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Sandia National Laboratories (SNL) and Oak Ridge National Laboratories (ORNL) Joint Development of SNL's Sample Tracking, Analysis & Reporting (STAR) Information System

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Sandia National Laboratories (SNL) and Oak Ridge National Laboratories (ORNL)

Joint Development of

SNL's Sample Tracking, Analysis & Reporting (STAR) Information System

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Computing and Telecommunications Services
based on work performed for
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Background

A comprehensive environmental sample management program allocates an extensive portion of its resources to information collection, management, and manipulation. Much of this data is difficult to obtain and even more costly to ensure that it is sufficiently accurate. Strict requirements for meeting holding times, analytical requests, and electronic data deliverables, etc., make an automated system desirable. A computerized system that collects information at the point at which a field sample is taken, tracks the sample to analytical labs and loads electronic data deliverables from these labs, while maintaining chain of custody and data integrity, is an efficient and cost effective approach to providing consistent and accurate, legally defensible sample data.

The Sandia National Laboratories, New Mexico (SNL/NM) Sample Management Office (SMO) contracted out the tracking of SNL sample data until an audit finding mandated an internal Sandia sample management system be implemented. In June, 1993, a team was formed to gather SMO requirements and begin development of a sample tracking system. As the team began the requirements phase, a review of existing software was performed for a make/buy decision. The commercial software available at that time was very limited, most only had limited tracking capabilities. A review of sample systems at various DOE labs was started with trips to EG&G Rocky Flats and ORNL to review DOE sample management processes and software.

Since sample collection processes vary very little between the different DOE laboratories, it was presumed that a good sample management data model and information system could be applied easily at different sites with only slight modifications. This paper is an overview of experiences encountered when SNL/NM transferred and implemented sample software from the Waste Area Group (WAG6) at Oak Ridge National Laboratories.

Sandia's Sample Management System Requirements

The Sandia SMO project was initially phased to computerize the following application system modules:

Phase I - Tracking sample data

- tracking of sample data from the field to the lab,
- batch reporting of sample tracking data,

Phase II - Analytical data loading and verification

- analytical data loads from multiple analytical labs,
- analytical data verification of non-CLP data deliverables,
- analytical data interface to Environmental Center systems, Environmental Restoration (ER), Waste Operations, Cradle-to-Grave Tracking, etc.
- analysis reporting on lab data using a statistical package,

Phase III - Billing sample data

- billing of lab invoices with charge back to internal SNL service center customers,

Phase IV - Sample Project Planning

- sample project planning allowing technical project leaders to submit and update sample plans on-line,

Phase VI - Sample data validation

- data validation of CLP (contract laboratory program) and
- non-CLP formats on multiple quality control (QC) levels,

Phase VII - Sample data bar-coding

- bar-coding of samples to enhance chain-of-custody requirements.

Sandia's Environmental Center information system standards made the use of a network Oracle 7.0 client/server data base system with Oracle Forms IV as the front-end interface desirable.

Sample Management System Make/Buy Decision

The following sample management systems were reviewed for possible application at Sandia:

Commercial:

- Analytical Compliance System (ACS),
- LUNA*Sample™ Eclipse Sample Tracking system (Oracle data base),
- Oracle Environmental Information System (Oracle data base).

DOE:

- EG&G Rocky Flats SMO Oracle data base system (Oracle data base),
- Analytical Services Organization - Sample Tracking System (Ingress),
- ORNL WAG6 Sample tracking system (Oracle data base).

The SMO Team did a complete review of the data models and application software for the systems listed above. WAG6 had the most complete sample management data model and came closest to Sandia SMO requirements and processes. As a result, Sandia initiated an ICO with ORNL to transfer the WAG6 analytical laboratory data models, software and enhancements to integrate with Sandia's Sample Tracking System.

SMO Technology Transfer

During the time involved in requesting, evaluating and transferring the Oak Ridge software, Sandia developed an in-house sample tracking module. This left Sandia with the decision to throw away their recently in-house developed sample tracking module, completely adopt the Oak Ridge WAG6 way of doing business, or integrate the WAG6 analytical data model with Sandia's sample tracking model. Data models can easily be modified to fit a new environment, but understanding the model requires knowledge of the thought and logic applied when the model was developed. To integrate the two models required that the Oak Ridge and Sandia analysts walk through the WAG6 model, comparing Sandia analytical requirements against the ORNL analytical data model, providing a way to integrate Sandia's sample tracking with WAG6's analytical software. This allowed Sandia's SMO to retain their SNL in-housed developed sample tracking module and continue to do business processes as they had in the past while adopting the WAG6 analytical software to load and verify data deliverables from analytical labs. This also allowed Sandia's SMO to implement the Oak Ridge analytical module in a few months, saving of three man years worth of development and programming effort. In addition, valuable expertise and lessons learned were acquired.

SMO/ORNL Working Agreement

The SNL and ORNL teams defined the following tasks required to transfer the Oak Ridge analytical module to SNL over a six month schedule:

- SNL and WAG6 analysts reviewed the WAG6 analytical data model to determine the WAG6 data model's use at Sandia,
- SNL provided ORNL with their SMO analytical requirements document and an example analytical laboratory electronic data deliverable (EDD),
- ORNL provided data for methods, sample test types, and sample bridge look-up tables,
- ORNL defined analytical processing rules for the analytical laboratories EDDs based on the SNL example EDD and analytical requirements,
- SNL reviewed and approve the analytical processing rules,
- ORNL set up a file server to develop and test software for Sandia,
- ORNL developed statistical analysis software using SAS™ based on Sandia's EDD processing rules,
- ORNL provided functional and system test plans,
- ORNL tested the functions and system,
- SNL accepted and implemented the SAS™ programs and the analytical software system,

- ORNL provided consultation to SNL to address technical issues associated with bringing SNL analytical laboratories on-line.

SNL placed an ICO purchase order, which was approved by DOE, to provided \$99,000 of funding to Oak Ridge for completing the required consulting and programming tasks.

SMO/ORNL lessons learned

The result of this collaboration between Sandia and Oak Ridge has been highly successful. The benefit of this teamwork has provided Sandia with the use of existing DOE software to solve similar environmental sample data management at a different DOE site and provided ORNL with valuable knowledge of how other DOE sites operate.

Conservative estimated savings of three man years of programming effort or \$500,000 for the ORNL automated analytical laboratory interface is significant. Additional benefit and saving includes the wide breadth of experience provided by Oak Ridge in implementation of interfacing electronically to analytical laboratories as well as extensive knowledge of radiochemistry and organic verification data processing rules. The transfer of experience and knowledge from ORNL to Sandia is difficult to quantify, but can easily be interpreted as one year of escalation in the development and implementation time or an additional \$500,000 in labor savings. The use of the Internet to communicate and efficiently transfer SNL and ORNL email, documentation and software was an extremely effective tool.

Due to cuts in Sandia funding, phase III through VII are currently not scheduled to be automated but further discussion on teaming efforts with Oak Ridge to implement ORNL data models and systems is being pursued.

The approach of transferring comprehensive application data models and software, that can easily be adapted and modified, allows DOE sites to keep their unique business processes while accepting existing software. This collaboration has provided proof that computer software can be successfully transferred between DOE sites at considerable savings of time and funds to DOE estimated at one million dollars for this one effort.

Appendix A

ORNL ENVIRONMENTAL RESTORATION INFORMATION MANAGEMENT SYSTEM

The ORNL Environmental Restoration Information Management System provides organization, integrity, security, traceability, and consistency of the environmental measurements data generated during an environmental restoration project life cycle. The system supports sample analysis planning, laboratory statements of work, field planning and logistics, sample collection and shipment, field measurements and validation, bar-coding, analytical laboratory results (electronic data deliverables and data validation), sample tracking, and assessment. The system was developed utilizing information engineering and an Integrated Computer Aided Software Engineering (ICASE) tool.

SYSTEM FUNCTIONALITY

Sample Analysis Planning (SAP)

The SAP contains the sampling locations, frequencies, analysis, containers, and field measurements to be collected. The software provides reference tables to populate the sampling tasks defined by the SAP prior to sampling for use in planning and sample collection. By entering tasks (e.g. quarterly groundwater quality) the user can re-use tasks and eliminate the need to re-enter similar information every time a sampling event occurs.

Laboratory Statement of Work (SOW)

The laboratory SOW specifies specific analytes, analysis methods, electronic and hardcopy deliverables, and cost for sample analysis. The software provides tables to populate the laboratory SOW information, it does not include cost information at this time.

Planning/Logistics

The software supports planning to go to the field by providing tools to bring the information populated from the SAP as tasks over to field forms (field activity sheet or field chain of custody) so that containers can be assembled and labeled prior to going to the field. The software can optionally generate sample container labels and bar code labels. The software also tracks the forms and log books associated with sampling events for traceability from the system to the hardcopy.

Sample Collection and Shipment

Using the field sheets generated in Planning and Logistics the field crews can add additional information on the forms and sample containers such as the Ph reading, sample collection date and time, and field measurements. The system also permits multiple QC sample ties (tracking the original sample and its duplicates, matrix spikes, and matrix spike dups). This information is entered into the system after the crews return from the field. After collection, the software can generate the Chain of Custody for sample shipment.

Field Measurements and Validation

The software can load and display information collected by automatic data collection devices such as groundwater levels, conductivity, water temperature, surface water levels, and meteorological data. Tools are provided to validate the field measurements collected to detect malfunctioning devices, missing data, or data out of range for the device.

Barcoding

The system has software to generate bar code labels for use on field forms, logbooks, and sample containers. Bar code readers can be used in the field to scan sample collection information and some field measurements, this information is then downloaded into the workstation from the readers and loaded into the database after verification by the field person. This reduces data entry and improves data quality by reducing errors in data entry. The bar coding features are all optional. The software will all work without using bar-codes.

Analytical Laboratory Results

The software supports electronic verification and validation of electronic data deliverables (EDDs) received from laboratories and allows this information to be loaded into a common data structure for all analytical data. This structure will accommodate both customer and Quality Control (QC) result information.

Electronic Data Deliverables (Sample Results)

The system has the ability to screen and load several types of data deliverables. Contract Lab Program (CLP) deliverables are screened using the Contract Compliance Screening (CCS) software and Computer Aided Validation and Evaluation Assessment Tool (CAVEAT) software. The CLP deliverables include inorganics, organic pesticides, and semi-volatiles. Non-CLP deliverables are loaded and include volatiles and radiological results. In addition to the sample results, the system loads 80% of the organic pesticide, 90% of all other organic, and 90% of the inorganic Quality Control (QC) data.

Analytical Data Validation

The system provides screens for data qualifiers to be added to the samples along with the CAVEAT reports.

Sample Tracking

Several sample tracking reports are either completed or under development to display sample status, holding time and turnaround times, validation status tracking, milestones, and laboratory SOW and data packet comparison to ensure the lab satisfied its requirements.

Assessment

Work is currently underway to provide assessment reporting.

Computing Environment

- Texas Instruments Information Engineering Facility (IEF) Data Model

- Oracle Database and Forms
- SAS
- C Programming Language
- SUN Workstation
- Solaris Operating System
- X-Windows Terminals
- IBM Personal Computers using X-windows Emulators.

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