SYNTHETIC AND VIRTUAL ENVIRONMENTAL MEDIA (SAVEM)

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ABSTRACT

The Synthetic and Virtual Environmental Media (SAVEM) Program, developed at the DOE Environmental Measurements Laboratory, responds directly to issues of improved data quality, increased regulatory confidence, analytical laboratory waste minimization, pollution prevention, worker safety/radiation exposure risk reduction, and environmental stewardship.

The SAVEM radiochemistry information analysis system uses digitally generated spectra to accurately model gamma-ray emission characteristics of radiological samples. A digital virtual sample can be specified that has the characteristics of any environmental media such as soil, sediment, or vegetation, and which exhibits the spectral characteristics of more than 2,000 gamma-emitting nuclides. The SAVEM system can duplicate the characteristics of 2,361 individual radionuclides with 47,902 gamma lines.

Over the past five years (1996-2001), EML analyses of SAVEM results indicate three key findings:

- A 50 % reduction in false negative results, e.g., 50% fewer analyses stating that a radionuclide is not detectable when, in fact, one was known to actually be present;
- A 42% reduction in false positive results, e.g., 42% fewer analyses having radionuclides indicated as present when in fact, they are not; and
- EML analyses of participating laboratories indicate a 12% overall increase in analytical accuracy when using SAVEM versus "conventional" analysis procedures.

INTRODUCTION

The Synthetic and Virtual Environmental Media (SAVEM) radiochemistry information analysis system uses digitally generated spectra to accurately model gamma-ray emission characteristics of radiological samples. A digital virtual sample can be specified that has the characteristics of any environmental media such as soil, sediment, or vegetation, and which exhibits the spectral characteristics of more than 2,000 gamma-emitting nuclides. In fact, the SAVEM system can duplicate the characteristics of 2,361 individual radionuclides with 47,902 gamma lines. The key difference between SAVEM and traditional libraries of stored gamma spectra is that initial raw data is not collected and measured from an actual prepared

standard or reference sample. In SAVEM, the raw data and final spectra are mathematically generated using defined physical and chemical relationships in conjunction with advanced computer simulation techniques.

KEY RESULTS

Once adopted, SAVEM will have many benefits. The most important of these is the increased level of regulatory and organizational confidence that will be placed in site radiological characterization data analyses and in waste characterizations performed prior to shipment and disposal. Increased confidence in analytical results leads directly to increased confidence in regulatory decisions about both site cleanup and closure decisions, and in approving waste shipments. Over the past five years (1996-2001), EML analyses of SAVEM results indicate three key findings:

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- EML analyses of participating laboratories indicate a 12% overall increase in analytical accuracy when using SAVEM versus "conventional" analysis procedures.

Another key feature of SAVEM is that by using virtual digital spectra for QC and QA evaluations, there can be a dramatic reduction in needs to produce, prepare and ship expensive laboratory-prepared radioactive samples and standards for quality control sample analysis requirements. Other benefits include reductions in laboratory waste generation, reductions in laboratory record-keeping requirements, and reductions in radiological waste disposal costs. As such, SAVEM represents a major step in "greening" radiochemistry processes and procedures, and simultaneously, improves analytical accuracy, reduces risks of accidental exposure, and provides a risk-free training tool for radiochemists and other laboratory staff.

BACKGROUND

The Department of Energy, Office of Environmental Management's (DOE/EM) Office of Safety, Health, and Security (EM-5) was created to consolidate safety, health, security, emergency management, risk management, package certification, quality assurance and characterization/monitoring/sampling/analysis activities and resources. EM-5 has engaged WPI through a DOE Chicago Operations Office Cooperative Agreement (DE-FC02-CH10849) to support efforts at the Department of Energy's Environmental Measurement Laboratory (EML) in communicating the features and benefits of the synthetic gamma spectrometry data evaluation program (the heart of the SAVEM system) to DOE remediation and cleanup projects. EML, located in downtown New York City, is a government-owned, government-operated laboratory that is programmatically an element of the EM Office of Science and Technology (EM-50). DOE's Chicago Operations Office (CH) administers the Laboratory.

EML provides program management, technical assistance and data quality assurance for measurements of radiation and radioactivity relating to environmental restoration, global nuclear non-proliferation, and other priority issues for the Department of Energy, as well as for other government, national and international organizations. WPI, as part of its cooperative agreement with DOE-Chicago Operations, works with EML staff in developing and improving stakeholder communication strategies focusing particularly on regulators, technology hardware and software vendors, end-users, and the international community. Specific areas of interest include:

- Disseminating information on the value and uses of advanced quality assurance, health and safety, and data validation and verification products;
- Developing communication plans and strategies to ensure the Gamma Spectrometry Data Evaluation Program and related quality programs are publicized and understood by stakeholders;
- Identifying strategies to manage data, information and knowledge to facilitate stakeholder communications; and
- Improving communications and knowledge sharing with international organizations whose mission(s) parallel EML's.

DATA QUALITY ISSUES

EML promotes best practices and management tools resulting in cost-effective, efficient, environmentally beneficial, and high quality analytical data and services for DOE. Making good decisions in environmental programs, particularly those with a radiological component, is critical in meeting DOE's missions. Key decisions about both specific recommendations concerning individual site cleanup actions and overall DOE radiological waste disposal actions and policies demand high quality data. Data quality evaluations and assessments of radiological data quality are the final steps in the overall environmental data decision process. [(1)] These decisions demand data of sufficient quality such that the level of confidence in these decisions is high and the risks of poor (incorrect) decisions are minimized.

A majority (>60%-70%) of the environmental analysis samples collected at DOE remediation and waste management sites and activities require a gamma spectral analysis as a central element of an overall site characterization process. Accurate site radiological condition characterization is essential in ensuring that both appropriate cleanup strategies are identified and selected, and that correct waste storage, treatment, transport, and disposal requirements are identified and met. A high precision, efficient and effective gamma spectrometry analysis system that quickly, accurately and cost-effectively identifies and quantifies radionuclides in waste samples is a critical need for several reasons. Specifically, such a tool has ready applications in cleanup activities, in implementing best waste management practices as EM progresses towards achieving organization-wide waste minimization and pollution prevention goals, in addressing long term monitoring needs, in establishing release criteria for contaminated sites, and in enhancing both site and programmatic risk assessments.

A majority of the environmental analysis samples collected across the DOE complex require a gamma analysis before final decisions can be made relative to the disposition of specific waste streams and/or specification of cleanup activities at a contaminated site. SAVEM does

not replace actual site environmental analysis samples, but it can replace radiological samples intended for quality control and data confidence (quality assurance) purposes. These QC and QA samples represent anywhere from 25% to 40% of all samples analyzed as part of DOE site characterization and waste stream analysis activities. SAVEM provides many features and benefits, because it:

- Improves laboratories' capabilities to accurately identify and quantify nuclides. This directly translates into better risk assessments and improved decision making processes;
- Quickly and efficiently identifies laboratories having problems with gamma spectroscopy software packages. This eliminates the need for submitting an additional battery of expensive QC samples to isolate specific problems and deficiencies;
- Is a training tool to educate health physicists and spectroscopists on analysis and data reduction process for complex spectra (without using actual QC samples). This improves consistency, accuracy, and reduces risks of accidental radioactivity exposure in training activities;
- Supports pollution prevention and waste reduction policies because no waste is produced when using SAVEM-produced synthetic gamma spectra;
- Supports risk reduction and health and safety principles because it limits worker and laboratory staff exposure to radioactive materials;
- Supports paperwork reduction principles because the technology promotes laboratory automation (reduces manual manipulation of spectra data); reduces waste inventory controls and record keeping; and reduces data requirements associated with radioactive waste generation, storage, transport and disposition; and
- Supports principles of long-term stewardship because the technology promotes continual quality improvements, sound knowledge and data management practices, and risk management.

DESCRIPTION OF THE TECHNOLOGY

The SYNTH program, the FORTRAN code written to generate synthetic gamma spectra, was developed by Pacific Northwest National Laboratory (PNNL) and is a key component of the SAVEM analysis system concept. The DOE/EML is the quality assurance/quality control reference laboratory for all contractor laboratories performing surveillance and monitoring activities for DOE/Environmental Management (EM) cleanup activities (DOE Order 414.1A and memorandum from EM-1). EML tested the accuracy of the SYNTH program by counting emissions from a known radiological standard using a germanium detector under specific conditions to generate actual Gamma emissions spectra. Subsequently, information describing relevant detector parameters, including specifications for detector diameter, length, % efficiency, end-cap type, resolution, nuclide, counts, etc. was entered into the SYNTH program. The spectra created by the SYNTH program were compared to the actual spectra obtained from counting the known standard using the germanium detector. The digitally-generated synthetic spectra produced using the SYNTH program were found to be within the expected tolerance range. The SYNTH program conforms to the guidelines and principles established in:

- DOE Order 203.1 *Software Quality Assurance*;
- U.S. Food and Drug Administration Center for Devices and Radiological Health, *General Principles of Software Validation*, Draft Guidance Version 1.1, June 1997;
- The National Institute of Standards and Technology (NIST) Special Publication 500-234, *Reference Information for the Software Verification and Validation Process*, March 1996, and
- EPA Office of Administration and Resource Management, Good Automated Laboratory Practices, Section 7.9 *Software*, December 1990.

USING SAVEM

The SAVEM analysis system is easy to use. A user contacts DOE/EML and provides specific information about their radionuclide detector configuration (type of detector, geometry, etc.) and the information format requirements of their specific radionuclide analysis software. EML produces a full set of SAVEM digital synthetic spectra files that include:

- A blank (to account for background signals);
- A calibration file to "zero" the analysis software; and
- Three separate digital spectra representing differing levels of analytical difficulty.

The three synthetic spectra would include, for example, an "easy" level of difficulty problem, e.g., usually a very simple single line or multiples with no interference, a "medium" level of difficulty problem, e.g., a spectra that includes some interfering and branching problems, and an analytically "hard" or difficult spectra that could include multiple radionuclides, a complex matrix, and complex branching.

After receiving the set of digital synthetic spectra files (typically on a diskette or tape, but in the future, obtained over the Internet from DOE/EML or any other SAVEM digital spectra provider), the analyst opens the files, and runs the gamma spectroscopy analysis software package. The analysis software interprets the SAVEM digital data information as if it was obtained from a real sample. The software captures the data, performs a radionuclide analysis, and produces an output file. The analyst checks the output to determine which specific radionucleide(s) and Gamma lines are present in the SAVEM digital virtual sample. These results are then sent to the SAVEM digital file producer (DOE/EML) for comparison with the parameters used to create the synthetic digital spectral file. Results of the comparison are sent back to the analyst to either 1.) confirm that the analyst's evaluation of the SAVEM digital synthetic spectra file is correct, or 2.) confirm that the analyst's evaluation is incorrect. In the event of an incorrect answer, additional information about possible sources of error is also included. Possible sources of error could, for example, include either software errors (corrupted files, incorrect use of SAVEM software calibration file, failure to consider background counts, etc.) or spectral output interpretation problems stemming from analyst errors or misunderstandings.

RESULTS FROM DIGITAL GAMMA SPECTRA DISTRIBUTION STUDIES

EML evaluated commercial available software packages for analyzing low-level environmental gamma-ray spectra in 1988, and again in 1991. The first evaluation indicated the software packages delivered poor accuracy and poor performance in peak analysis. [2] The second evaluation indicated better performance, but problems still existed. [3] In 1996, EML began distributing synthetic digital radionuclide spectra to participating laboratories to evaluate commercially available and "in-house" developed analytical software package capabilities for accurately identifying and quantifying nuclides in complex gamma-ray spectra. Currently, more than 65 laboratories (both domestic and international) participate in the program. Results collected during the past five years indicate a 42% reduction in laboratories reporting false positive results, and an overall 12% increase in accuracy in comparing laboratory values relative to established reference values. [4,5] In addition, the synthetic gamma spectra software in SAVEM can serve as a training tool to teach laboratory personnel and health physicists proper techniques in nuclide identification and quantification of highly radioactive samples without risks of either excessive radiation exposure or potential risks of contamination.

Table I presents an overview of the laboratories participating in the synthetic gamma data evaluation program conducted under the direction and supervision of EML.

Table I:
Category of Laboratories Participating in Evaluation Program

Laboratory Type	# of Participants	Percentage of Total
National Labs	8	12.1%
Commercial Labs	16	24.2%
State Labs	13	19.7%
International Labs	19	28.8%
University Labs	10	15.2%

PRELIMINARY ESTIMATES OF SAVEM-DERIVED ECONOMIC AND ENVIRONMENTAL BENEFITS

Since 1990, EML has been actively involved in supporting the radiation measurement industry as it moves from a mainframe-based, manually operated system to PC-based, digital analysis systems. The major benefits of the SAVEM technology include:

- SAVEM reflects the principles of As Low As Reasonable Achievable (ALARA), and supports the new Nuclear Safety Management Rule (10 CFR830, effective August 2001).
- SAVEM can revolutionize analytical laboratory QA Audit/Assessment Processes (both the extent of resources needed and the time required). An Audit/Assessment

Team, which can be as many as 2 to 3 people, can spend up to a week at laboratory certifying laboratory capabilities and reviewing data. Using SAVEM, an EM quality assurance lab audit could send 1 or 2 persons and spend 1or 2 days at the laboratory instead of a full week. The basic concept is that the auditors could send sample digital spectra to the laboratory one or two weeks prior to the actual audit team visit, and have the desired analysis data waiting for them upon arrival. Today, it is possible to conduct at least part of the audit on a remote basis, with sample digital spectra sent to the lab and analysis results transmitted back to the audit team via the Internet before it ever arrives at the location being audited.

- SAVEM revamps disposal site waste verification/certification processes (and reduces costs, resource use and time). Disposal sites are required to verify and certify waste packages from hazardous waste generators to meet their waste acceptance criteria. This process can be greatly facilitated if the waste generator and waste disposal site have a web-based quality control system that can be assessed via the Internet on a secure line.

- SAVEM serves as an excellent training tool. It produces accurate, realistic data, and at the same time does not expose personnel (particularly untrained or partially trained staff) to unnecessary and avoidable radiation exposure and other health and safety risks (chemical exposure, inhalation, etc.)

- SAVEM improves risk assessment confidence levels and both site-specific and programmatic decision-making capabilities by reducing uncertainty levels that accompany analytical results. The SAVEM technology improves on the precision and accuracy of analytical results. This directly translates into better knowledge on the contaminants of concern and improves the likelihood that selected remedial actions are, in fact, the most appropriate remedial action.

The limitations of the SAVEM process are:

- The process does not validate that the detector and the electronic components of the system are working properly. It is designed to be both a check of the spectroscopic analysis software and the person performing the data interpretations; and

- The SAVEM analysis system is a single blind process. Many laboratory quality assurance managers prefer systems that are designed as double blind processes. (A single blind process is when an analyst suspects a specific sample is a quality control sample, but does not know its value. A double blind process uses samples that prevent the analyst from knowing both that the sample is a quality control sample and the analyst does not know the result).

CONCLUSIONS AND FUTURE APPLICATIONS

We have only begun to define the extent of SAVEM's full development potential in protecting and promoting both national security issues and environmental stewardship needs.

The SAVEM system is truly "Faster, Cheaper, Better and Safer". These attributes are clearly demonstrated in the context of both DOE (and other) site characterizations and in waste stream analyses. In the particular context of waste stream content analyses, there are specific requirements governing the security and disposition of radioactive wastes at both federal and commercial disposal sites. Waste generators must supply precise waste characterization information, demonstrate that the information satisfies defined requirements, and meets applicable data quality objectives. [(6)] In this context, SAVEM supports a wide range of potential applications in:

- Verifying and Validating waste disposal programs at commercial and federal waste disposal facilities;

- Preparing and producing site-specific performance standards (particularly heterogeneous materials), and in simulating radionuclides that are both exotic, e.g., very short half lives, and very expensive to produce;

- Helping agencies involved in laboratory certification and capabilities approval (SAVEM provides agencies with an ability to certify laboratories safely, quickly and at a reduced cost);

- Promoting green chemistry technology (this process can: replace needs to produce expensive radioactive standards, reduce worker exposure, and reduce waste generation and disposal volumes, reduce disposal costs, and reduce record-keeping requirements that accompany radioactive waste generation, storage, transportation and disposal, and finally, reduces requirements for radioactive waste disposal facility capacity); and

- Potential development of a paperless, near real time, web-based synthetic gamma spectra quality control/quality assurance sample preparation and analysis results reporting service.

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