for background spectra
• review Tc-99m/Ge-75m isotopes, option
• reprocess and release the results.
• Other necessary features identified in the task 1 of this contract and build currently available the SAINT2 software earlier should also be included. Figures 3-6 contain examples of some tools in SAINT review software.

b) The source code, a system design document, an installation guide and a user guide for the software delivered.

c) The system design document should include doxygen documentation for the main elements of the software.

Meetings:  
When the basic part of particulate data review is ready (review relevant nuclides and unidentified peaks, review of critical limits and MDC and background spectra review) the contractor should present the results for the commission (2 days)
In the end of task 4 the contractor should deliver the product and present its capability for the Commission (3 days). In this meeting the acceptance of task 3 is considered.

Figure 3. Special nuclide review tool that shows the gamma lines and actual possible peaks in the spectrum.

Figure 4. Tc-99m/Ge-75m review tool, this tool is used to differentiate between Tc-99m, Mo-99 (fission products) and Ge-75m (cosmogenic interaction).
4.2 Meetings

Meeting schedule is introduced in 4.1.1. – 4.1.4, all meetings shall be held at the Commission’s premises.
4.3 Other Provisions

- The Commission strongly recommends the use of the Qt widget toolkit for building the GUI and of C++ for developing the software. The C programming language can be used for computational routines if preferred.

- All IDC radionuclide software uses a central database, with a defined structure which runs under an Oracle RDBMS. The software developed under this contract must also work against this database. Should the need arise to define new database tables or to change the structure of existing database tables, the Contractor shall inform the Commission of the required changes early on. The Commission will decide on the feasibility of such changes. The Qt SQL classes can be used for database access from the C++ application.

- The software packages developed in task 2, task 3 and task 4 contain several tools that are similar in appearance and user experience, like spectrum display, manipulation and calibration tools. The software should be developed in such a way that common functionality is identified at the design stage and common widgets/components can be shared by the two software packages, For instance common components could be placed in a library that each of the two software packages links against.

- All software shall function under standard Linux Red Hat 5.3 or later. Special care shall be taken not to use any platform-specific extensions in the code developed under the contract.

- The source code written shall be in line with IDC coding and documentation standards. Specification of these standards will be provided to the Contractor at the start of the Work. Doxygen-style comments shall be included into the source code and a Doxygen documentation shall be generated by the Contractor based on such comments.

- The Commission prefers to use the GNU Scientific Library (GSL) for mathematical routines not available in the C++ Standard Library.

- The Contractor shall be required to submit monthly progress reports by email, describing the status of the work and any problems encountered.

- As a general rule, the Schedule for provision of the deliverables (based on section 3 of this document and to be provided in the Statement of Work written by the Contractor in the proposal) shall be followed, unless otherwise agreed with the Commission during the course of the activity.

- The delivery of the software can be made electronically or by mail on CD/DVD.
5 Acceptance Criteria

- The Commission shall consider the work under the Contract complete following acceptance of the final report and all the deliverables. After the completion of each subtask within tasks 2, 3 and 4 the Contractor shall deliver the software together with an updated software design description, software user guide and software installation guide to the Commission. The Commission will test the software and report bugs within 2 weeks following the delivery. For the final deliverable the Commission requires a testing period of 1 month. After task 3 and 4 the Contractor shall assist the Commission in implementing the software at the Commission’s headquarters and in conducting a test program with analysts (review approx 50 spectra).

- All deliverable material, comments, meetings, presentations and other communications with the Commission shall be written or conducted in the English language.

- Deliverable documents shall be delivered in both Microsoft Word (Word XP or newer) and Portable Document Format (PDF) version 6.0 formats, unless otherwise specified.

- Final reports for each task shall be provided in draft to the Commission for review and comments three weeks before the final version is delivered.

6 Work location

The staff designated by the Contractor for this work assignment shall perform their tasks in their own offices, except for the meetings that shall take place at the Commission.

7 Required technical skills of the Contractor

The Contractor’s staff performing the Work must have the following qualifications:

6.1 A university degree in Computer Science (or other scientific/technical subject with a high computing content).

6.2 At least 3 years of recent professional experience implementing and testing software on Unix and Linux systems.

6.3 At least 3 years of recent professional experience developing scientific software systems.

6.4 At least 3 years of recent professional experience using C++ with Qt on a Unix platform.

6.5 Experience using object-oriented design and development methods.

6.6 At least 3 years of professional experience with database programming using an RDBMS (preferably Oracle). Experience using Qt SQL Classes is a plus.

6.7 Experience with radionuclide data processing systems is highly desirable.

6.8 Experience using the GNU Autotools series of development tools is desirable.

6.9 Professional experience in MATLAB programming is desirable.

6.10 Fluency in written and spoken English.
8 Requirements for the company

It is expected that the Contractor respond to the following technical and financial requirements;

a) Proven experience in building scientific analysis software.

b) Experience in high resolution gamma ray spectrum analysis is an asset

c) The company needs to possess the necessary hardware/software tools to perform the work with Linux Redhat 5.3 environment.

9 Responsibilities of the Commission

9.1 For designated Contractor Personnel, and to the extent necessary for the Contractor to fulfil the requirements of these TOR when carrying out work approved by the Commission on site, the Commission will provide:

9.1.1 Infrastructure, including office space and standard office supplies, hardware and software.

9.1.2 Access to E-mail, telephone and facsimile.

9.2 The Commission will make related technical documentation available to the Contractor.

9.3 The Commission will make qualified staff available to provide assistance and cooperation in responding to information requests from the Contractor in order to allow the Contractor to carry out the Work.

10 Intellectual Property Rights

All title, ownership rights and intellectual property rights in and to the Software shall remain with the Contractor. The Commission shall acquire no title, right or interest in the Software, other than the licence(s) specifically granted by the Supplier under the Licence Agreement attached as Annex A to the Contract, and the title to the media upon which the Software is delivered.

11 CTBTO Policy for Data Access by Contractors

The CTBTO PrepCom document CTBT/PC-13/1/Annex II defines the policy for provision of access to IMS data and IDC products to organizations contracted by the PTS to do work for the PTS as follows:

- "Each contractor will access only those IMS data and IDC products necessary for fulfilling its task.

- The IMS data and IDC products will be used only for research associated with the development of the IMS and IDC or for the purposes stated in the contracts.

- Access provided to an organization for the purposes of fulfilling a contract will terminate when the contract is completed."
The restrictions placed on all users will not exclude the presentation of data or products (or information derived from there) for peer review at scientific meetings or in scientific journals and other scientific publications. The inclusion of IMS data and IDC products in scientific journals and other scientific publications will be limited to those required to reflect the scientific achievements. The contractor should not redistribute these data to third parties.”

IDC bulletins that incorporate event screening criteria shall not be included.

12 CTBTO Policy for Publications and Presentations

The CTBTO PrepCom document CTBT/PC-13/1/Annex II defines the rules for publications and presentations of results of PTS Contractors as follows: The contractor will provide the PTS with a copy of any publication or presentation in advance. If the PTS does not raise any objections within five working days after the receipt by the PTS of the advance copy, the publication or presentation shall be considered as approved. While considering the request for publication or presentation, the PTS will verify that the publication or presentation is limited to the reflection of scientific achievements only. A disclaimer, stating that the PTS is not responsible for the views of the author, should be included in the publication or presentation.