External Technical Review for Evaluation of System Level Modeling and Simulation Tools in Support of Savannah River Site Liquid Waste Process

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ABBREVIATIONS AND ACRONYMS

ANL	Argonne National Laboratory
ANS	American Nuclear Society
ANSI	American National Standards Institute
ARP	Actinide Removal Process
AFP	Actinide Finishing Process
COTS	Commercial off-the-shelf
CRESP	Consortium for Risk Evaluation with Stakeholder Participation
CSSX	Caustic-side Solvent Extraction
CSV	Comma-separated values
DDA	Deliquification, Dissolution and Adjustment
DOE	Department of Energy
DSA	Documented Safety Analysis
DWPF	Defense Waste Processing Facility
EM	DOE Office of Environmental Management
EPA	U.S. Environmental Protection Agency
ERD	Emergency Response Data
ETAF	Evaluated Transfer Approval Form
ETR	External Technical Review
FTF	F Tank Farm
GM	GlassMaker II
GUI	Graphical User Interface
GWSB	Glass Waste Storage Building
HLLCP	High liquid level conductivity probe
HLW	High-Level Waste
HLW-IPT	High-Level Waste System Integrated Project Team
HQ	Headquarters
HTF	H Tank Farm
IEEE	Institute of Electrical and Electronics Engineers
I/O	Input/Output
IT	Information Technology
LAW	Low-Activity Waste
LCCM	Life-cycle cost model
LIMS	Laboratory Information Management System
LLWP	Life-cycle Liquid Waste Disposition System Plan
LOI	Line(s) of Inquiry
LWO	Liquid Waste Operations
LWS	Liquid Waste System
MCU	Modular CSSX Unit
MST	Monosodium Titanate
NNDC	National Nuclear Data Center
NNSA	National Nuclear Security Administration
ORNL	Oak Ridge National Laboratory
ORP	Office of River Protection

OS	Operating System
PCCS	Product Composition Control System
PUREX	Plutonium–Uranium Extraction
QA	Quality Assurance
RAM	Reliability Availability and Maintainability
SB	Sludge Batch
SDIP	Salt Disposition Integrated Program
SME	Slurry Mix Evaporator
SPF	Saltstone Processing Facility
SpG	specific gravity
SQA	Software Quality Assurance
SQL	Symbolic Query Language
SQAP	Software QA Plan
SRNL	Savannah River National Laboratory
SRS	Savannah River Site
SWPF	Salt Waste Processing Facility
SWS	Sludge Washing Spreadsheet
TSR	Technical Safety Requirement
VBA	Visual Basic for Applications
V&V	Verification and Validation
VB	Visual Basic
WAC	Waste Acceptance Criteria
WCS	Waste Characterization System
WMF	Windows Metafile

EXECUTIVE SUMMARY

This report presents results of the External Technical Review (ETR) Team that evaluated the system-level modeling and simulation tools in support of Savannah River Site (SRS) liquid waste processing. A short description of the relevant experience of the team members and observers is given in Appendix A.

The SRS Liquid Waste System (LWS) is a highly integrated operation that involves safely storing liquid waste in underground storage tanks; removing, treating, and dispositioning the Low-Activity Waste (LAW) fraction as in concrete vaults on-site; vitrifying the higher-activity waste; and storing the vitrified waste until permanent disposition at a Federal Repository. After waste removal and processing, the storage and processing facilities are cleaned and closed. In order to integrate all required activities, the Life-cycle Liquid Waste Disposition System Plan (LLWP) has been developed. It establishes a planning basis for processing the constituents of the liquid waste system to the end of the program mission. The LLWP is a qualitative evaluation based on modeling and simulation estimates.

This review was chartered[1] to focus on three primary areas:

- Assess the assumption that the tools used for liquid waste process simulation yield reasonable estimates
- Evaluate if additional tools are needed to guide execution of individual processing steps
- Evaluate methods to improve the rate at which system model predictions are performed

The foci of the charter were "operational" aspects of the modeling at SRS, i.e. reasonableness of estimates, prediction speed, tool integration, etc. Software Quality Assurance (SQA) was not a primary focus area of this ETR. However, during the course of the review, the team noted a number of relatively simple to execute improvements of the overall SRS modeling process that were related to SQA. Therefore, a discussion of SQA topics relevant to SRS is included as Appendix C. In addition, SQA is mentioned (where appropriate) in Section 6.0 of the report that discusses the individual models used at SRS. Section 6.0 covers observations and recommendations for each of the tools that support the LLWP.

The review centered on several existing software tools, including:

- **Waste Characterization System Version 1.5 (WCS 1.5)** – a set Microsoft Excel workbooks used to track the inventory of selected chemicals and radionuclides in SRS High-Level Waste (HLW) tanks to represent real-time conditions.

- **Sludge Batch Toolkit** – a set of Microsoft Excel workbooks – including GlassMaker II (i.e. a set of Sludge Washing Spreadsheets and a stand-alone version of PCCS) – used to

[1] A copy of the ETR Charter is included in Appendix B. The Charter was established by EM-HQ and SRS personnel to ensure that both parties agreed to the broad goals of the review.

help plan and assemble sludge batches to feed to the Defense Waste Processing Facility (DWPF).

- **Product Composition Control System (PCCS) –** a Microsoft Excel spreadsheet used to guide the acceptability decision for each DWPF process batch.

- **SpaceMan Plus™ –** a Visual Basic 6 model used in planning to model material flows throughout the entire LWS to the end of the program mission.

- **COREsim™** – a discrete-event model used to evaluate bottlenecks in the LWS and to simulate facility processes.

Note: There is no software planning or acceptability tool analogous to PCCS for salt processing or Saltstone Processing Facility feed acceptability. Current acceptability methodology requires a manual system.

Main Observations

There are four main Observations:

1. ***The current System Plan relies on a collection of software tools to organize and analyze information, and guide processing of high-level waste at SRS. These tools currently provide reasonable estimates; however, no integrated system planning tool presently exists.***

   As utilized by experienced/qualified staff, the current tools have been effective in supporting processing of liquid waste at SRS. This has resulted in successful production of over 8 million pounds of radioactive glass at the DWPF, through processing five different batches of tank waste. The software tools were originally designed to meet Documented Safety Analysis (DSA), waste acceptance criteria (WAC) requirements and regulatory commitments. These codes have evolved over a number of years and have been modified to serve many of the requirements of the planning system. However, they are not optimal for system planning. Because the codes were developed independently to meet the immediate needs of different users, the codes do not integrate well, and often, are not integrated at all. A large number of manual actions are required to input data and transfer information among various spreadsheets, workbooks, systems and organizations.

2. ***The capabilities and integration of current tools are limited. These limitations hamper process optimization and mid to long-term planning***

   The current tools are limited by several factors. Data transfers are not automated, and there is not a data element dictionary common to all modeling platforms. Therefore, porting information from one model to another requires human intervention to interpret what the data means and how to input/export information so that it can be used in other models. This makes the model update process both slower and vulnerable to various types of human error. In some cases, the need for detailed familiarity with the codes or processes limits their uses to a small group of specialized experts. Also, the planning tools and processes are maintained by different owners, which makes coordination of a common process model structure, and approach to documentation, more difficult. Information Technology (IT) professionals are not routinely used to perform software functions (e.g. code revision and database management) and are not part of the modeling team; as a result, software selection is not optimal, and there appears to be an over-reliance on spreadsheet-based tools and legacy methods. Finally, the speed of calculation is often limited by computer hardware; the Team was briefed that access to more capable systems appears to be constrained by procurement issues and cyber-security concerns.

3. ***There is a need to increase system planning flexibility and the turnaround time at which system model predictions are performed***

   Tools should be revamped to decouple planning and operations support functions. Current planning tools are operated with the same level of rigor as operations-support (e.g., safety basis) tools, lengthening the scenario analysis process. Uncertainty management and error propagation should be managed using a more systematic approach. There is currently no WAC tool for the Saltstone Processing Facility that is analogous to PCCS for high-level waste vitrification. All of the codes should incorporate consistent, appropriately graded, Quality Assurance (QA) documentation and programming practices.

4. ***There is a need to relate system planning results with cost***

   Existing planning tools do not incorporate LWS processing costs. Cost-related evaluations are conducted by other methods and are not integrated with planning tools. Life-cycle plans assume funding is available at whatever levels are required to meet the project timeline: "*This Plan assumes full funding of the estimated costs to accomplish the required project - and operations activities. It supports justification for requesting necessary funding profile*" [CHEW 2007]. Therefore, waste handling is optimized on a purely technical basis in order to meet project timelines for completion of the mission. Modeling tools often incorporate cost as a factor, and the planning tools should be upgraded to factor in processing costs.

Recommendations

Several actions are recommended, based on the observations listed above.

1. ***Recommended short-term actions (6 to 12 months) include:***

   - Improve capability of computer resources (i.e., processor, memory and software)
   - Engage modeling experts and data-management professionals to develop and modernize present systems and integrate tools
   - Review current QA software design against most recent Department of Energy (DOE) policy guidance and implement simple SQA improvements as suggested in Appendix C

(e.g. lock down spreadsheet cells, embedded "error checking", use of named ranges instead of individual cell references, etc.)

- Develop a consistent approach to uncertainty management among tools to better understand error propagation and evaluate overall system uncertainty
- Define and implement SRS "best practices" to improve awkward spreadsheet procedures for data management and thereby improve data integrity
    - Participate in complex-wide technical exchanges to identify and adopt best practices and new software approaches
    - Develop standard approach for spreadsheet documentation
- Begin planning for development of data systems and integrated models for operations and planning and evaluate needs and opportunities for long-term optimization
- Develop a tool analogous to PCCS for Saltstone Processing Facility WAC

2. Recommended mid-term (next 2 years) actions:

- Develop a "tank inventory database" to support:
    - Independent safety analysis and DSA requirements
    - Near-term operations
    - Long-range planning estimates
- Develop integrated planning models to include the capability to run:
    - "What-if" scenarios
    - Risk, Sensitivity, and Reliability, Availability, and Maintainability (RAM) analyses
    - Faster revisions of the System Plan to take advantage of new and emergent information and opportunities
- Develop the ability to compare historical model predictions with actual data, i.e., put in place a mechanism whereby inputs and outputs are archived in a database so that modeling accuracy over time, or data forensics, can be evaluated
- Relate system planning results to cost
- Develop the capability to propagate uncertainties through the planning process
- Explore computing environments for long-term planning needs, including optimization
- Contribute to DOE Office of Environmental Management (EM) Headquarters (HQ) complex-wide effort to identify opportunities and approaches for system optimization

3. Recommended long-term (3 to 4 years) actions include:

- Integrate the "tank inventory database" and safety-basis ("WCS") system
- Develop the capability to ensure the consistency of assumptions and calculations among safety, planning, operations and WAC tools
- Implement improved tools for optimization and decision making
- Work with the DOE-EM HQ and other program offices to adopt consensus standards for material properties across all models

External Technical Review for Evaluation of System Level Modeling and Simulation Tools in Support of Savannah River Site Liquid Waste Process

1.0 Background

The Savannah River Site, a 300-square-mile DOE Complex located in the State of South Carolina, has produced nuclear material for national defense, research, medical, and space programs. Since 1954, SRS Tank Farms have received more than 140 million gallons of liquid waste. Periodically the liquid waste has been evaporated to reduce its volume. To date, over 100 million gallons have been evaporated; the SRS Tank Farms currently store over 36 million gallons of waste containing approximately 400 million curies of radioactivity (Figure 1.1). Most of the tank waste inventory was generated during processing of irradiated targets and spent fuel using the Plutonium–Uranium Extraction (PUREX) process in F Canyon and the modified PUREX process in H-Canyon (H-Modified or HM process). Waste generated from the recovery of Pu-238 in H-Canyon for the production of heat sources for space missions is also included. More recently 30,000 gallons of highly radioactive Americium/Curium solution was transferred from F-Canyon to Tank 51H in the H Tank Farm.

Because the liquid radioactive waste storage tanks at SRS are constructed of carbon steel and the canyon wastes are acidic, the wastes were neutralized via additions of sodium nitrite and sodium hydroxide. These additions have resulted in formation of metal hydroxide solids that settled as sludge, and a supernate containing the soluble salt. The supernate volume was reduced by evaporation, which concentrated the soluble salts to their solubility limit, and resulted in precipitation of crystalline salt solids or “saltcake”. The salt cake and supernate in combination are referred to as salt waste.

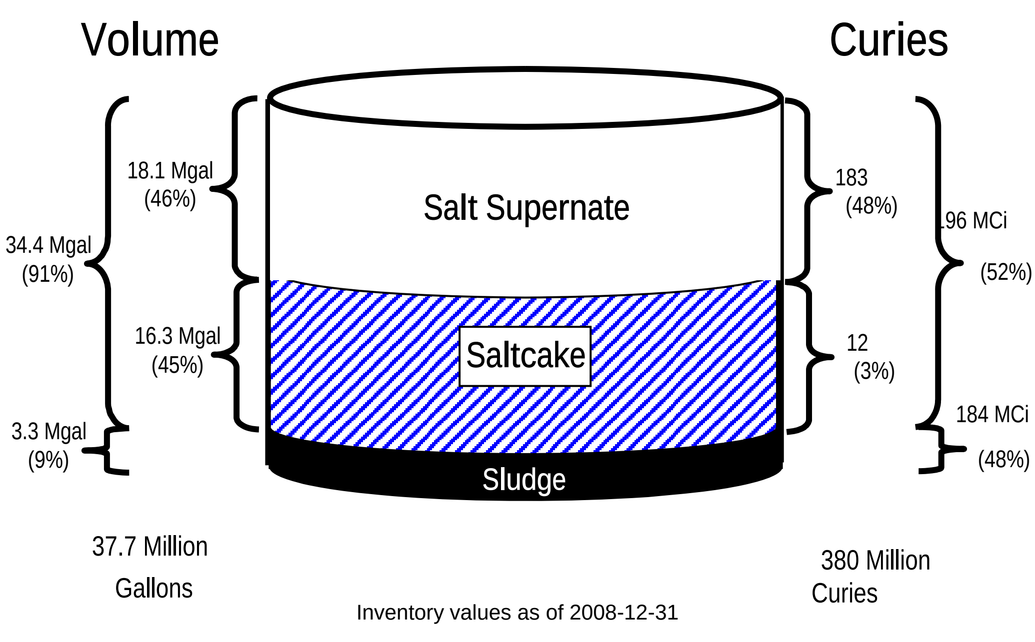

Figure 1.1 SRS Liquid Waste Composite Inventory as of December 31, 2008 [CHEW 2007]

The sludge contains the majority of the long-lived (half-life > 30 years) radionuclides and strontium. It is currently being stabilized at DWPF as a borosilicate glass. Greater than 95% of the radioactivity of the salt waste is short-lived (half-life of 30 years or less), mainly due to Cs-137 and its daughter product Ba-137m; the actinide contamination is low. The salt waste is treated to separate the high radioactivity and low radioactivity fractions. The high radioactivity fraction is immobilized at DWPF in a borosilicate glass and the low radioactivity fraction is immobilized in grout matrix at the Saltstone Processing Facility (SPF). The current plan for salt waste treatment is [CHEW 2007]:

- Deliquification, Dissolution and Adjustment (DDA) – mainly used for Tank 41 which has a relatively low radioactive content. The treated salt solution is sent to SPF for immobilization in grout.

- Actinide Removal Process (ARP) – Actinides are sorbed on monosodium titanate (MST) and sent to DWPF for immobilization in glass and the remaining liquid is sent to the Modular CSSX Unit (MCU) for further treatment.

- Modular CSSX Unit (MCU) – Reduces the Cs concentration by solvent extraction. The Cs-containing product is send to DWPF for stabilization as glass and the remaining decontaminated salt solution is sent to SPF for stabilization as grout. The MCU will be replaced by the Salt Waste Processing Facility (SWPF) in 2013 (based on approval of SWPF Critical Decision-3, Construction Start).

The tank waste removal process is a multi-year process and consists of the following steps:

1. Adding water to dilute concentrated salt re-dissolve the saltcake and assist in the suspension of sludge
2. Mixing to form a slurry
3. Pumping of the slurry from the waste storage tanks to the waste treatment tanks for further processing.

Tank space is carefully tracked. A portion of the tank space is reserved as contingency space in the event that a tank leaks. Currently, tank farms receive waste from the H-canyon stabilization program, liquid waste from DWPF, and waste water from sludge washing operations. Transfer to and from waste tanks and the three operating evaporators are routinely done. SRS has 51 underground waste tanks that were placed in operation between 1952 and 1986. There are 49 active waste tanks located in two separate facilities, H-Tank Farm (29 tanks) and F-Tank Farm (20 tanks). Two tanks in F-Tank Farm are not active; they have been isolated, operationally closed, and grouted. Categorization of the waste tanks is given in table 1.1

Table 1.1 SRS Waste Tanks Types

Type	Total Number of Tanks	Current Waste Inventory	Comments
I	8	3 Mgal	Oldest, constructed between 1952 and 1953
II	8	3 Mgal	Constructed between 1955 and 1956
III	27	28 Mgal	Newest tanks, placed into operation between 1969 and 1986. Only tanks that meet Environmental Protection Agency requirements for full secondary containment and leak detection
IV	8	4 Mgal	Constructed between 1958 and 1956

The Liquid Waste System is a highly integrated operation (Figure 1.2) that involves safely storing liquid waste in underground storage tanks; removing, treating, and dispositioning the LAW fraction in concrete vaults on-site; vitrifying the higher-activity waste; and storing the vitrified waste until permanent disposition at a Federal Repository. After waste removal and processing, the storage and processing facilities are cleaned and closed. In order to integrate all required activities, the Life-cycle Liquid Waste Disposition System Plan (LLWP) has been developed. It establishes a planning basis for processing the constituents of the liquid waste system to the end of the program mission. The LLWP is a qualitative evaluation based on modeling and simulation estimates.

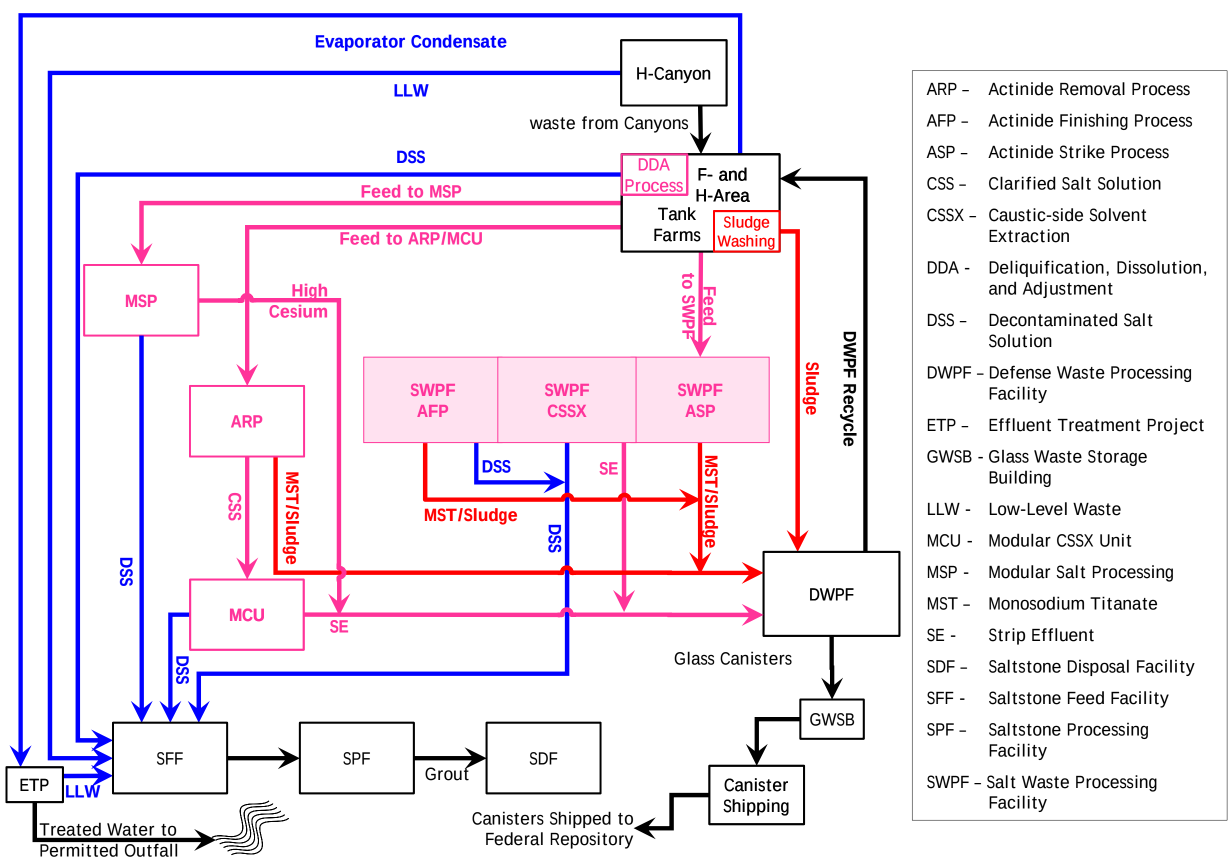

Figure 1.2 SRS Process Flowsheet [CHEW 2007]

2.0 Scope of the Review

The objective of this review was to evaluate the current Process Simulation Tools that support the planning basis for the SRS Life-cycle Liquid Waste Disposition System Plan. It covers a collection of software tools used to organize and analyze information, and to guide the management and processing of high-level waste at SRS. The liquid waste system at SRS is a highly integrated operation that involves a number of activities. The LLWP was developed to meet key mission requirements (DSA and WAC) and schedules based on modeling and simulation estimates generated by the software tools.

This review was chartered to focus on three primary areas:

- Assess the assumption that the tools used for liquid waste process simulation yield reasonable estimates
- Evaluate if additional tools are needed to guide execution of individual processing steps
- Evaluate methods to improve the rate at which system model predictions are performed

The foci of the charter included in Appendix B, were "operational" aspects of the modeling at SRS, i.e., reasonableness of estimates, prediction speed, tool integration, etc. Software Quality Assurance was not a primary focus area of this ETR. However, during the course of the review, the team noted a number of relatively simple to execute improvements of the overall SRS modeling process that were related to SQA. Therefore, a discussion of SQA topics relevant to SRS is included as Appendix C. In addition, SQA is mentioned (where appropriate) in section 6.0 of the report that discusses the individual models used at SRS.

3.0 Team Membership

The team was comprised of six independent experts whose credentials and experience align with the specific lines of inquiry (LOI) listed in section 4.0 and who collectively provided to the team sufficiently broad capability and flexibility to address the full range of issues that emerged during the review. Technical expertise included, but was not limited to design, engineering and management of chemical processing, and computer software development. Members of the team for this review were Monica Regalbuto, Lead (EM-21), Kevin Brown (Vanderbilt University/ CRESP), David DePaoli (ORNL), Candido Pereira (ANL), John Shultz (EM-21), Sahid Smith (EM-21).

Two observers from Hanford participated in the review. The observers were Paul Certa and Gail Allen. Short descriptions of the relevant experience of the team members and observers are given in Appendix A.

4.0 Lines of Inquiry

In order to process the liquid waste at SRS, an adequate overarching strategy (master plan/schedule) that integrates all systems and operations under consideration is necessary. A systems approach ensures that all operations and interfaces, risks and alternatives are evaluated to ensure that throughput, schedule, budget, and other requirements are met. The plan must account for the variable maturity of different aspects of the project with respect to schedule and address two basic questions:

1. Is the degree of development and planning sufficient to meet the schedule for implementation?
2. What aspects of a systems approach are in place, and which aspects need further development or are missing?

The following section covers the primary LOI for the review and has been organized into three categories: Category 1: Current Overall Software Performance and Process Structure; Category 2: Current Individual Tools; and Category 3: Additional Tools Needed.

<u>Category 1: Current Overall Software Performance and Process Structure</u>

1. How did SRS select the various software modeling tools they are using?

The majority of tools do not appear to have been selected through a formal evaluation process. Rather, the tools were developed by engineers to meet immediate mission needs and have evolved to address expanded roles. No periodic evaluation of software tools or modeling approaches was described during site presentations or in provided documentation. SRS staff indicated their recognition of the need for improved tools/systems and briefly described current efforts to improve modeling and information management/software approaches. As evidenced by success to date in the generation of acceptable glass waste forms, the functionality of the current tools appears to be suitable for operational support. However, two issues reduce the level of confidence that the current system of tools will optimally meet future needs:

Operational Support: The current software tools (1) are not integrated, requiring manual transfer/input of data through cumbersome and tedious means, (2) require adaptation of calculations by subject-matter experts through undocumented logic and (3) require exploration of possible processing options by manual iteration. This limits the capability to accommodate emergent management, technical or operational/facility issues.

Planning: The current tools ability to quickly perform mid- to long-term planning is limited. The time requirements in tool use, particularly the expert-driven calculations in Sludge Washing Spreadsheets and the creation of input card decks for SpaceMan Plus™, limits exploration of "what-if" scenarios and sensitivity analyses. SpaceMan Plus™ projections of future activities are not tied to glass or Saltstone Processing Facility acceptability.

2. ***Has the quality of the process simulation tools been adequately assured (i.e., is the QA plan adequate)?***

   Engineering Analysis Documentation is very good. Software QA Documentation appears to be adequate but not consistent across all models, while implementation and execution of SQA could be improved in almost all models. In general, SQA is performed by personnel at SRS. The SQA documentation is generated by site personnel, and the sufficiency of that documentation is reviewed and approved by SRS personnel. None of the SQA plans specifically require a "user's manual" for the models. The process by which information flows through the modeling system is derived from logic imparted by a select few experts, thereby making the training of new personnel (or implementing software to incorporate expert logic) difficult or impractical. SRS personnel should conduct an initial evaluation of methods to improve the data management process, particular of the level "B" software.

3. ***How do previous simulation tools predictions compare with actual process performance?***

   As noted earlier, SRS has produced over 8 million pounds of waste forms that are acceptable for permanent disposal in a Federal geologic repository. However, for most models, there appears to be limited comparisons of historical model predictions with actual data, i.e. there does not appear to be a process in place whereby the history of the inputs and outputs have been archived (e.g., in a database) so that modeling accuracy over time, or data forensics, can be evaluated. No examples of sensitivity or uncertainty analyses were presented.

4. ***How do the simulation tools predictions compare to other tools used in other sites?***

   With the exception of COREsim™ evaluation for National Nuclear Security Administration (NNSA) programs, no efforts to benchmark software usage from other sites were identified.

5. ***Is the time required to do a study of model predictions acceptable to evaluate project risks?***

   There is limited capability for sensitivity analyses or optimization in the current system tools because there is no automation of cases. Some modeling activities are limited by computer processing time, and it appears that some spreadsheets strain the capability of current hardware; for example, the automatic recalculate feature is often disabled in WCS during data input to allow the user to avoid the delays required for recalculation of the large spreadsheet after each entry. It appears that a large amount of time is consumed in expert-driven manual calculations in the Sludge Washing Spreadsheets. A significant opportunity appears to be available for enhancement of optimization capability, through development of an automated tool that captures the logic utilized in creating and adapting these spreadsheets. For the existing software tools, computer processing time can be significantly improved by increasing memory and processor capability on workstations. SRS staff indicated difficulties in updating hardware with improved capabilities due to procurement issues and cyber-security concerns.

   Modeling is also limited by the transfer of information between codes. Each code requires manual input, manipulation, transfer, and verification of data. This process is both time consuming, and prone to induce transcription and other errors. Generation of input data decks for SpaceMan Plus^{TM} appears to be the task with greatest time impact, as generation of the input for a single scenario can take as long as three months. It appears clear that the tools and their implementation can be significantly improved through the involvement of data management professionals and modeling experts.

6. ***Does SRS have adequate resources (current equipment, number of licenses, number of trained personnel, etc.) to perform the modeling scope that is needed?***

In some cases, the existing computer hardware hampered performance, notably for COREsim^{TM}. SRS personnel indicated that in some cases run-time could be reduced from several hours to less than one with a more powerful workstation. SpaceMan Plus^{TM} was developed using Visual Basic 6 which is no longer supported and is limited to two users. WCS 1.5 is a single-user/single-platform system limited by computer runtime. Microsoft Excel is used as a platform for many models, but Excel does not have the performance capability (e.g. encoding of expert logic and performance of unit operations) that other modeling software packages provide. To a significant extent, key codes were reliant on specific experts either for efficient utility (SpaceMan Plus^{TM}) or logic basis (Sludge Washing Spreadsheet). The absence of these experts would severely impact planning, notably sludge batch management. In general, an effort to upgrade the codes should be undertaken in the near-term to enable efficient planning. As codes are upgraded, computer resources would also require upgrades.

7. ***Is the output of models provided in a user friendly format (Graphical User Interface (GUI))?***

With the exception of COREsim^{TM}, a commercial discrete event platform [COREsim], the models do not have user-friendly GUIs. SpaceMan Plus^{TM} does have a limited graphical user-interface providing the user with tank characteristics during execution, but the majority of codes required significant manual input of data and manipulation of outputs to generate graphical forms or manageable datasets. In general, comparison of different processing scenarios is difficult or impractical because the generation of graphs and reports is not straight-forward, making rapid data analysis difficult. In some cases, (particularly for Glassmaker II and the Sludge Washing Spreadsheets), an expert user was required to supply logic to the operations.

<u>Category 2: Current Individual Tools</u>

1. ***Does the Waste Characterization System (WCS), a series of workbooks, adequately estimate the composition and inventory of the liquid waste tanks?***

The generation of critical supporting reports (e.g., Emergency Response Data, Evaluated Transfer Approval Forms, etc.) using the WCS for safety evaluations and the approval of tank transfers has been effective. However, the use of WCS for multiple functions (including both safety and non-safety calculations) complicates planning, maintenance, and verification of the results. The safety basis inventory estimates require significant adjustments before they are used in planning.

2. ***Does the Sludge Washing Spreadsheet (SWS), a spreadsheet model, adequately estimate the composition and inventory of the washes resulting from each sludge batch?***

   The Sludge Washing Spreadsheet has been used by experts to successfully guide near-term washing operations including those responding to emergent information and operations. Description of the “sludge washing logic" needed to produce the washed sludge batches is incomplete. In addition, there is no user guide or procedure for the system. The spreadsheet facilitates and guides expert sludge washing evaluation for near-term, operational purposes, but is not time-efficient for long-term planning or for “what-if” analyses required for scenario testing. The spreadsheet does not directly incorporate the sludge washing logic needed to produce acceptable washed sludge batches as feed to the DWPF. Any optimization is performed by the user, which makes error checking difficult and may produce suboptimal or different answers for different users. Also, since this process is so heavily reliant on human intervention, an overall, hard-coded waste management “Systems” model has not been developed.

3. ***Does GlassMaker II, a Visual Basic program, adequately estimate the composition of each sludge batch?***

   The Sludge Batch Planning Toolkit (Glassmaker II) has been used to plan future acceptable washed sludge batches for all remaining sludge in the SRS Tank Farm. The program output includes summaries of predicted sludge compositions to be fed to DWPF, canisters produced, acceptability results, and anticipated transfers. The spreadsheet practices needed to evaluate and plan future washed sludge batches are burdensome. The current system does not have immediate feedback on waste acceptability.

4. ***Does PCCS adequately estimate the acceptability by DWPF?***

   PCCS determines whether a glass composition representing the content of a SME batch is acceptable for the DWPF based on meeting all of the constraints on a set of glass properties. It includes both measured properties and properties that must be derived from chemical models based on the composition. The spreadsheet accounts for uncertainties related both to the property models and the measurement of the properties. The spreadsheet has been used successfully to fulfill its intended purpose as it has resulted in the production of over 8 million pounds of acceptable radioactive glass at the DWPF.

5. ***Does SpaceMan Plus™, a Visual Basic program, adequately simulates operation of all the processes in the entire Liquid Waste System?***

   Although data manipulation (input and output) is cumbersome, the SpaceMan Plus™ code appears to adequately simulate operation of all processes in the LWS. The program does not have internal process logic, but rather runs through a sequence of user-defined activities. As a result, significant user input is required to operate the program, making it extremely timeintensive, in particular for long-range planning. There are several practical limitations to the software (e.g. 48-week years, conflicts must be resolved manually, etc.), and as a result, SpaceMan Plus™ is better suited for short-term planning and development where a short series of activities can be evaluated readily. SpaceMan Plus™ Plus appears to be the tool that most limits planning efforts; generation of the input for a single scenario can take as long as three months.

6. ***Does COREsim™, a discrete-event simulation logic, adequately simulate the process?***

COREsim™ is a discrete-event simulator that tracks timing and movement within a process. It has proven adequate for modeling and debottlenecking specific processes and for debottlenecking. Although it has not been applied to the entire LWS for long-range planning, it has been used successfully to simulate a number of operations at SRS including operations within SWS. Examples include time and motion studies of the MCU, the Saltstone facility, salt feed and DWPF liquid recycle processing, Application of COREsim™ has resulted in major cost reduction in facilities and operations at SRS--investment of about $500K has resulted in greater than $15M in savings. SRS management should evaluate whether COREsim™ or other similar tool has the capability to take over more of the current modeling effort (e.g. potential to replace Excel files used in SWS and possibly SpaceMan Plus™).

7. ***What is the relationship between COREsim™ and SpaceMan Plus™?***

SpaceMan Plus™ is a software planning tool written in Visual Basic 6. The code is used to predict system-wide chemical, radiological, mass, and volume conditions, providing input to the LLWP. SpaceMan Plus™ is used to model operation in the LWS and to predict tank inventories resulting from future actions. The model manages input that defines timing of individual activities, including liquid transfers and processing. COREsim™ is a discrete-event platform that is used at SRS to predict resource availability. According to SRS personnel, it apparently has limited capabilities for detailed chemistry which may limit its overall utility for long-range system planning. COREsim™ has been used to identify process bottlenecks, resource needs, and queuing effects on system performance. COREsim™ is not currently used for the LLWP. There is an effort underway to implement COREsim™ as an alternative to SpaceMan Plus™. The team recommends that this process continue.

<u>Category 3: Additional Tools Needed</u>

1. ***Are all critical processing steps characterized?***

The LWS modeling tools address the critical process steps required for tank inventories, transfers, sludge processing and feed acceptability to DWPF. There is no software tool for salt processing and Saltstone Processing Facility acceptability analogous to PCCS. Critical current or future processes that may require additional model development include DWPF (melter, sludge receipt and adjustment, SWPF (MST strikes, filtration, CSSX); DWPF/SWPF coupling and DWPF water recycle; salt dissolution [CHANG 2009].

2. ***Given that SpaceMan Plus ™ modeling is the time-limiting process in program life-cycle scenario evaluation, is there a better platform/tool that could be used for life-cycle modeling that would decrease model run time?***

   In the longer term, SpaceMan Plus™ should be replaced with a discrete-event model with embedded logic. Expanding the CORESim™ models is one possibility. The software should be able to model the operations included in SpaceMan Plus™ to the extent possible; this objective may require specialized discrete analysis software or interface between multiple codes. The new planning code would continue to support operations and system planning functions. With automated life-cycle model output, it would also enable comparative evaluation of multiple scenarios which is not generally feasible with SpaceMan Plus™.

5.0 Overall System Observations and Recommendations

The LLWP was developed to establish the planning basis for processing the constituents of the liquid waste system and is based on estimates derived from chemical and system models, and process simulations. Process activities include: (1) storage of liquid waste in underground tanks, (2) removal, treatment, and disposition of low-active waste in concrete vaults, (3) vitrification of high–level waste, and (4) storage of the vitrified waste prior to permanent disposition.

The scope of the review was to evaluate the current process simulation tools that support the planning basis for the SRS System Plan to assess if the modeling and simulation tools used for the LWS yield reasonable estimates of the operations and timetables required to complete all liquid waste treatment activities. Based on a review of the relevant software tools on hand, the team evaluated the adequacy of the available tools and the need for development of additional tools. Finally, the team evaluated methods that can improve the rate at which system model predictions are performed. The Observations of this review overlap the three primary lines of inquiry. Therefore, the Observations may not directly correspond one to one with the scope questions listed in the Charter given in Appendix B.

5.1 Main Observations

There are four main Observations:

1. ***The current System Plan relies on a collection of software tools to organize and analyze information, and guide processing of high-level waste at SRS. These tools currently provide reasonable estimates; however, no integrated system planning tool presently exists.***

   As utilized by experienced/qualified staff, the current tools have been effective in supporting processing of liquid waste at SRS. This has resulted in successful production of over 8 million pounds of radioactive glass at the DWPF, through processing five different batches of tank waste. The software tools were originally designed to meet DSA, WAC requirements and regulatory commitments. These codes have evolved over a number of years and have been modified to serve many of the requirements of the planning system. However, they are not optimal for system planning. Because the codes were developed independently to meet the immediate needs of different users, the codes do not integrate well, and often, are not integrated at all. A large number of manual actions are required to input data and transfer information among various spreadsheets, workbooks, systems and organizations.

2. ***The capabilities and integration of current tools are limited. These limitations hamper process optimization and mid to long-term planning***

   The current tools are limited by several factors. Data transfers are not automated, and there is not a data element dictionary common to all modeling platforms. Therefore, porting information from one model to another requires human intervention to interpret what the data means and how to input/export information so that it can be used in other models.

This makes the model update process both slower and vulnerable to various types of human error. In some cases, the need for detailed familiarity with the codes or processes limits their uses to a small group of specialized experts. Also, the planning tools and processes are maintained by different owners, which makes coordination of a common process model structure, and approach to documentation, more difficult. IT professionals are not routinely used to perform software functions (e.g. code revision and database management) and are not part of the modeling team; as a result, software selection is not optimal, and there appears to be an over-reliance on spreadsheet-based tools and legacy methods. Finally, the speed of calculation is often limited by computer hardware; the Team was briefed that access to more capable systems appears to be constrained by procurement issues and cyber-security concerns.

3. ***There is a need to increase system planning flexibility and the turnaround time at which system model predictions are performed***

   Tools should be revamped to decouple planning and operations support functions. Current planning tools are operated with the same level of rigor as operations-support tools (e.g., safety basis) thereby lengthening the scenario analysis process. Uncertainty management and error propagation should be managed using a more systematic approach. There is currently no WAC tool for the Saltstone Processing Facility that is analogous to PCCS for high-level waste vitrification. All of the codes should incorporate consistent, appropriately graded, QA documentation and programming practices.

4. ***There is a need to relate system planning results with cost***

   Existing planning tools do not incorporate LWS processing costs. Cost-related evaluations are conducted by other methods and are not integrated with planning tools. Life-cycle plans assume funding is available at whatever levels are required to meet the project timeline: "*This Plan assumes full funding of the estimated costs to accomplish the required project - and operations activities. It supports justification for requesting necessary funding profile*" [CHEW 2007]. Therefore, waste handling is optimized on a purely technical basis in order to meet project timelines for completion of the mission. Modeling tools often incorporate cost as a factor, and the planning tools should be upgraded to factor in processing costs.

5.2 System Planning Modeling Tools

The output from a collection of multi-use software tools is required to support system planning. These tools are also used to provide operational support. The modeling tools currently used by SRS for liquid waste system planning are summarized in Figure 5.2.1 and Table 5.2.1. These tools include:

- **WCS 1.5** – a set of Microsoft Excel workbooks used to track the inventory of selected chemicals and radionuclides in SRS HLW tanks to represent real-time conditions.

- **Sludge Batch Toolkit** – a set of Microsoft Excel workbooks – including GlassMaker II (i.e. a set of Sludge Washing Spreadsheets and a stand-alone version of PCCS) – used to help plan and assemble sludge batches to feed to DWPF.

- **PCCS** – a Microsoft Excel spreadsheet used to guide the acceptability decision for each DWPF process batch.

- **SpaceMan Plus™** – a Visual Basic 6 model used in planning to model material flows throughout the entire LWS to the end of the program mission.

- **COREsim™** – a discrete-event model used to evaluate bottlenecks in the LWS and to simulate facility processes.

Note: There is no software planning or acceptability tool analogous to PCCS for salt processing or Saltstone Processing Facility feed acceptability. Current acceptability methodology requires a manual system.

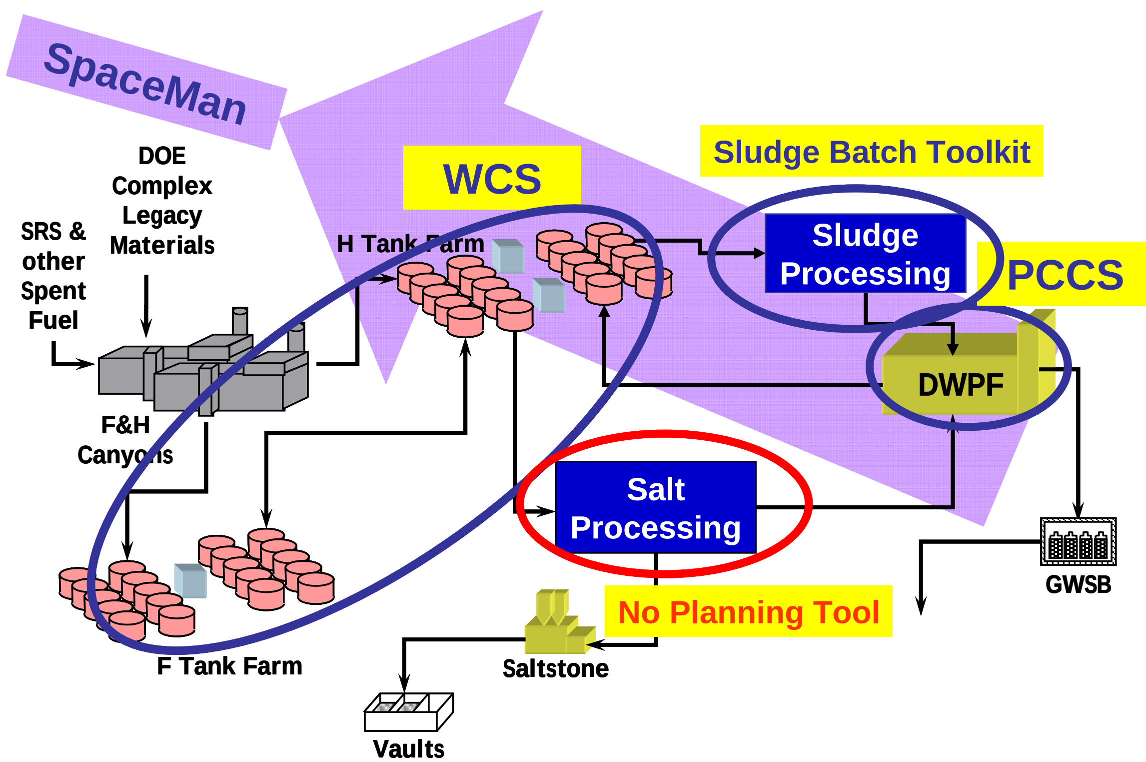

Figure 5.2.1 Overview of SRS Liquid Waste System Planning Modeling Tools

The software tools provide data that are used as the basis for several key functions including safety basis, operational support, planning, and waste acceptance. The roles of these software tools and information flows between tools are outlined in Figure 5.2.2. Input/output information from these tools is in multiple formats. Transfers of information are performed manually.

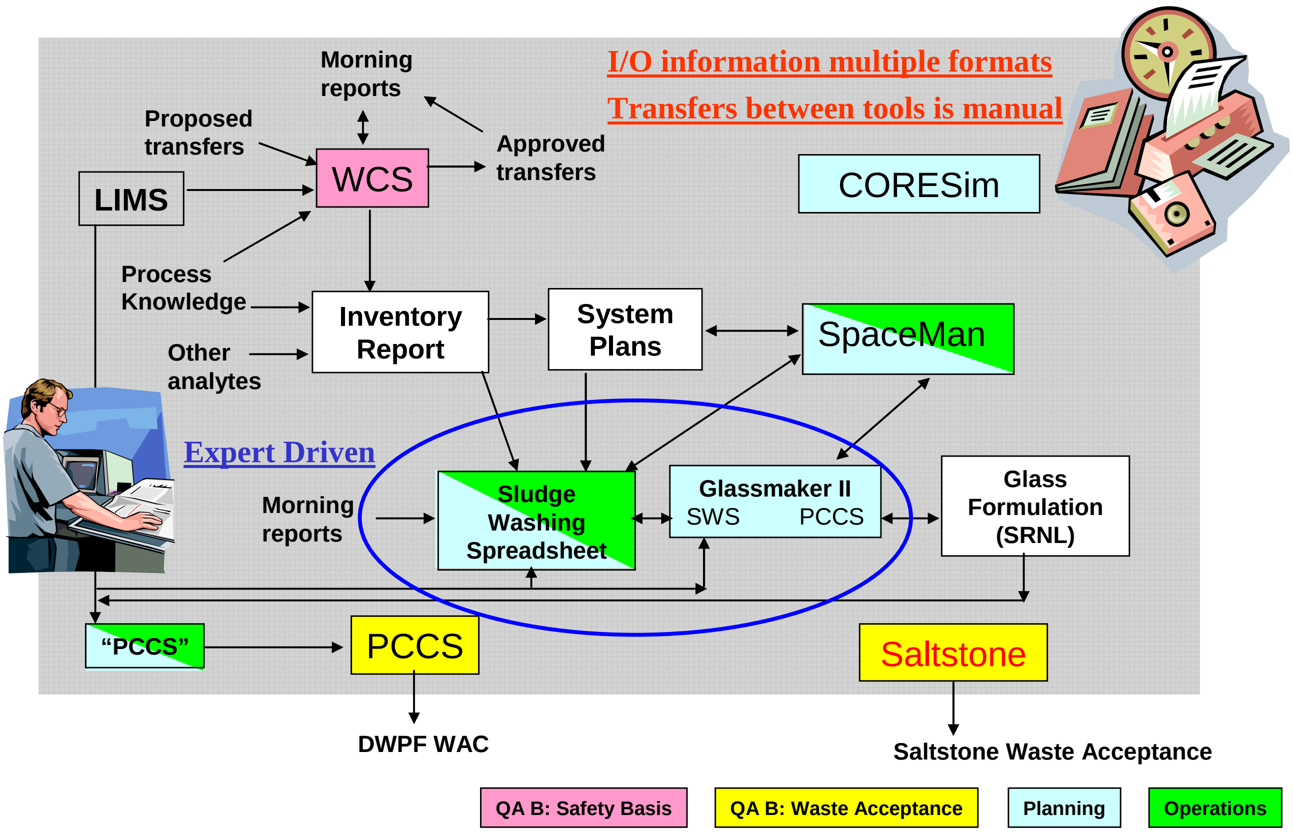

Figure 5.2.2 Information Flow in Current Operation & Planning Systems

Safety Basis Tools

WCS 1.5 is used to calculate limits associated with various DSA programs, including flammability, corrosion, and transfer control programs. WCS inventory data is based on sample analyses, canyon process records, composition studies, and theoretical relationships. Inputs include engineering evaluations, mapping/morning reports, DSA and Technical Safety Requirements (TSR), and flammability/corrosion limits. Primary outputs include Emergency Response Data (ERD) and Evaluated Transfer Approval Forms (ETAF), flammability/corrosion status, WAC/Feed Qualification/Salt Out/engineering evaluations, morning reports, and safety basis inventory.

Operational Support Tools

Multiple software tools provide operational support. This support has become increasingly important as DWPF sludge processing has been moving towards "just-in-time" processing reducing contingency for accommodating emergent technical or facility issues [CHEW 2007]. The Sludge Washing Spreadsheet is used by subject matter experts as an operational support tool to calculate near-term sludge washing steps. The GlassMaker II tool uses sludge composition output from multiple Sludge Washing Spreadsheet to project batch acceptability and provide input to SRNL glass-formulation experiments. CORESim™ has been used to conduct time and motion studies of a number of LWO operations including the Salt Disposition Integrated Program (SDIP) Strip Effluent Process, Saltstone Feed Preparation System, DWPF, and MCU.

<u>Planning Tools</u>

Several software tools are used for planning. The inventory data in WCS serves as the basis for planning. The WCS data require extensive manipulation, as described in the Tank Inventory Report [TRAN 2008] to remove conservatism incorporated for safety calculations so the data can be used as tank inventories for planning purposes.

The Sludge Batch Toolkit (GlassMaker II) is used for mid- and long-term planning of sludge batches to feed to DWPF. Outputs include the composition estimates of the washed and sludge and melter feed batches to be processed in DWPF.

SpaceMan Plus™ is used for long-range planning of waste tank-related operations through final site closure. SpaceMan Plus™ is used to model operation of the LWS and to predict tank inventories resulting from future actions. Key outputs include tank inventories, evaporator operation, and transfer schedules.

COREsim™ is a discrete-event tool that predicts resource availability. COREsim™ has been used to identify process bottlenecks, resource needs, and queuing effects on system performance, but is not currently used for the Life Cycle System Plan.

<u>Waste Acceptance Tools</u>

PCCS is used to meet requirements of the Glass Product Control Program [BRICKER], as part of the DWPF waste acceptance strategy. The model is used to predict process and product quality from analytical measurements of the composition of SME samples. The Slurry Mix Evaporator (SME) acceptability is based on a number of process and product-quality constraints.

Table 5.2.1 Summary of Current SRS Liquid Waste System Planning Modeling Tools

	WCS 1.5	**Sludge Washing Spreadsheet**	**GlassMaker II**	**PCCS**	**SpaceMan Plus™**	**COREsim™**
Description	Excel sheets (tank inventories and safety-related information)	Excel sheets (calculate sludge washing steps)	Excel sheets (input to glass formulation experiments)	Excel sheets (verify acceptability of glass)	Visual Basic 6 code (predict tank inventories with future actions)	Discrete-event simulation model (operations research)
Function	Planning Safety Operation Support	Planning Operation Support	Planning	Planning Waste Acceptance	Planning	Planning
Manual Inputs	Samples, process knowledge, historical transfers	LIMS, morning reports, inventory report, WCS	Waste tank composition, sample results from LIMS	LIMS data: Glass sample compositions	Card file depicting scenario and GlassMaker II output	Scenario, tank connectivity, operating logic, reliability and availability data
Manual Outputs	Emergency Response Data, Evaluated Transfer Approval, Waste Characterization Data	Process steps, transfers and material balances	Compositions for glass formulation testing	Acceptance decision relative to multiple criteria for WAC	Transfers and tank inventories	Identification of pinch points for processing
QA	Level B (Originally level D)	Level D	Level D	Level B	Level D	Level D

5.3 Overall Recommendations

Figure 5.3.1 depicts recommended elements of an upgraded set of system tools for support of LWS planning and operations with several substantive changes from the current approach. The principal tank inventory database upon which planning and safety calculations are derived would be maintained in a database of the tank values for concentrations and volumes, with identified uncertainties. The current functionality of WCS 1.5 would be captured in a safety-basis tool that applied appropriate conservatism to the values in the best estimate tank inventory database. The recommended approach is in contrast to the current situation, in which the necessary conservatism is incorporated in the WCS entries, and the values must be revised to provide estimate values for operational support and planning. It is strongly recommended that the tank inventory database be developed in a suitable database format, rather than in a spreadsheet.

Tools for planning and operational support would be de-coupled so that planning tools are developed and operated at a lower level of detail and rigor than tools used for near-term operational support, facilitating scenario analysis. An integrated, discrete-event model that incorporates the functionality of current tools, including the Sludge Washing Spreadsheets, GlassMaker II, stand-alone versions of PCCS, and SpaceMan Plus™ would be used for planning. A tool for salt processing and Saltstone Processing Facility acceptance, comparable to

PCCS in function would be developed. This tool would become even more important as SWPF comes online during the next few years, which will result in a significant volume flow increase to SPF when compared to current processing rates.

Enhancement of SRS system planning tools should be done in concert with Complex-wide integrated planning and development. Development of SRS system tools should be aligned with the overall High Level Waste System Integrated Project Team (HLW-IPT) goals for development of a life-cycle cost model (LCCM). The LCCM will take data from SRS and ORP tank inventories and discrete-event modeling tools to evaluate scenarios to reduce cost and identify technical needs.

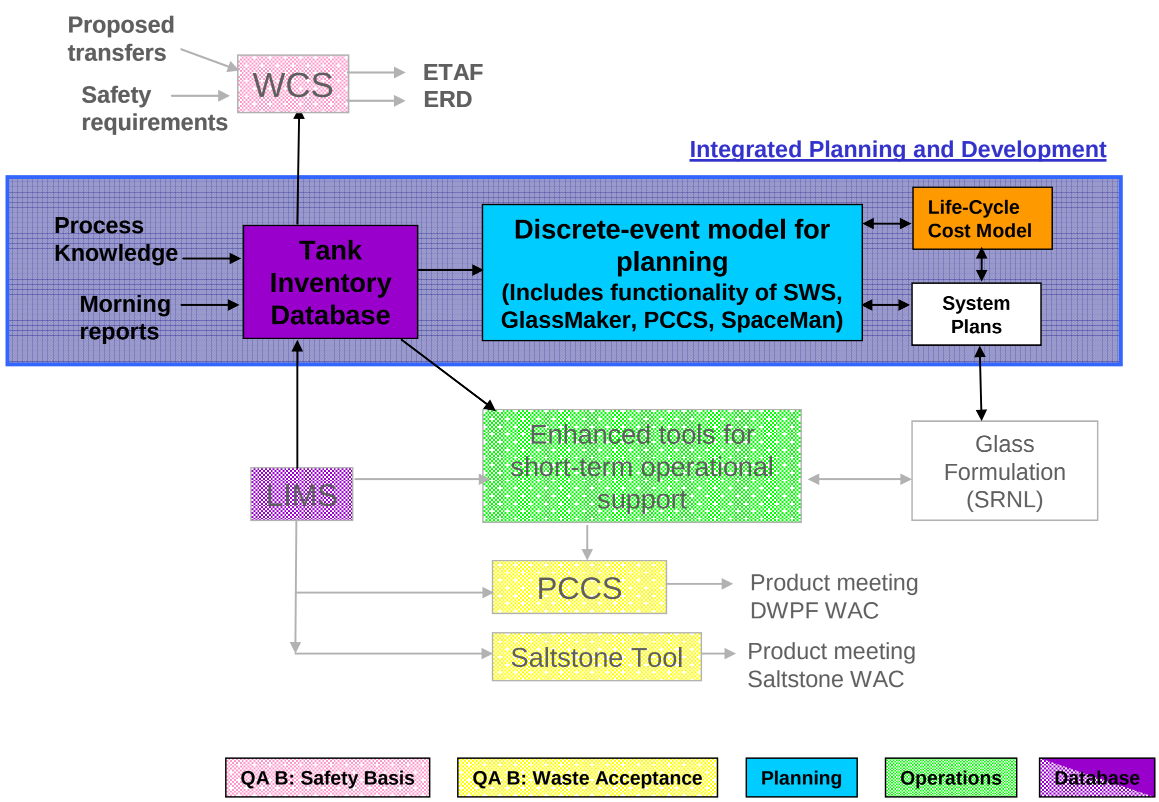

Figure 5.3.1 Integrated Planning and Development Tool, De-couple from Safety, Operations and Waste Acceptance Tools

Specific recommendations based on the listed observations for implementation within the next 6 to 12 months (short-term), 2 years (mid-term) and 3 to 4 years (long-term) are given below:

1. ***Recommended short-term actions (6 to 12 months) include:***

- Improve capability of computer resources (i.e., processor, memory and software)
- Engage modeling experts and data-management professionals to develop and modernize present systems and integrate tools
- Review current QA software design against most recent Department of Energy (DOE) policy guidance and implement simple SQA improvements as suggested in Appendix C (e.g. lock down spreadsheet cells, embedded "error checking", use of named ranges instead of individual cell references, etc.)
- Develop a consistent approach to uncertainty management among tools to better understand error propagation and evaluate overall system uncertainty
- Define and implement SRS "best practices" to improve awkward spreadsheet procedures for data management and thereby improve data integrity
    - Participate in complex-wide technical exchanges to identify and adopt best practices and new software approaches
    - Develop standard approach for spreadsheet documentation
- Begin planning for development of data systems and integrated models for operations and planning and evaluate needs and opportunities for long-term optimization
- Develop a tool analogous to PCCS for Saltstone Processing Facility WAC

2. ***Recommended mid-term (next 2 years) actions:***

- Develop a "tank inventory database" to support:
    - Independent safety analysis and DSA requirements
    - Near-term operations
    - Long-range planning estimates
- Develop integrated planning models to include the capability to run:
    - "What-if" scenarios
    - Risk, Sensitivity, and RAM analyses
    - Faster revisions of the System Plan to take advantage of new and emergent information and opportunities
- Develop the ability to compare historical model predictions with actual data, i.e., put in place a mechanism whereby inputs and outputs are archived in a database so that modeling accuracy over time, or data forensics, can be evaluated
- Relate system planning results to cost
- Develop the capability to propagate uncertainties through the planning process
- Explore computing environments for long-term planning needs, including optimization
- Contribute to DOE-EM-HQ complex-wide effort to identify opportunities and approaches for system optimization

3. Recommended long-term (3 to 4 years) actions include:

- Integrate the “tank inventory database” and safety-basis (“WCS”) system
- Develop the capability to ensure the consistency of assumptions and calculations among safety, planning, operations and WAC tools
- Implement improved tools for optimization and decision making
- Work with the DOE EM-HQ and other program offices to adopt consensus standards for material properties across all models

6.0 Individual Tools Observations and Recommendations

This section covers each of the current tools used for the LLWP. For each of the tools a brief description is given, followed by observations and short-term, mid-term and long-term recommendations. The time table for each of these recommendations is the same as for the overall recommendations given in Section 5.0. Short-term is within the next 6 to 12 months, mid-term within the next 2 years and long-term within the next 3 to 4 years.

6.1 Waste Characterization System, Version 1.5 (WCS 1.5)

Brief Description

The Waste Characterization System, Version 1.5 documents the composition of the waste in each of the 49 HLW tanks at SRS that have not been grouted [BUI 2005]. The components of the tanks, sludge, salt, and supernate are characterized separately. Waste characteristics come from monthly sample analyses, canyon process records, composition and solubility studies, and theoretical relationships [HESTER, CAMPBELL]. WCS 1.5 provides the basis for performing safety calculations (e.g., flammability, corrosion, etc.) as required by the 10 CFR 830 DSA and production planning [CAMPBELL].

The current WCS application consists of multiple Microsoft Excel workbooks containing multiple spreadsheets as illustrated in 6.1.1 The applications run in a networked environment under Microsoft Windows but is restricted to a single user at a time for reasons of security and data integrity. WCS translates requirements and technical data from various sources (including engineering evaluations, morning reports, safety requirements, flammability/corrosion limits, etc.) into formulae, criteria, and logic relationships. User application of data from the WCS includes ERD; ETAFs; flammability and corrosion statuses; Waste Acceptance, Feed Qualification, and engineering evaluations, morning reports, and Safety Basis inventory predictions [LANG]. WCS is used for safety and non-safety related applications and has been classified as Level B software based on the SRS Manual E7, Procedure 5.01 [HEVEL]. Subject matter experts review and approve the data commensurate with their use in WCS [CAMPBELL]. Figure 6.1.2 depicts the basic WCS workflow including interactions with other systems (i.e., SpaceMan Plus^{TM}, GlassMaker, and PCCS) reviewed by the team.

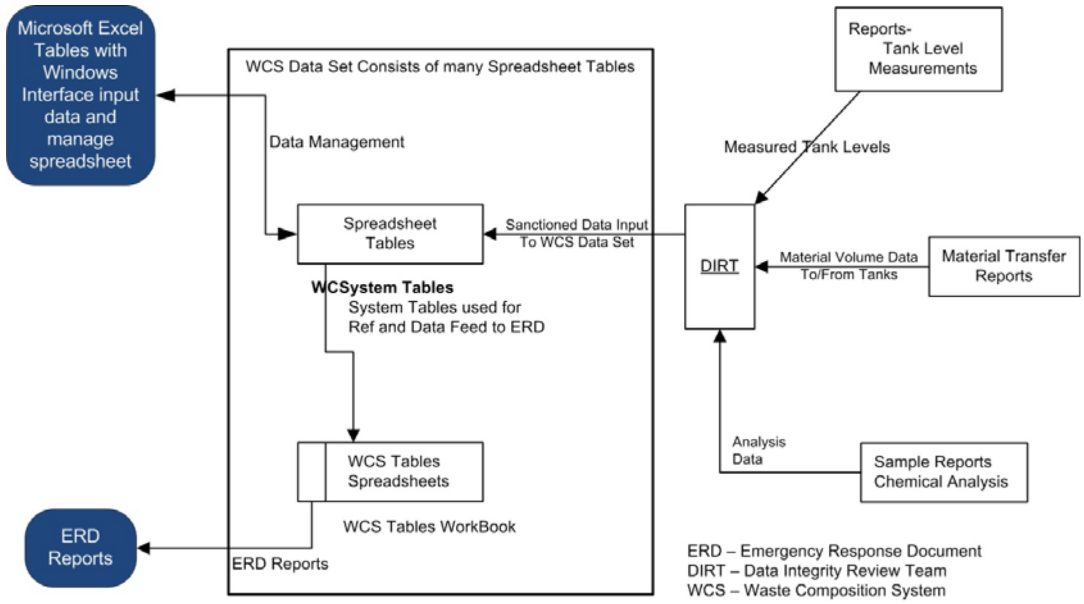

Figure 6.1.1 WCS Applications Systems Architecture [CAMPBELL]

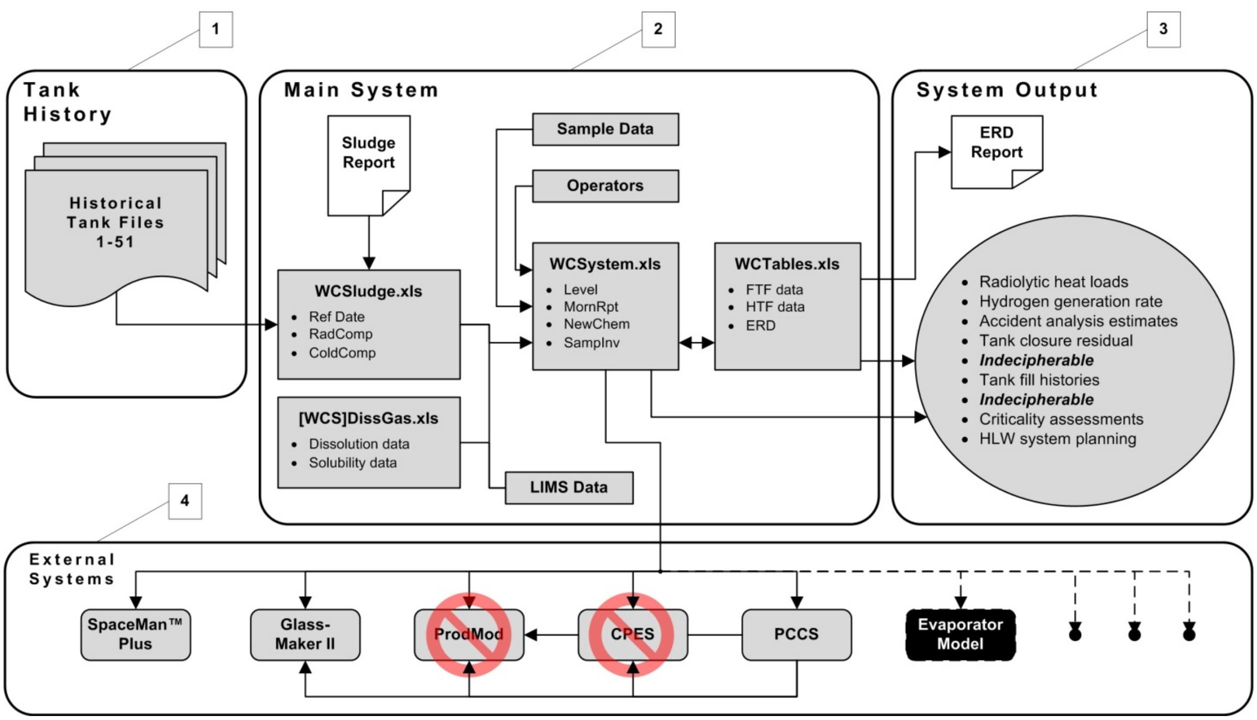

Figure 6.1.2 WCS Workflow Diagram [CAMPBELL]

Observations

The generation of critical supporting reports (e.g., ERD, ETAF, etc.) using the WCS for safety evaluations and the approval of tank transfers has been effective. However, the use of WCS 1.5 for multiple functions (including both safety and non-safety calculations) complicates planning, maintenance, and verification of the results. Furthermore, the WCS is a single-user/single-platform system that uses only manual inputs and verification and is thus limited by computer runtime. The safety basis inventory estimates in WCS require significant adjustments before they are used in planning. These adjustments are executed as described in the pertinent Tank Inventory Report [TRAN].

SQA documentation for the WCS 1.5 should be reviewed based on current standards. Particular attention should be paid to verification and maintenance of calculations, and the underlying relationships and formulae in the workbook. Further discussion of techniques to improve SQA is provided in Appendix C (including: "locking down" of cell references to disallow unintentional changes in calculations; embedded "error checking" that would alert a user that an erroneous data value had been entered, or an out-of-range (or nonsensical) calculated value had occurred.

Recommendations

Short-term

To reduce potential vulnerabilities associated with WCS software documentation, SRS should review the current software and design specifications against the most recent DOE policy and SQA guidance. SRS should also improve current WCS documentation to facilitate mapping out traceable paths from underlying conceptual relationships to spreadsheet calculations especially for Safety Basis calculations.

Planning should begin to develop the next generation of WCS to include a "tank inventory database" and a separate safety basis database or calculation system. The data inputs appear to be adequate for the current application of WCS. However, the necessary inputs to both the WCS [LANG, BUI 2005] and Tank Inventory Report [TRAN] should be evaluated and divided into those needed to estimate inventories and those required for Safety Basis calculations. Uncertainties in tank inventories and associated calculations should be characterized and documented in a systematic and transparent fashion based on historic information and process knowledge from DWPF for both planning and Safety Basis purposes. Finally, SRS should evaluate the adequacy of computing environments to execute the current version of WCS.

Mid-term

SRS should develop and document a software design compliant with accepted industrial standards for the next generation of the WCS to decrease vulnerability and enhance software understanding, improve maintenance and transferability, etc. The software design should be used to develop: (1) a database in a more standard format (e.g., Access, SQL Server, Oracle, etc.) to generate tank inventory data for planning purposes and (2) a database and/or calculation system to generate Safety Basis inventories (i.e., “adjusted” tank inventory data), information, and reports for tank transfer and other safety-related processing steps to capture current WCS functionality. The “tank inventory database” and Safety Basis calculation system (“WCS”) should be integrated to the extent practical to improve efficiency and reduce transcription errors. New computing environments should be evaluated to allow efficient operation for long-term planning purposes.

The uncertainties associated with tank inventories should be generated for planning purposes and reconciled with the adjustments needed for Safety Basis calculations. This may be accomplished either by modification of the “tank inventory database” or developing a new system to maintain uncertainties.

Long-term

SRS should investigate the need to develop improved computational tools for characterizing uncertainties, estimating tank inventories, and optimizing the planning process. The “tank inventory database” should be integrated with the other planning tools (e.g., GlassMaker II, Sludge Washing Spreadsheet, SpaceMan Plus™, etc.) to the extent practical to improve efficiency and reduce the likelihood of transcription errors. Extending the integration of the “tank inventory database” with a system that captures current WCS functionality and the other planning tools would allow propagation of inventory uncertainties through both the Safety Basis and planning processes. The manner in which computations are performed for uncertainty and sensitivity analyses will impact the interactions among the various databases and tools. SRS should evaluate new computing environments (e.g., high-end desktop) for long-term planning needs including optimization (under uncertainty) for planning purposes.

6.2 Sludge Batch Planning Toolkit (Glassmaker II)

<u>Brief Description</u>

The Sludge Batch Planning Toolkit (Glassmaker II) program uses inventories from WCS 1.5 adjusted to remove conservatism (as described in the Tank Inventory Report [TRAN 2008]) to calculate a sludge batch composition based on the batch recipe input by the planner. GlassMaker II then simulates the sludge washing process to reach the desired sodium endpoint; the acceptability of the resulting composition vector is checked using the PCCS [BROWN]. GlassMaker was originally developed using Visual Basic for Applications (VBA) in Microsoft Excel; however, because updating the original GlassMaker program was deemed not cost-effective, a simple Excel-based "Sludge Batch Planning Toolkit" (a.k.a., GlassMaker II) was developed. The Sludge Batch Planning Toolkit was built to allow the evaluation of multiple sludge batch processing scenarios.

Observations

The Sludge Batch Planning Toolkit has been used to plan future acceptable washed sludge batches for all remaining sludge in the SRS Tank Farm. The program output includes summaries of sludge compositions to be fed to the DWPF, canisters produced (on a batch and total basis), acceptability results, and projected transfers. The spreadsheet practices needed to evaluate and plan future washed sludge batches are burdensome (and often cumbersome). All data input is manual and comes from multiple sources over varying timeframes. Furthermore, the current system does not have immediate feedback on waste acceptability. As a result, comparisons of multiple scenarios are complex and time-consuming.

Recommendations

Because the Sludge Batch Planning Toolkit (GlassMaker II) is based on versions of the Sludge Washing Spreadsheet developed for planning purposes, recommendations for both are similar and will be provided after the Sludge Washing Spreadsheet is described in the next section.

6.3 Sludge Washing Spreadsheet (SWS)

Brief Description

Documentation for the use of this tool was included within the spreadsheet, but no documentation was provided (or appears to be available) to describe the logic used to generate the Sludge Washing Spreadsheet., The purpose of the spreadsheet is to project the pertinent composition and characteristics for each processing step needed to prepare a washed sludge batch for DWPF feed [GILLAM 2009a]. As sludge processing proceeds, the workbook inputs (including sludge masses, radiolytic heat rates, analyses, control requirements, etc.), formulae, and potentially the structure for the sludge batch under evaluation may be updated as needed.

In essence, the SWS workbook is an *expert-driven platform* that can be used by the subject matter expert to evaluate the impact of emergent conditions and compare different potential sludge batch processing options [GILLAM 2009b]. Model inputs include estimates of sludge masses, the order and sizes of waste transfers, timing and quantity of corrosion inhibitor additions, settling times, decant sizes, and the position of the high liquid level conductivity probe (HLLCP). The constraints under which the washing process is developed include maximizing sludge mass, minimizing the volume and number of washes, maximizing use of evaporator capacity, and minimizing necessary operations. The SWS is also used to ensure, to the extent possible, that planned sludge processing steps will be within the safety constraints provided by the flammability, corrosion, and transfer control programs.

Observations

The Sludge Washing Spreadsheet has been used by experts to successfully guide near-term washing operations including the management of emergent information and operations. The documentation provided in the worksheet itself is considered the best practice for the SRS spreadsheet planning tools reviewed by the team. However, the description of the sludge washing logic needed to produce washed sludge batches is incomplete, and there is no user guide or procedure for the system.

The spreadsheet facilitates and guides expert sludge washing evaluation for near-term, operational purposes but is not time-efficient for long-term planning or for “what-if” analyses required for scenario testing. The spreadsheet does not directly incorporate the sludge washing logic needed to produce acceptable washed sludge batches as feed to the DWPF. The spreadsheet is a single-expert-driven system that performs calculations developed by the expert to guide sludge washing. There are numerous, competing end-points that are not integrated. Any optimization is performed by the user, which makes error checking difficult and may result in suboptimal or different answers for different users. Uncertainties are addressed in a non-systematic fashion based on expert judgment and uncertainties in the outputs are not provided.

Recommendations

Because the Sludge Batch Planning Toolkit (GlassMaker II) is based on versions of the Sludge Washing Spreadsheet developed for planning purposes, recommendations for both are provided here.

Short-term

The knowledge and process logic from the single expert who developed and currently runs the Sludge Washing Spreadsheet should be captured in a format that will lend itself to subsequent software design. A mentoring program should be instituted to develop additional knowledgeable users for both operational and long-term planning support. Planning should begin to develop a new sludge washing tool for planning purposes.

Uncertainties in the sludge washing processing calculations for both operational and planning purposes should be characterized (and documented) in a systematic and transparent fashion based on historic information and knowledge obtained during processing the first four sludge batches and other pertinent information.

Mid-term

Expert functional and logic descriptions should be used to develop (1) an operational tool for near-term sludge washing calculations and (2) a long-term planning tool that would incorporate sufficient functionality and logic from the current spreadsheet. Optimization needs for both operational and long-term planning should be evaluated. The new tools should be integrated with the “tank inventory database” and provide the capability to generate uncertainties associated with sludge washing operations for both operational and the long-term planning. The computing environment needed to support the new tools for long-term sludge washing and planning needs, including potential optimization and learning (e.g., artificial intelligence), should be evaluated.

Long-term

A mechanism or capability is needed to assure consistency between the near-term operational tool and the long-term planning tool. The "tank inventory database" and new WCS system should be integrated with the sludge batch planning tools to allow propagation of inventory and sludge washing uncertainties through the planning process. Optimization methods should be implemented as needed both locally in the sludge washing operational evaluation and globally in the planning process.

6.4 Product Composition Control System (PCCS)

Description

The Product Composition Control System is an Excel-based application run on Windows NT 4.0 Workstation [BROWN]. It is used for the Glass Product Control Program as part of the DWPF waste acceptance strategy [RODRIGUEZ]. The system contains models that are used to predict glass process and product quality from the composition of SME samples. The acceptability of SME batches is evaluated based on process and product quality constraints required for the DWPF and calculated by application with outputs displayed on the PCCS spreadsheet.

PCCS determines whether a glass composition representing that derived from the content of a SME batch is acceptable for the DWPF. The determination is based on meeting all of the constraints placed on the glass for a set of properties at appropriate confidence levels. Some of the properties are measured directly (sample collection, compositions) while others (viscosity, durability) are predicted from models based on the measured composition. The spreadsheet calculations account for uncertainties associated with both the property models and those associated with direct measurement of the properties. A glass composition is deemed within the acceptable range for DWPF if all of the applicable constraints are satisfied after accounting for the modeling and measurement uncertainties.

Inputs to the spreadsheet are analytical measurements of SME samples including: weight percent solids, specific gravity (SpG), and elemental and anion compositions. These inputs are taken from the average composition of four SME samples determined by chemical analysis. The output is a workbook that yields the predicted acceptability results for the glass that would be produced from the SME batch based on process and product quality constraints that are incorporated into the spreadsheet calculations.
The confidence levels are user defined but set to meet the Waste Acceptance Criteria (WAC) requirements. The software QA is documented in the PCCS Software QA Plan (SQAP) [GILMORE].

Observations

The spreadsheet has been used successfully to fulfill its intended purpose as it has been used for the production of over 8 million pounds of radioactive glass at the DWPF, through processing five different batches of tank waste. Because the difference in QA levels precludes direct linkage between codes, Laboratory Information Management System (LIMS) data are currently input manually into PCCS. Manual input increases the time required for data processing, and it also introduces potential for errors associated with data entry. However, it provides for an independent check of the input data to be processed.

The analyses carried out in the spreadsheet are based on two sets of analyses of six samples. Four of the six samples are selected for product acceptability determination based on the total quantity of oxides. An average composition is then derived from the four samples and serves as the basis for the acceptability determination. Although the sample selection appears adequate based on success in meeting the product constraints, the down-select from six to four samples was not formally documented in the PCCS documentation. The minimum number of samples selected (four) was originally intended to account for sample recovery although it is not apparent that the down-select is currently needed based on the information presented.

Recommendations

Short-term

Because the QA level for the PCCS spreadsheet is Level B, higher than required for the LIMS database, data is input manually into the PCCS spreadsheet. Automation of the data input should reduce the time required for turnaround on waste acceptability and reduce the chance of input errors. A mechanism for transferring LIMS data with limited manual manipulation should be investigated, perhaps through an intermediate spreadsheet. Such a system should include an independent comparison of the LIMS source data and the PCCS input data to serve as an error check. There does not appear to be any documentation of the selection of the four samples from the original six or more that serve as the basis for waste acceptance. The technical basis for this sample selection should be documented.

Mid-term

PCCS does not integrate readily with the other tools being used by LWO. The potential benefit of a more accessible platform to facilitate integration with other tools should be evaluated. Actual initiation of this effort should be balanced with the relative time and effort required to rework and qualify the new code. The glass properties predictions in the PCCS are semi-empirical where experimental data are used to define coefficients for mechanistically-based models. SRS should initiate a program to define the requirements of a model to predict melt-rate from the melter-feed composition. The goal is to develop a more complete science-based system for glass acceptability characterization. A similar approach should also be applied in improving current physicochemical models used to predict other critical glass properties such as the possibility of nepheline formation, ,and leach rates. for various disposal environments (e.g., tuff, salt, clay, etc.).

Long-term

DOE-EM should support the development of a more rigorous thermochemical model to predict melt-rate from the composition of the starting mixture and melter conditions. The goal is to increase confidence in the acceptability of any particular glass formulation, potentially reducing the amount of waste glass waste that is produced. This approach may also simplify sludge management, potentially broadening the allowable sludge composition space and reducing composition manipulation steps. Such a model or set of models should be of particular benefit where waste compositions are more variable.

6.5 SpaceMan Plus™

Description

SpaceMan Plus™ is a software planning tool written in Visual Basic 6 and running on an IBM workstation. The code is used to predict system-wide chemical, radiological, mass, and volume conditions in order to project the long-range effects of operational plans [HOPKINS]. It is used for both long-range and operational planning of waste tank-related operations through the final completion of the liquid waste program [HAMM]. In this function, SpaceMan Plus™ is used to identify and sequence the individual activities related to tank farm operation, sludge batch manipulation, DWPF and SWPF production rates. It is used to evaluate and resolve processing conflicts and identify opportunities or improvement as well as to evaluate the operability and effectiveness of the activities as laid out.

The model processes inputs that define the scale and timing of individual activities including liquid transfers liquid processing and tank properties. The inputs to the code are a series line commands based on "cards," a format held-over from earlier versions of the software. Each line of code defines a specific activity including the start and end dates, repeats, start and end points, and other characteristics (volumes, tank type, operating points, etc.) of the action. Each action is represented by a numeric code in a defined order with dates, volumes, etc. specified [DNFSB]. Actions that are coded include liquid transfers between tanks, evaporator properties, saltcake dissolution, tank fills, Saltstone parameters, etc. A graphical user-interface provides information to the user on tank characteristics during execution. The program outputs are text files that are manually exported to spreadsheets or other formats for creation of charts and tables to represent the series of activities that define the overall System Plan. The output data includes information on tank inventories, monthly volume balances, evaporator operations, space recovery, and overheads, as well as reports on outages, transfers and other activities. The results are examined by subject-matter experts for conflicts, opportunities, operability, and effectiveness. The software QA level is D and is described in the Liquid Waste Planning Software Quality Plan [GILMORE].

Observations

Although the SpaceMan Plus™ code has been used for long-term system planning, the data construct used to represent each activity is awkward. The data input is derived from a previous version which used inputs based on a series of card commands. Cards are no longer used but each activity is represented by a single line of numeric code, a legacy from the original version. Thus, setting up a run is time-consuming and requires specialized knowledge of this coding. Because each activity must be defined, a series of activities must be carefully worked out prior to running the code. Conflicts must be resolved by trial and error and generation of the input for a single scenario can take as long as three months. As a result, there are a limited number of users who are proficient in SpaceMan Plus™. In addition, graphical output reports which enable interpretation of results must be manually generated. As result, SpaceMan Plus™ is better suited for short-term planning and development where a short series of activities can be evaluated readily.

There are several practical limitations to the software. For example, schedules are represented by 48-week years (4 wks/mo, 12 mo/yr), activities are assumed to operate at steady state within each week, and calculations performed once-a-week calculations have to be spread over multiple weeks to model evolving processes. Actions are limited to 100 per week. Although the cost is a key variable in operational planning, there is no cost-related analysis within the code. There are no restrictions on number or type of transfers, non-operation is not specifically flagged, and error handling is limited. In terms of computer support, the code is written in Visual Basic 6 which is no longer supported and the site has only two development licenses. The SpaceMan Plus™ code is used in Appendix C as an example of where application of SQA analysis and techniques can improve modeling throughout SRS.

Recommendations

Short-term

As SpaceMan Plus™ will continue to be used extensively, several improvements should be made to the code. The data input should be redesigned to facilitate creation of scenarios and improve turnaround. Creation of the card deck should be automated to minimize or at least shorten process time for the current trial-and-error approach. Also, generation of reports and graphics should be automated, perhaps by creating an interface with commercial project planning or standard spreadsheet software.

More fundamentally, the code should be updated to a currently supported version of Visual Basic. Practical limitations within the code should be addressed, notably the time-related limitations (48 wks/yr, once/week, etc.) and error handling and flagging. The gas generation model should be updated to better predict free space in tanks. Updating and upgrading the code should be weighed against the benefits of switching to a more modern framework.

Mid-term

In the longer term, SpaceMan Plus™ should be replaced with a discrete-event model with embedded logic. The software should be able to capture operations included in SpaceMan Plus™ to the extent possible; this objective may require specialized discrete analysis software or an interface between multiple codes. The new planning code should be able to perform all of the functions of SpaceMan Plus™, but without the trial and error that requires significant user manipulation of input forms. Such a model would continue to support operations and system planning functions, but with automated life-cycle model output rather than require the user to conduct evaluations prior to running the scenarios. A discrete event model would also enable comparative evaluation of multiple scenarios which is not generally feasible with SpaceMan Plus™ due to the requisite preparation time. As a discrete event model would require an upgrade in computer requirements, an evaluation of the optimum computing environment should be conducted.

6.6 COREsim™

Description

COREsim™ is a discrete event simulation framework that is currently being used to conduct time and motion studies for a number of liquid waste disposition operations [CHANG]. It is a commercial product that runs on a Microsoft Windows platform. COREsim™ has been used to evaluate processing cases in order to provide inputs to Liquid Waste Disposition System Plan [PARKINSON]. In support of this effort, the software has been used for throughput analysis, de-bottlenecking, identification of potential interface issues, process timing, resource utilization, and resolving model inconsistencies. Other COREsim™ utilities include design verification and validation, evaluation of alternative processing, and determining confidence level for achieving milestones. It has been used to validate SpaceMan Plus™ output. Inputs used to conduct time and motion studies include the facility availability, resource requirements, cycle time, process steps, process sequence, constraints, conflict matrix, what-if logic variables, and several tank parameters. For each "what-if" case, a description document is created.

The primary outputs include throughputs for several facilities: DWPF canister production, SWPF salt waste processing rate, Saltstone processing rate, and the DWPF Recycle water management system. Timelines are generated for all resources and functions used or specified in process models. Data is output in a number of formats including graphical Windows Metafile (WMF), text (comma-separated values, (CSV)), and as timelines.

The software is QA Level D as described in the Liquid Waste Planning Software Quality Plan: [GILMORE]. Verification and validation requirements are listed in report: [CHANG].

Observations

The application of COREsim™ to a number of facilities at SRS has resulted in major cost reduction in facilities and operations at SRS--investment of about $500K has resulted in greater than $15M in savings. Although it has been used for time and motion studies of a number of LWO operations (e.g., SDIP Strip Effluent Process, Saltstone Feed Preparation System, DWPF, and MCU, etc.), it has not been applied to long-term planning system due to computing power limitations. The current liquid waste model run time is limited by the computing platform that is available. However, models created in COREsim™ may be able to capture SWS logic flow, enabling evaluation of multiple processing scenarios which could result in significant improvements in process efficiency and ultimately cost savings.

Recommendations

Short-term

In order to increase the utility of COREsim™ to liquid waste treatment, the simulations should be run on a faster processor with more memory to boost productivity. This would enable fast evaluation of a number of what-if studies, a current limitation of the planning project. Because it has demonstrated value in a relatively short time, the feasibility of employing COREsim™ to replace some currently outmoded, though still utile, software should be explored. There is an effort underway to implement COREsim™ as an alternative to SpaceMan Plus™. The team recommends that this process continue.

Mid-term

In the mid-term, the utility of COREsim™ as a system planning model should be fully evaluated. Many of the limitations of SpaceMan Plus™ would be overcome with a discrete-event model such as COREsim™. While COREsim™ may not be ideal in this role (SRS personnel indicated that it may not be well-suited for the process chemistry), because it has been widely applied at SRS and is currently being employed within the program. Expanded CORESim™-based models could automate life-cycle model output while supporting operations and system planning. Multiple processing scenarios may be evaluated, which is difficult to do currently with SpaceMan Plus™. Other discrete event analysis tools may be better suited for the needs of the SWS project in terms of long-range planning and interfacing with the other project codes, so a survey of such software is warranted before COREsim™ is fully expanded for complete life-cycle analysis. In order to fully utilize the program's functions, an evaluation of the optimum computing environment should be conducted.

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Appendix A – Biographies of Review Participants

Team Members

Monica C. Regalbuto, Lead Dr. Regalbuto is the head of the Process Chemistry and Engineering Department in Argonne's Chemical Sciences and Engineering Division. She is an affiliated researcher with the Massachusetts Institute of Technology, Cambridge, MA and currently holds an IPA position with DOE-EM. Dr. Regalbuto has made key contributions to nuclear fuel cycle technology, beginning with the TRUEX process for removing transuranic elements from aqueous acidic solutions such as those found at DOE waste sites throughout the United States. She led the development of AMUSE, a computer model used by researchers to optimize processes for separating dissolved spent nuclear fuel. Under Dr. Regalbuto's leadership, Argonne conducted a highly successful demonstration of CSSX, a process for separating cesium-137 from high-level radioactive waste at DOE's Savannah River site. She maintains technical leadership in the development of advanced separations processes as alternatives for recycling spent fuel. Dr. Regalbuto is a key contributor to the development and demonstration of the UREX+ processes and pre-conceptual engineering design. Dr. Regalbuto's research supporting the development of nuclear fuel cycle technologies combines her experience in separations, computer simulations and proliferation resistance areas. In 2007 Dr. Regalbuto received both the Hispanic Engineer National Achievement Award Corporation (HENAAC) Professional Achievement Award and the American Nuclear Society (ANS) Jane Oestmann Professional Women's Achievement Award. Dr. Regalbuto's publications include over 30 journal articles, reports and presentations and five patents. She received a B.S. from ITESM, Mexico and an M.S. and Ph.D. from the University of Notre Dame, IN.

Kevin G. Brown. Dr. Brown is Senior Research Scientist in the Department of Civil and Environmental Engineering at Vanderbilt University. His research has been supported by the multi-university Consortium for Risk Evaluation with Stakeholder Evaluation (CRESP). Dr. Brown's current research focuses on life-cycle risk evaluation, model integration, and waste management issues related to proposed advanced nuclear fuel cycles and cementitious barriers for nuclear applications. Between 1986 and 2002 at the Savannah River Laboratory, he was recognized as a DOE Complex-wide authority in process and product control for high-level waste vitrification. His activities supporting the Defense Waste Processing Facility (DWPF) included: 1) optimizing waste loading, 2) modeling critical properties, 3) managing uncertainties, and 4) supporting variability studies and waste form acceptance. He served a similar role across the DOE Complex supporting vitrification projects at Idaho, Hanford, and West Valley. Dr. Brown spent 2002-2003 at the International Institute for Applied Systems Analysis (IIASA) in Austria where he estimated potential transboundary radiation doses from hypothetical accidents at Russian Pacific Fleet sites. They were the first such studies known in the West. Dr. Brown led the CRESP evaluation of life-cycle risks for the DOE Idaho Site Subsurface Disposal Area (SDA) where wastes contaminated with radioactive and hazardous materials were buried in pits, trenches, and soil vaults before 1970. He supported the corresponding risk evaluation for the Idaho Site Calcined Bin Sets containing high-level wastes. The results were presented to the Idaho Site Citizens Advisory Board (CAB), who strongly endorsed the clarity of the approach and the results. He holds a BE in Chemical Engineering, an MS in Environmental and Water Resources Engineering, and a Ph.D. in Environmental Engineering from Vanderbilt University.

David W. DePaoli is currently Group Leader of the Separations and Materials Research Group, Nuclear Science and Technology Division at Oak Ridge National Laboratory. David has worked at ORNL for over 23 years and has been involved in a wide range of chemical- and energy-related research and development projects, including demonstration of environmental-cleanup and waste-treatment technologies, basic research on separations employing external fields, and development of separation processes to recover materials for medical isotope production. For the past 12 years, he has been group leader of the Separations and Materials Research Group in the Chemical Technology and Nuclear Science and Technology Divisions at ORNL, which conducts fundamental and applied R&D aimed at applying chemical engineering principles to develop energy-related technologies. He is currently involved in efforts to develop advanced materials for electrochemical double-layer capacitors, devise new routes for production of chemical feedstocks from renewable sources, improve centrifugal contactor performance models for solvent extraction, and demonstrate real-time characterization tools for nanomaterials production processes. David has also been active in recent roadmapping activities for Nuclear Energy Advanced Modeling and Simulation (NEAMS) in the Department of Energy's Office of Nuclear Energy. David is Associate Editor for the journal *Separation Science and Technology*, and has acted as General Chairman for the 11th through 15th Symposia on Separation Science and Technology for Energy Applications. David has been an Adjunct Associate Professor in the Department of Chemical and Biomolecular Engineering at the University of Tennessee since 1999, and a director of the Separations Division of the American Institute of Chemical Engineers from 2003 through 2007. David received a BS in chemical engineering from the University of Michigan, and a Ph.D in chemical engineering from the University of Tennessee. He is author of over 40 peer-reviewed publications, and holds four patents.

Candido Pereira has been a researcher in the Chemical Sciences and Engineering Division of Argonne National Laboratory for the past 16 years. He received his PhD in Chemical Engineering from the University of Pennsylvania. At Argonne, he has worked on several programs related to the processing of spent nuclear fuel. In the Integral Fast Reactor program, he led efforts to develop an ion exchange process for cleaning spent salt from the electrorefining of spent metallic fuels to allow its recycle, and to develop a ceramic waste form for the sequestration of active metal fission product chlorides. He conducted research on the processing of gasoline and diesel fuel using catalytic systems to generate hydrogen for fuel cell applications. He currently conducts research on the treatment of spent commercial reactor fuel through the Advanced Fuel Cycle Initiative. He played a lead role in the UREX+ demonstrations that were run at Argonne between 2003 and 2007, authoring several summary reports. He has also worked on enhancing the AMUSE solvent extraction code, and on the conceptual design and simulation of an advanced spent fuel treatment plant based on the UREX+1a process. Recent research has also centered on the implementation of safeguards in spent fuel treatment facilities, both through AFCI and NNSA programs. He currently leads the Process Simulation and Equipment Design Group.

John R. Shultz. Dr. Shultz currently works in the DOE Office of Environmental Management but formerly worked in the DOE Office of Security, where he helped draft the DOE Safety Software Guide (DOE G 414.1-4) and provided input on the DOE Quality Assurance Order (DOE O 414.1C). For this work he received a commendation from the Assistant Secretary for the Office of Environment, Safety and Health (John Shaw). In addition, Dr. Shultz is acknowledge as a contributor to ANSI/ANS-10.4-2008 *"Verification and Validation of Non-Safety Related Scientific and Engineering Computer Programs For the Nuclear Industry"* and is currently on the standards development team for ANSI/ANS-10.7-200x; *"Non-Real Time, High Integrity Software for the Nuclear Industry".* While in the Office of Security, Dr. Shultz revised DOE M 474.1-2A, which governs the reporting of nuclear material inventories and transactions to the Nuclear Materials Management Safeguards System (NMMSS), a summary-level database of all nuclear material in the United States. Furthermore, Dr. Shultz was a member of an item-level nuclear material accountability software development team (Local Area Network Material Accounting System-LANMAS) that received the DOE CIO Technical Excellence Award. In addition, Dr. Shultz has worked with a team of DOE engineers and scientists to help the Russian Federation design and implement a nuclear materials database and accountability system. Dr. Shultz was previously employed as a lead research engineer and senior policy analyst with the National Energy Technology Laboratory, US Department of Energy, Morgantown, WV. Dr. Shultz is a Certified Software Quality Engineer (CSQE) and a former active duty and reserve Army military policeman (enlisted) and engineer (officer).

Sahid C. Smith. Dr. Smith is a general engineer in the K Basin Closure project group at the Richland Operations Office of the U. S. Department of Energy. He received his B.S. and Ph.D. in chemical engineering from Florida A&M University. He has worked on projects related to processing and disposition of spent nuclear fuel and transuranic waste. His technical expertise includes radioactive waste management, heat and mass transfer simulation, and CFD modeling of non-Newtonian flows.

Team Observers

Gail K. Allen. Mr. Allen is a senior engineer in the Mission Analysis and Strategic Planning group at Washington River Protection Solutions LLC. He is a chemical engineer with 35 years experience in process engineering and radioactive waste management at Hanford. Technical expertise includes heat and mass transfer simulation, steady state and dynamic process flowsheet development and modeling, PUREX plant plutonium and uranium reprocessing, and chemical processing associated with the current waste treatment plant design being built at Hanford. He is the lead developer for the system planning model HTWOS which has been in use at Hanford for 15 years.

Paul J. Certa. Mr. Certa is a senior engineer in the Waste Feed Delivery and System Planning group at Washington River Protection Solutions, LLC. He is a chemical engineer with over twenty-seven years experience in strategic planning and analysis of complex chemical processes, in leading technical teams in conducting complicated engineering studies (seven years) and in processing nuclear waste and reprocessing plutonium (eleven years). He has led or has participated in the development of five system plans for the retrieval and treatment of the tank waste at Hanford for the U.S. Department of Energy, Office of River Protection. He is a licensed chemical engineer in Washington State and a certified manager.

Appendix B – Charter

Evaluation of System Level Modeling and Simulation Tools in Support of Savannah River Site Liquid Waste Planning Process

1.0 Background

The Savannah River Site (SRS), a 300-square-mile DOE Complex located in the State of South Carolina, has produced nuclear material for national defense, research, medical, and space programs. Since 1954, SRS Tank Farms have received more than 140 million gallons of liquid waste. Periodically the liquid waste was been evaporated to reduce its volume. Over 100 million gallons have been evaporated; the SRS Tank Farms currently store over 36 million gallons of waste containing approximately 400 million curies of radioactivity (figure 1). Most of the tank waste inventory was generated during processing of irradiated targets and spent fuel using the Plutonium–Uranium Extraction (PUREX) process in F Canyon and the modified PUREX process in H-Canyon (H-Modified or HM process). Waste generated from the recovery of Pu-238 in H-Canyon for the production of heat sources for space missions is also included. More recently 30,000 gallons of highly radioactive Americium/Curium solution was transferred from F-Canyon to Tank 51H in the H Tank Farm.

Because the liquid radioactive waste storage tanks at SRS are constructed of carbon steel and the canyon wastes are acidic, the wastes were neutralized via the additions of sodium nitrite and sodium hydroxide. These additions have resulted in metal hydroxide solids settling as sludge and soluble salt supernate. The supernate volume was reduced by evaporation, which concentrated the soluble salts to their solubility limit. The resulting crystalline solids are referred to as saltcake. The salt cake and supernate combined are referred to as salt waste.

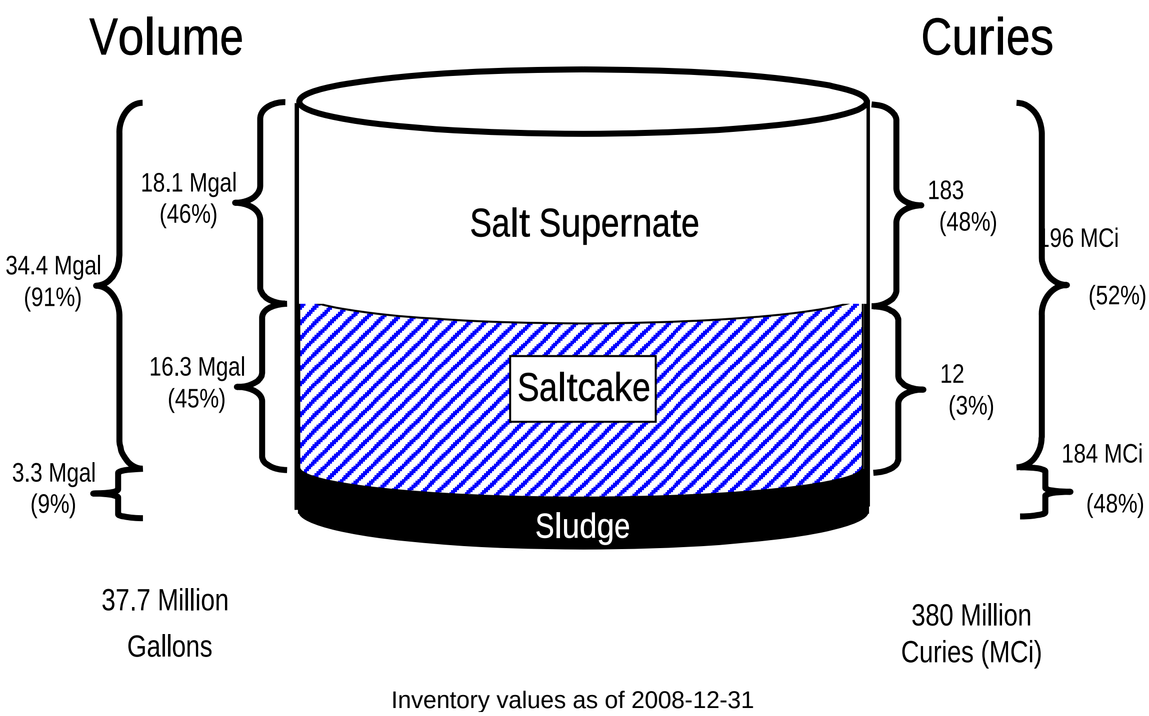

Figure 1. SRS Liquid Waste Composite Inventory as of December 31, 2008 [LWO-PIT-2007-00062]

The sludge contains the majority of the long-lived (half-life > 30 years) radionuclides and strontium. The sludge is currently being stabilized at the Defense Waste Processing Facility (DWPF) as a borosilicate glass. Greater than 95% of the radioactivity of the salt waste is short-lived (half-life < 30 years), mainly due to Cs-137, its daughter product Ba-137m and lower actinide contamination. The salt waste is treated to separate the high radioactivity and low radioactivity fractions. The high radioactivity fraction is immobilized at DWPF in a borosilicate glass and the low radioactivity fraction is immobilized in grout matrix at the Saltstone Production Facility (SPF). The current plan for salt waste treatment is [LWO-PIT-2007-00062]:

- Deliquification, Dissolution and Adjustment (DDA) – mainly used for tank 41 which has a relatively low radioactive content. The treated salt solution is sent to SPF for immobilization in grout.
- Actinide Removal Process (ARP) – Actinides are sorbed on monosodium titanate (MST) and sent to DWPF for immobilization in glass and the remaining liquid is sent to the Modular CSSX Unit MCU unit for further treatment.
- Modular CSSX Unit (MCU) – Reduces the Cs concentration by solvent extraction. The Cs-containing product is send to DWPF for stabilization as glass and the remaining decontaminated salt solution is sent to SPF for stabilization as grout. The MCU will be replaced by the Salt Waste Processing Facility (SWPF) in 2013 (based on approval of SWPF Critical Decision-3, Construction Start).

The tank waste removal process is a multi-year process and consists of the following steps:

- Adding de-ionized water to dilute concentrated salt or re-dissolved the saltcake and assist in the suspension of sludge
- Mixing to form a slurry
- Pumping of the slurry from the waste tanks to the waste treatment tanks for further processing.

Tank space is carefully tracked. A portion of the tanks space is reserved as contingency space in the event that a tank leaks. Currently, tank farms receive waste from H-canyon stabilization program, liquid waste from DWPF, and waste water from sludge washing operations. Transfer to and from waste tanks and the three operating evaporators are routinely done. SRS has 51 underground waste tanks that were placed in operation between 1952 and 1986. There are 49 active waste tanks located in two separate facilities, H-Tank Farm (29 tanks) and F-Tank Farm (20 tanks). Two tanks in F-Tank Farm are not active; they have been isolated, operationally closed, and grouted. Categorization of the waste tanks is given in table 1.

Table 1. SRS Waste Tanks Types

Type	Total Number of Tanks	Current Waste Inventory	Comments
I	8	3 Mgal	Oldest, constructed between 1952 and 1953
II	8	3 Mgal	Constructed between 1955 and 1956
III	27	28 Mgal	Newest tanks, placed into operation between 1969 and 1986. Only tanks that meet EPA requirements for fully secondary containment and leak detection
IV	8	4 Mgal	Constructed between 1958 and 1956

The Liquid Waste System is a highly integrated operation (figure 2) that involves safely storing liquid waste in underground storage tanks; removing, treating, and dispositioning the Low-Activity Waste fraction in concrete vaults; vitrifying the higher activity waste; and storing the vitrified waste until permanent disposition at a Federal Repository. After waste removal and processing, the storage and processing facilities are cleaned and closed. In order to integrate all activities required, the Life-cycle Liquid Waste Disposition System Plan (LLWP) has been developed. It establishes a planning basis for processing the constituents of the liquid waste system to the end of the program mission. The LLWD is a qualitative assessment based on modeling and simulation estimates.

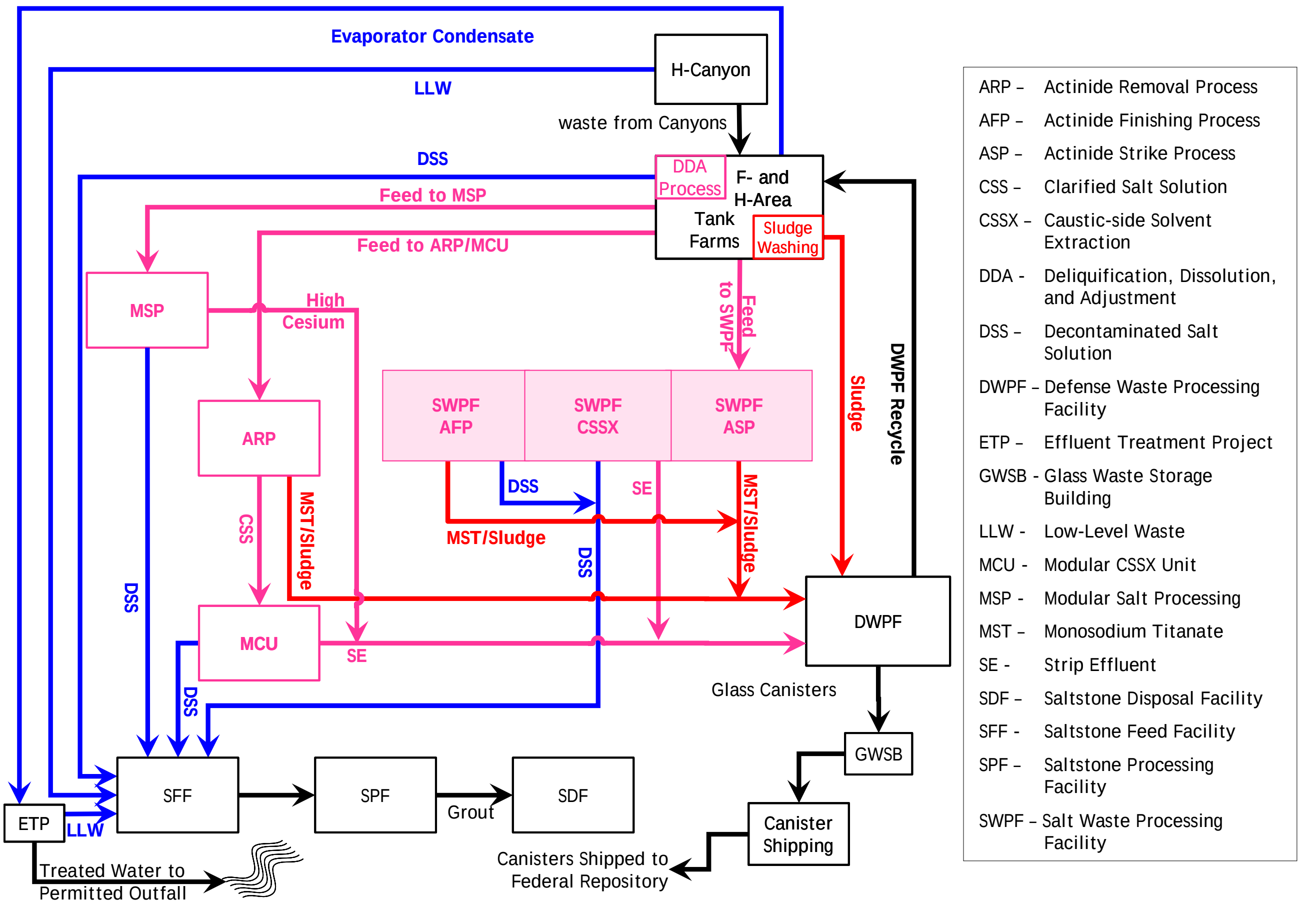

Figure 2. SRS Process Flowsheet [LWO-PIT-2007-00062]

2.0 Scope of the Review

The objective of this review is to evaluate the current Process Simulation Tools that support the planning basis for the SRS Life-cycle Liquid Waste Disposition System Plan.

This review will focus on three primary areas:

- Assess the assumption that the tools used for liquid waste process simulation yield reasonable estimates
- Evaluate if additional tools are needed to guide actual execution of individual processing steps
- Evaluate methods to improve the rate at which system model predictions are done

3.0 Team Membership

The team will include five or more independent experts whose credentials and experience align with the specific lines of inquiry (LOI) listed below and who collectively provide to the team sufficiently broad capability and flexibility to address the full range of issues that may emerge in this review. Technical expertise includes, but is not limited to design, engineering and management of chemical processing and computer software development. Individual expertise and experience will be commensurate with the LOI. The experts must be free of any conflicts of interests with Savannah River Operations Office.

Each team member is responsible for conducting a thorough, professional and independent review, for supporting the identification and resolution of technical issues, for participating in the development of draft and final reports, and for supporting resolution of comments and any points of disagreement. Collectively, the team is responsible for producing a high quality review report that is responsive to this charter, that includes unambiguous conclusions regarding the identified lines of inquiry, and that presents clearly any dissenting viewpoints. All team members will sign the final report.

Team members for this review:

Monica Regalbuto (EM-21)
John Shultz (EM-21)
Candido Pereira (ANL)
David DePaoli (ORNL)
Kevin Brown (Vanderbilt University)
Sahid Smith (EM-21)
Modeler from DOE-ORP as an Observer

4.0 Period of Performance

This review will formally begin in late March 2009, although the collection of background information began in mid March. The review shall include a combination of presentations, interviews with key personnel, information gathering sessions, independent document reviews, and group discussions. The review is expected to be completed at the end of May 2009. The key milestones for the review team are as follows:

- Provide Supporting Documentation — March 27, 2009
- Site Visit to SRS — April 20-24, 2009
- Status Briefing to EM Senior Management — April 27-30, 2009
- Team Meeting – Draft Report — May 14, 2009
- Final Report Approved by Team Members — May 28, 2009

5.0 Lines of Inquiry

Is there an adequate overarching strategy (master plan/schedule) developed to integrate all systems and operations under consideration that will be necessary for processing liquid waste SRS? A systems approach ensures that all operations and interfaces, risks and alternatives are evaluated to ensure that throughput, schedule and budget and other overall requirements are met. "Adequate" considers maturity of each aspect with respect to schedule; is the degree of development and planning sufficient to meet the schedule for implementation? What aspects of a systems approach are in place, and which aspects are missing?

5.1 How those SRS selected the various software modeling "tools" they are using?

5.2 Does the Waste Characterization System (WCS), a series of spreadsheets, adequately estimate the composition and inventory of the liquid waste tanks?

  5.2.1 What calculations are performed in the spreadsheets?

  5.2.2 What are the pertinent data needed to perform the estimation?

  5.2.3 How is gas generation calculated within WCS

5.3 Does the Sludge Washing Spreadsheet (SWS), a spreadsheet model, adequately estimates the composition and inventory of the washes resulting from each sludge batch?

  5.3.1 What calculations are performed in the spreadsheets?

  5.3.2 What are the pertinent data needed to perform the estimation?

5.4 Does GlassMaker, a Visual Basic program, adequately estimates the composition of each sludge batch?

  5.4.1 What are the program inputs?

5.5 Does PCCS adequately estimate the acceptability by DWPF?

  5.5.1 What are the program inputs?

5.6 Does SpaceMan Plus™, a Visual Basic program, adequately simulates operation of all the processes in the entire Liquid Waste System?

  5.6.1 Is the information from WCS, SWS, and GlassMaker accurately transferred and at the same level of development in order to estimate volumes and compositions in each tank and each process as waste is processed through the system?

5.7 Does CORESim™, a discrete-event simulation logic, adequately simulate the process?

  5.7.1 Does the model adequately predicts resource availability, identifies process bottlenecks, resource needs, and queuing effects on system performance?

5.8 What is the relationship between CORESim™ and SpaceMan Plus™?

5.9 Has the quality of the process simulation tools been adequately assured (i.e., is the QA plan adequate)?

  5.9.1 What is the traceability of data used to support the models?

  5.9.2 Has Validation and Verification (V&V) been conducted?

  5.9.3 Are there any benchmark validation study reports?

  5.9.4 How are version and revision controlled?

  5.9.5 How are users instructed on software execution?

  5.10 Are all critical processing steps characterized?

  5.11 How does previous simulation tools predictions compared with actual process performance?

  5.12 How do the simulation tools predictions compare to other tools used in other sites?

  5.12.1 Have side to side comparisons been done?

  5.13 Is the time required to do a study of model predictions acceptable to evaluate project risks?

  5.14 Given that SpaceMan Plus ™ modeling is the time-limiting process in program life-cycle scenario evaluation, is there a better platform/tool that could be used for life-cycle modeling that would decrease model run time?

5.15 Is the current equipment available, number of licenses purchased, number of personnel trained adequate to perform the modeling scope needed?

5.16 Is the output of models provided in a user friendly format (Graphical User Interface)?

6.0 Approvals

Mark Gilbertson, Deputy Assistant Secretary — 4/3/09 (Date)
Office of Engineering and Technology
Office of Environmental Management
U.S. Department of Energy

Terrel J. Spears, Assistant Manager Waste Disposition Project — 3-25-09 (Date)
Savannah River Operations Office
Office of Environmental Management
U.S. Department of Energy

Appendix C - Software Quality Assurance Overview

This Appendix covers two areas: Part 1 provides an overview of SQA and the relevant standards and Part 2 discusses SQA specific to the SRS modeling program.

Part 1

SQA in Software Development

Ideally, the QA process for software development begins when there is a mere “glimmer in the eye” that a software tool will be used to answer some question. The earlier in the process software QA references are consulted and their guidance is incorporated in software development, the easier (overall) the QA process. Poor QA practices can lead to errors that can have serious adverse impacts on program operations. Therefore, not only as a good business practice, but to avoid or lessen the chance of operational impacts, it is incumbent upon the software owner to do a thorough SQA review.

SQA Standards

The operant standards for software development are published by the Institute of Electrical and Electronics Engineers (IEEE). Over 140 standards related to software engineering are available from the IEEE website.[2] In addition to IEEE, there are a number of software development standards specifically applicable to the nuclear industry.[3] Also, the Defense Nuclear Facilities Safety Board (DNFSB) has strongly recommended that DOE do a better job of software QA[4], particularly for software used in “Safety Class” systems.

An important aspect of software QA is to use a “graded” approach, based on the importance of the software in process/program operations. For software that is used in “Safety Systems” a very rigorous software QA process must be implemented. For non-safety systems, the appropriate level of rigor is less than for “Safety Systems”, and the references upon which the QA review is conducted are different.[5] The following sections (in italics) are excerpts of requirements for SQA noted in the NQA-1 standard[6]. This is not an exhaustive list, but should impress upon the reader the seriousness with which the nuclear safety community takes SQA.

> *401 Use of Computer Programs*
> *To the extent required in paras. 401(a) and (b) of this Requirement, computer program acceptability shall be preverified or the results verified with the design analysis for each application. Preverified computer programs shall be controlled in accordance with the requirements of this Standard.*

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[2] See IEEE Software Engineering standards at http://standards.ieee.org/ ; “IEEE Software & Systems Engineering Standards Collection VuSpec CD-ROM and Road Map to Software Engineering Book”
[3] See 10 CFR 830, ASME NQA-1, ANSI/ANS 10.4-2008; DOE G 414.1-4 “Safety Software Guide”
[4] Letter to Secretary Spencer Abraham, September 23, 2002 which discusses the Department’s corrective actions to addresses deficiencies documented in the Board’s technical report: “DNFSB/TECH-25, Quality Assurance for Safety –Related Software at Department of Energy Defense Nuclear Facilities”
[5] See ANSI/ANS-10.4-2008
[6] ASME NQA-1–2008(Revision of ASME NQA-1–2004). Quality Assurance Requirements for Nuclear Facility Applications. Copyright ASME International

(a) The computer program shall be verified to show that it produces correct solutions for the encoded mathematical model within defined limits for each parameter employed.

(b) The encoded mathematical model shall be shown to produce a valid solution to the physical problem associated with the particular application.

801.2 Software Design.
The software design shall be documented and shall define the computational sequence necessary to meet the software requirements. The documentation shall include, as applicable, numerical methods, mathematical models, physical models, control flow, control logic, data flow, process flow, data structures, process structures, and the applicable relationships between data structures and process structures. This documentation may be combined with the documentation of the software design requirements, or the computer program listings resulting from implementation of the software design.

801.4 Software Design Verification.
Software design verification shall be performed by a competent individual(s) or group(s) other than those who developed and documented the original design, but who may be from the same organization. This verification may be performed by the originator's supervisor, provided (a) the supervisor did not specify a singular design approach or rule out certain design considerations and did not establish the design inputs used in the design, or (b) the supervisor is the only individual in the organization competent to perform the verification. Cursory supervisory reviews do not satisfy the intent of this Standard.

801.5 Computer Program Testing.
Computer program testing shall be performed and shall be in accordance with Requirement 11.

802 Software Configuration Management.
Software configuration management includes, but is not limited to configuration identification, change control, and status control. Configuration items shall be maintained under configuration management until the software is retired.

Elements of a Good SQA Process

There are a number of key elements in any good SQA process. Those elements can be broadly by binned into three categories: Documentation, Verification, and Validation (V&V). Though Verification and Validation are two separate processes, the software industry generally lumps the two together and refers to a general "V & V" of software. The following describes key elements of both the documentation and V&V of software.

SQA Documentation

The most basic element of software QA is proper process documentation. The following are examples of some of the documentation that would be present in a robust software QA process.

- Plans that explain in detail the following:
    - The problem to be solved
    - Specifications for hardware
    - Source code
    - Software
    - Operating system
    - Programming language
    - The test plan for evaluating software/model accuracy
    - Configuration management plan, including revision/version control

- Documentation of assumptions used in development of software
- Documentation of sources of data used in the model, including traceability of information to accepted reference standards when appropriate
- Documentation of program variables, i.e. the use of a data element dictionary
- Documentation of the data management process
- Provision of user's manuals and/or technical manuals as appropriate

SQA Verification & Validation (V&V)

The simplest, easiest way to do at least a "first pass" of software V&V is to step through ANSI/ANS-10.4-2008. The standard is quite brief. Also, the checklists in the back of the standard can be especially helpful to ensure that important software QA steps are not missed. Additionally, this standard should be considered a starting point for "safety" systems, with the recognition that safety software evaluations are more rigorous, and that meeting the 10.4 requirements is a "necessary but not sufficient" component of safety software V&V. Key elements of V&V include:

- Ensuring program logic is accurate and accomplishes the desired task
- Performing tests to ensure data calculations and output are accurate
- Performing tests to gauge what happens if erroneous/false/accidental data is input into the software. For example: Are warning flags or error checks used?
- Revision control – Is there a good process for updating the software based on new information, new software, or new needs the software must perform.

Part 2

SRS Modeling Quality Assurance (QA)

This section analyzes the implementation of general engineering QA and Software Quality Assurance (SQA) principles used in the models at SRS. This section is not intended to be a formal SQA review, which is a task beyond the scope of the ETR charter. However, good QA/SQA is critical to ensuring model accuracy and sufficiency. Therefore, this section reviews SRS QA and SQA processes/procedures and analyzes how QA impacts the overall SRS modeling effort.

General Impressions Regarding QA

VERY GOOD – Engineering Analysis Documentation
ADEQUATE – SQA Documentation (but not good across all models)
LESSER QUALITY – SQA Implementation and Execution (could be improved in most models)

Perhaps one of the reasons why the implementation of SQA principles is not consistent, is the lack of involvement of IT professionals in the modeling team. The following sections use the SpaceMan Plus^{TM} code development process to illustrate how the software models evolved at SRS and how this evolutionary process impacted SQA.

Example Discussion of SpaceMan Plus™ –Engineering Analysis Documentation

The SpaceMan Plus™ program does a really fine job of documenting the engineering analysis that is fed into the software. An excerpt from one of the SpaceMan Plus™ documents (Figure C.1 below) shows a very comprehensive explanation regarding how data are derived and then hard-coded into the software.

3 Mathematical Functions

- Supernate specific gravity is calculated as a function of sodium molarity, which is initially calculated from the sum of the anions (see section 4.1.16). For molarities between 0M and 6M, specific gravity follows an empirical curve (Equation 1) developed using a 2000+ population set from tank farm historical data (1973 to 2001) with the aid of JMP statistical software (Figure 1).

Equation 1. Supernate Specific Gravity for [Na]<6M

$$SpG_{[Na]<6} = -0.0017254 * [\mathrm{Na}]^2 + 0.057012490236 * [\mathrm{Na}] + 1.01293648396792$$

Figure 1. Specific Gravity versus Sodium Concentration (Tanks 1 through 51 Sample Data)

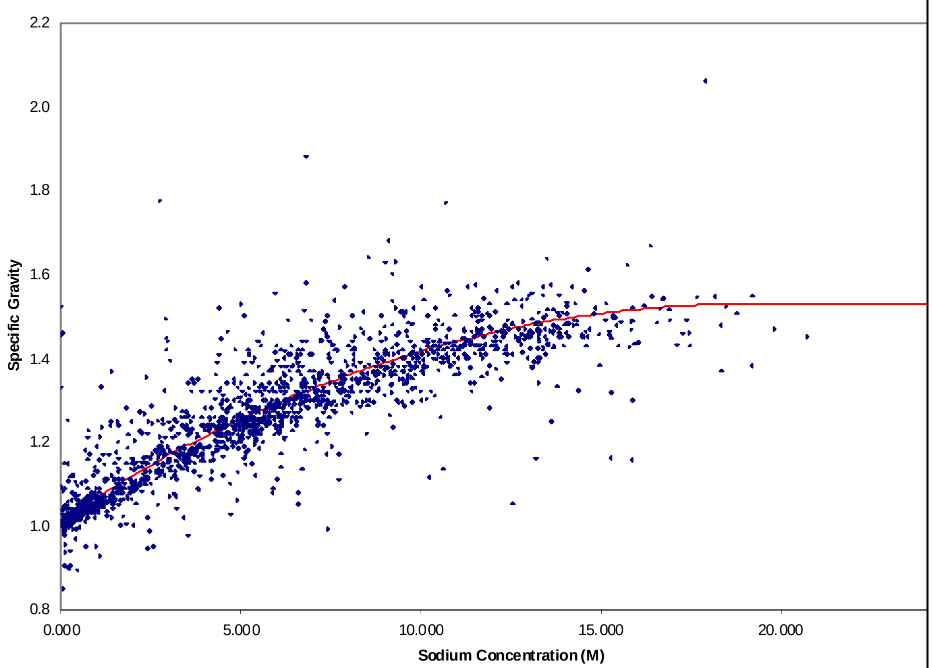

Figure C.1 The figure above is copied from SpaceMan Plus Plus™ Assumption List for v1.1.2; M. D. Hopkins, 766-H document number CBU-PIT-2006-00059, REVISION: 0, November 29, 2006; pages 7 and 8

Example Discussion of SpaceMan Plus™ –Standards and Data Documentation

The "SpaceMan Plus™ Assumptions List" provides additional detail regarding material property constants that are used in the model. For example, Figure C.2 shows information from Appendix B of the Assumptions List.

Table B-1 SpG of solids tracked in SpaceMan Plus

Component	SpG	Source
Hg	13.546	7 (20°C)
$NaNO_3$	2.261	8
$NaNO_2$	2.168	2 (0°C)
NaOH	2.13	2
$NaAlO_2$	2.5	
Na_2CO_3	2.532	8
Na_3PO_4	2.537	2 (17.5°C)
Na_2SO_4	2.68	8
NaCl	2.165	8
NaF	2.558	9
KNO_3	2.109	8
NaHgO(OH) (Assumed)	5.001	
$CaSO_4$	2.96	2

Figure C.2 The figure above is copied from SpaceMan Plus™ Assumption List for v1.1.2; M. D. Hopkins, 766-H document number CBU-PIT-2006-00059, REVISION: 0, November 29, 2006; page B-1

This is again a very good, methodical, approach to documenting the assumptions made regarding model inputs. Unfortunately, there are three issues with how SRS documents material properties for SpaceMan Plus™ that apply to all the other models: 1) There are a number of areas in the SpaceMan Plus™ material property appendices where the concept of "referencing the source", and thereby ensuring traceability, breaks down; 2) It is not clear whether or not some of the reference sources come from the best available source. For example, the National Nuclear Data Center[7], Brookhaven National Lab may be a better source for decay information; 3) After reviewing the other SRS software spreadsheets/models it is clear that there is not a coordinated effort to use the same material property information for all models. It is a much better modeling practice to use a universal material properties database (with revision controls and traceability) from which all models draw, rather than to have each model develop it's own set of "constants". This approach would also cut down on sources of possible error and result in less work for the individual modelers.

[7] In March 2002, the Department of Energy headquarters standardized all DOE inventory reporting to one source - The sixth edition of Nuclear Wallet Cards (2000). See http://www.nndc.bnl.gov/wallet/wcdoe.html

Discussion of SpaceMan Plus™ – Software QA Implementation and Execution

SpaceMan Plus™ was developed by an engineer in his "spare time" as a planning tool for waste transfers. The original version was written in the Basic programming language. For this review, we were provided the actual Basic source code, and a great many supporting files and documents. In addition, SRS personnel gave a presentation that explained how the software is used, and the shortcomings/problems that exist with the software. During the SR presentation, it was noted that they (SRS) could no longer purchase the version of Basic for which SpaceMan Plus™ was written[8]. Therefore, SRS could only update the software and use the compiler they had, and could not update to a more current programming language. This issue (old compiler) should not be terribly difficult to fix if the modeling team had some dedicated IT personnel on staff. The source code should be compilable under another Basic version without much modification. A second issue that came up during the presentation was that SpaceMan Plus™ used 48 weeks per year in its calculations. When we inquired as to why, SRS stated they were not sure why, that this was not intentionally done, but that it did provide some useful "slack" in the system in order to account for outages or problems that otherwise were not considered. A review of the source code shows why a year is defined as 48 weeks. Essentially, the algorithm defines a "year" as 4 weeks per month, for 12 months (see Figure C.3). Although this is a conservative estimate, there are more appropriate and less restrictive methods to add conservatism to a model. If programming specialist were assigned to the SpaceMan Plus™ project, the code would likely have been programmed differently.

```
Public Sub SortEngine()
Description:   Initializes the general array "xz()" to zero
'          and determines the number of steps based on a
'          user defined start and end date. The number
'          of steps is then defined in the "dte()" array
'          for use in other subroutines.

Dim NumSteps As Integer
Dim DateFlag As Integer

NumSteps = 0 'Initiates step counter
DateFlag = 1 '"Date Flag" determines if counter started
        'and ensures the correct number of steps
  'Initializes xz() array to zero (0)
  'For yr = StartYear To EndYear
  For yr = StartYear To EndYear
     For mn = 1 To 12
     If DateFlag = 1 Then mn = StartMonth
        For wk = 1 To 4
        If DateFlag = 1 Then wk = StartWeek
           NumSteps = NumSteps + 1 'Counts the number of steps
           For i = 0 To 12
              For j = 0 To NumOfActions
                 DateFlag = 0
                 xz(yr, mn, wk, i, j) = 0
              Next j
           Next i
        Next wk
     Next mn
  Next yr
```

Figure C.3 The section above was copied from SpaceMan Plus source code that was opened up in MS Wordpad (filename SpaceMan Plus.Bas)

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[8] Version 6 of the BASIC programming language

SQA Process and Documentation at SRS

In general, SQA is performed by personnel at the SRS site. The SQA documentation is generated by site personnel, and the sufficiency of that documentation is reviewed and approved by SRS personnel. The primary documents governing SQA at SRS are as follows:

- Manual 1Q "Quality Assurance Manual" Procedure 20-1, Rev. 11, "Software Quality Assurance", effective date 12/17/2008. This Manual requires maintenance of a "Safety Software Inventory List"[9]. In addition, for the two "Level B" software systems[10] noted in this review (the WCS and PCCS models), there are individual software QA plans which are described below.
- Level B: WCS Software QAP B-SQP-H-00041 Revision: 2 CBU/LWDP Waste Characterization System Date: 6/28/07 Software Quality Assurance Plan (SQAP), rev. 2, 2007
- Level B: DWPF Software Quality Assurance Plan, B-SQP-S-00006, rev. 4, 2007
- Levels D and E: Liquid Waste Planning Software Quality Assurance Plan; B-SQP-H-00060; Revision 1; March 12, 2009. This plan applies to all software developed, supported, and maintained within the Liquid Waste Planning (LWP) group and includes commercially acquired software and custom software applications developed for hand-held computers with a design classification of Level D and Level E.

SQA External Reviews at SRS

The team is only aware of one external safety SQA audit performed since 2004 of "Safety Software Currently Used to Support the Analysis and Design of Defense Nuclear Facilities".[11] This review was limited in scope and only reviewed two specific codes: GTSTRUDL, a purchased structural analysis code package, and Tank Top Loading, an SRS developed code.

Modeling Software Development at SRS

This is a review of the SQA documentation provided both prior to and during the ETR visit. The top level document which guides the general software QA process is Manual 1Q "Quality Assurance Manual" and, Procedure 20-1, Rev. 11, "Software Quality Assurance". This QA of the review focuses on the QA documentation that was provided, the QA process as noted during the model presentations, and the implementation of QA in the models (e.g. as data is input by users, and as the software tools are used over time).

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9 Available online at: http://shrine01.srs.gov/eshqa/QAhp/sqa/ssilr00.htm

10 See DOE G 414.1-4 "Safety Software Guide" for a discussion of what constitutes a "Safety System" and what constitutes "Level B" software.

11 "Assessment of Savannah River Site's Software Quality Assurance Processes for Design & Analysis Software for Safety Systems (SQAIP 4.2.4.3), On-site Assessment 2/18/04-2/19/04, report number FSS-TQS-2004-00002

Documentation of SRS Software Development Process

In this instance, it appears that many of the software modeling efforts began as an answer to a specific need, and the general process of software QA was not applied in a systematic way across all models. In fact, some models/spreadsheets attempt to incorporate QA principles to a much higher degree than others. Those systems that are currently doing a better job should be used as examples for the other systems and those "SRS Software Best Practices" should be incorporated in other systems.

Topical area: Plans that explain in detail the following: the problem to be solved; specifications for hardware, source code, software, operating system, and programming language; the test plan for evaluating software/model accuracy

Analysis: There are inconsistencies among the documents that guide the QA process at SRS.

- Manual 1Q "Quality Assurance Manual" Procedure 20-1, Rev. 11, "Software Quality Assurance", effective date 12/17/2008.

  - Comment 1 - The Procedure has much of the language that one would expect in an overall SQA program document. For example, the plan notes that "version control", and "configuration change control" will be instituted. However, as noted earlier in this report, the requirements in the SQA plans vary in their implementation. An example of this is that in most of the spreadsheets, anyone can change the fundamental spreadsheet equations any time they like (even unintentionally). Essentially, this creates a new "version" of the software that has not undergone the appropriate V&V process. This Procedure attempts to address in writing most of the key elements of SQA, but there is a breakdown regarding practical guidance (e.g. example documents for software owners at SRS would be helpful in ensuring they implement the requirements consistently).

  - Comment 2 - The references in this Procedure are out of date (e.g. NQA-1-2000 is listed as current, which would be at least 1, perhaps 2 revisions behind as of the last revision date of the Procedure) or lacking in appropriateness. The fundamental standards on which software design is based are published by IEEE. This Procedure does not mention IEEE as a source for SQA. Of most concern is the lack of reference to ANSI/ANS-10.4-2008 "Verification and Validation of Non-Safety-Related Scientific and Engineering Computer Programs for the Nuclear Industry". That standard (10.4-2008) has some really helpful features to ensure the sites overall SQA program is properly evaluated and documented.

- WCS Software QAP B-SQP-H-00041 Revision: 2 CBU/LWDP Waste Characterization System Date: 6/28/07 Software Quality Assurance Plan (SQAP), rev. 2, 2007

  - Comment 1 - P. 5 states that: "There is no commercial off-the-shelf (COTS) software within the scope of the SQAP". This is not an accurate statement. The WCS is an MS Excel workbooks. Therefore, by definition it is a COTS product. Also, it is VERY NECESSARY to keep track of the current version of Excel the spreadsheet uses because not all versions of Excel handle calculations or embedded Visual Basic macros in the same manner.

- Comment 2 - From this Plan it is difficult to access how the spreadsheet model owners implement “version control”, or “configuration control”, or “Provide a revision history that includes for each change; a description of the change, the rationale and significance of the change, the date, the change identifier, the document sections that were revised and references to other documents affected by the change.”[12] There was no documentation provided regarding the practical way that if changes are made to the cells that those changes are documented.

- DWPF Software Quality Assurance Plan, B-SQP-S-00006, rev. 4, 2007

  - Comment 1 - The Plan speaks at a high level regarding the aspects of SQA that should be present, but does not guide what the software owner how to do so. For example, PCCS relies heavily on Visual Basic macros. Each of those macros is essentially a “program”. What is the guidance for documenting those macros? None was observed.

  - Comment 2 - An observation common to the WCS and to PCCS spreadsheet SQA plans is a lack of practical guidance regarding how some of the language in the plan is implemented for spreadsheets

  - Comment 3 - The Plan says “no functional analysis will be done”[13]. Functional analysis (testing of accuracy of model output) MUST be conducted periodically to check the accuracy of the calculations and program logic. This is especially true when users can change fundamental aspect of the program (as is the case with PCCS).

- Levels D and E: Liquid Waste Planning Software Quality Assurance Plan; B-SQP-H-00060; Revision 1; March 12, 2009. This plan applies to all software developed or used other than level “B” or higher (e.g., not to be used for safety software).

  - Comment 1 - This Plan, as noted in the other plans, includes some reasonable “language” regarding SQA, but does not provide sufficient guidance for practical use by model owners.

  - Comment 2 - This Plan does not reference ANSI/ANS-10.4-2008, which is the relevant standard for the types of software covered in this Plan. Therefore, key elements of adequate SQA noted in 10.4-2008 are left out of the Plan.

[12] See B-SQP-H-0041, page 10 of 11
[13] See B-SQP-S-00006, page 7 of 16

Topical area: Documentation of assumptions used in development of software

Analysis: As mentioned during the example using SpaceMan Plus™, the documentation of engineering analyses and assumptions is very good. However, there are a number of shortcomings regarding the documentation of assumptions within the spreadsheets and software itself.

Topical area: Documentation of sources of data used in the model, including traceability of information to accepted reference standards when appropriate

Analysis: The particular standards (e.g. thermodynamic data, molecular weights, radioactive decay constants, etc.) are not documented consistently across the models. In some cases, it is not evident where data comes from, and it may be very difficult to go "back in time" to determine the source of constants that are hard-coded into either spreadsheets or programs. SRS needs to consistently document sources of data and constants across all models. For spreadsheet models, a good process is to use comments within the cells (for a positive example, see how the sludge washing spreadsheets are implementing this approach). Also, the team would recommend that a new "material properties database" be constructed to ensure data used in all calculations are drawn from the same source[14]. In addition, SRS needs to adopt the best available standards for material properties (see discussion of NNDC earlier) and provide documentation as to the source of those standards (a traceable path).

Topical area: Documentation of program variables, i.e. the use of a data element dictionary

Analysis: There was no evidence of a data element dictionary common to all modeling platforms. Therefore, porting information from one model to another requires human intervention to interpret what the data mean and how to input/export information so that it can be used in other models. This makes the model update process both slower and vulnerable to various types of human error.

Topical area: Documentation of the data management process

Analysis: The general data management process can be greatly improved. Simply using a database for information that is read into SpaceMan Plus™ would greatly improve the data management process.

Topical area: Provision of user's manuals and/or technical manuals as appropriate

Analysis: None of the SQA plans specifically say that a "user's manual" is required for the models. That is simply not the case. The process by which information flows through the

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[14] A good starting point for this database is the SpaceMan Plus ™ Assumptions List mentioned earlier in this section.

modeling system is kept in a select few experts "heads", thereby making the training of new personnel (or implementing software to incorporate expert logic) very difficult.

Verification and Validation (V&V)

Topical area: Ensuring program logic is accurate and accomplishes the desired task

Analysis: Linked spreadsheets are very difficulty to verify/validate. Mention is made in the various SQA plans that there are "test plans" to verify model accuracy. However, the users have access to the source code, spreadsheets, and macros. The user could introduce errors simply by referencing a wrong cell, putting a data element out-of-bounds, or deleting a row or column. The "static" test plans alluded to in the SQA plans would not catch these logic errors. There needs to be an ongoing, and automated (hard coded), process for logic error testing.

Topical area: Performing tests to ensure data calculations and output are accurate

Analysis: As mentioned above, linked spreadsheets are very difficulty to verify/validate. The complexity of the spreadsheet (and the used of embedded macros) means that it is very difficult to figure out if the calculations are correct or accurate. Also, there was no mention of planning for data quality analysis using statistical quality control checks. For example, no provision was mentioned for trending of key parameters to check whether errors or present.

- Provisions for verification and validation of calculations and program logic
  - Use "check data" input sets to make sure no spreadsheet lines have been deleted or critical formulas have been changed
  - Walk through (stepwise) the macros that are used and/or write output files with intermediate calculations to prove that they are done correctly
  -
- Archiving of input and output data sets should be conducted so that forensic examination can be conducted if a significant error occurs

Topical Area: Performing tests to gauge what happens if erroneous/false/accidental data is input into the software. For example: Are warning flags or error checks used?

Analysis: Error checking is generally not embedded in cells. For example, a logic strategy could be used that says: "if this occurs, then set an error flag and tell the user". Some of this error checking logic occurs in some spreadsheets, but there should be a much wider use of this technique.

Topical area: Revision control – Is there a good process for updating the software based on new information, new software, or new needs the software must perform

Analysis: Generally, anyone with access to the software can change the underlying software/spreadsheet calculations. Changes to the input or output data can be performed by anyone that has access to the spreadsheet or the software. There is essentially no "revision" control with the possible exception of PCCS.

Crosscutting Observations and Recommendations:

It would be a useful investment for SRS to invite IT professional (knowledgeable in current modeling “best practices” and SQA requirements) to evaluate the existing models and provide a list of items that can be improved, and a detailed strategy/explanation on how to improve those items. In addition, a “first cut” evaluation of how to improve SQA should be conducted by site personnel to improve the data management process. For example, consider the following:

- Locking down certain spreadsheet cells/columns so that unintentional (or intentional) model errors can not be introduced. This would limit the potential for users to inadvertently change the formulas and thereby generate erroneous data

- Consider implementing error checking within the spreadsheet itself

- Consider archiving Excel files based on changes on some reasonable basis. For example, archive and maintain the data sets at the end of the day and use a unique filename or identifier for that data set or file. Another approach would be to write the data from the spreadsheets (both the data inputs and calculated values) into a database for data archive purposes

- Access to the software code/calculations should be restricted to only those with a need, and the knowledge, to make changes

- Use of drop-down or check box menus for data entry should be used. This would reduce the possibility of introducing human-caused error in the data input process.

- Use “named values” for calculations within Excel instead of cell references when possible. The enormous length of calculation being done within certain cells (greater than 1000) characters, not with data names but cell references makes verification of data calculations and data flow very difficult

- Need to note the version of Excel in which the spreadsheets are used, and note on what Operating System (OS) the version of Excel is used.

- There are many Visual Basic (VB) macros in the various spreadsheets. However, there appeared to be no documentation (other than within the code of the macro itself or the name of the macro) regarding what those macros do. This is especially problematic for Level B software. There are 12 Macros in “WCS 1.5 Revision”. There should a separate discussion/explanation what those macros are doing. Also, any user has access to not only changing the Excel cell values and cell calculation, but also has access to the VB code and could change the program.

- As a short-term easy fix, use a database to store inputs/outputs from SpaceMan Plus^{TM}. This would allow both SpaceMan Plus^{TM} and COREsim^{TM} to read in files efficiently, and would ensure that both models start with the same data. SRS should consult with software professionals on how best develop the database. There is a great likelihood that experienced software developers or modelers could improve the efficiency of data management.

- SRS should port SpaceMan Plus^{TM} to another (supported) version of Basic, and change the routine that calculates 48 weeks for a year instead of the appropriate 52 weeks per year.

- SRS should encourage the use of COREsim^{TM} (or other discrete-event modeling package) for both SpaceMan Plus^{TM} and the SWS. The SWS logic is not captured in any of the current models. If COREsim^{TM} can be adapted to take over the SWS functions, the modeling program would have the beginnings of a tool that could someday become and true “Overall Liquid Waste Systems” model, rather than of a series of manually derived and linked spreadsheets.