Cementitious Barriers Partnership (CBP): Training and Release of CBP Toolbox Software, Version 1.0 – 13480

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ABSTRACT

The Cementitious Barriers Partnership (CBP) Project is a multi-disciplinary, multi-institutional collaboration supported by the Office of Tank Waste Management within the Office of Environmental Management of U.S. Department of Energy (US DOE). The CBP program has developed a set of integrated tools (based on state-of-the-art models and leaching test methods) that improve understanding and predictions of the long-term hydraulic and chemical performance of cementitious barriers used in nuclear applications. Tools selected for and developed under this program are intended to evaluate and predict the behavior of cementitious barriers used in near-surface engineered waste disposal systems for periods of performance up to or longer than 100 years for operating facilities and longer than 1,000 years for waste management purposes.

CBP software tools were made available to selected DOE Office of Environmental Management and field site users for training and evaluation based on a set of important degradation scenarios, including sulfate ingress/attack and carbonation of cementitious materials. The tools were presented at two-day training workshops held at U.S. National Institute of Standards and Technology (NIST), Savannah River, and Hanford included LeachXS™/ORCHESTRA, STADIUM®, and a CBP-developed GoldSim Dashboard interface. Collectively, these components form the CBP Software ToolBox. The new U.S. Environmental Protection Agency leaching test methods based on the Leaching Environmental Assessment Framework (LEAF) were also presented. The CBP Dashboard uses a custom Dynamic-link library developed by CBP to couple to the LeachXS™/ORCHESTRA and STADIUM® codes to simulate reactive transport and degradation in cementitious materials for selected performance assessment scenarios. The first day of the workshop introduced participants to the software components via presentation materials, and the second day included hands-on tutorial exercises followed by discussions of enhancements desired by participants. Tools were revised based on feedback

obtained during the workshops held from April through June 2012. The resulting improved CBP Software ToolBox, including evaluation versions of and LeachXS™/ORCHESTRA and STADIUM® has been made available to workshop and selected other participants for further assessment.

Inquiries about future workshops and requests for access to the ToolBox software can be made via the CBP website [1].

INTRODUCTION

Cementitious materials are widely used in nuclear applications (e.g., waste disposal systems and nuclear facility components); Fig. 1 provides examples of cementitious barriers used in such applications. Often cement barriers are primary controls to prevent radionuclide releases from nuclear facilities; however, these barriers are typically either ignored or "conservatively" considered in assessments of the potential performance of the effectiveness of the barriers in preventing or limiting contaminant release. Improved test methods and models are needed to better reflect the actual long-term effectiveness of cement materials in nuclear applications. This is a national concern that potentially affects those waste disposal sites that use cementitious waste forms and structures, decontamination and decommissioning activities, service life determination of existing structures, and design of future public and private nuclear facilities.

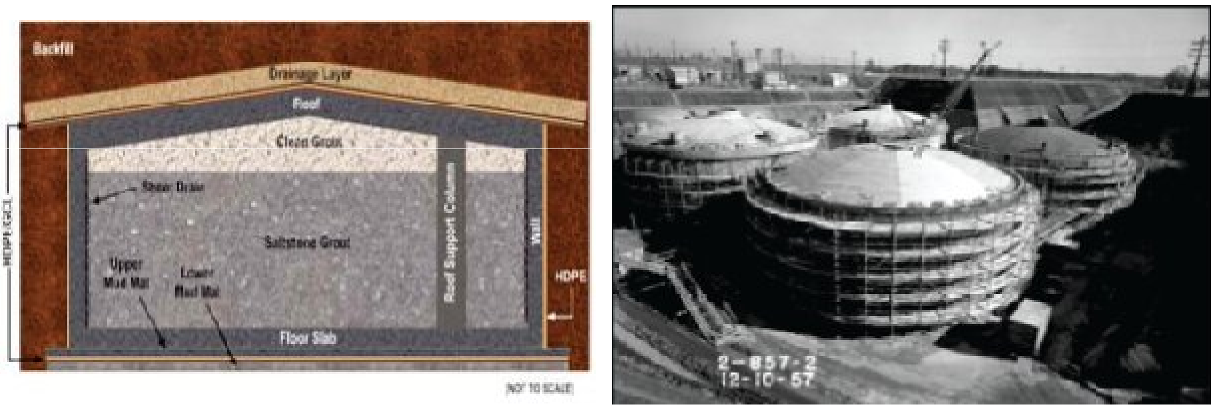


Fig. 1. Examples of Cementitious Barriers: Schematic of Saltstone Waste Form in a Concrete Vault (left) and High-Level Waste Tank under Construction (right) [2]

The Cementitious Barriers Partnership (CBP) Project [3] is a multi-disciplinary, multi-institutional collaborative effort supported by the U.S. Department of Energy (US DOE) Office of Tank Waste Management and managed under a Cooperative Research and Development Agreement (CRADA). The goal of the CBP is to develop the next generation of simulation tools and corroborative experimental methods needed to evaluate the structural, hydraulic and chemical performance of cementitious barriers used in nuclear applications over extended time frames.

The CBP has developed and released a set of integrated tools (using state-of-the-art models and leaching test methods) that improve understanding of the performance of cementitious materials used in nuclear applications. Collectively these tools form the CBP Software ToolBox [3]. Tools selected for and developed under this program have been used to evaluate and predict the behavior and performance of cementitious materials used in near-surface engineered waste disposal systems for periods of performance up to or longer than 100 years for operating facilities and longer than 1,000 years for waste management purposes.

THREE TOOLBOX TRAINING WORKSHOPS

The CBP tools were presented to selected DOE Office of Environmental Management (DOE-EM) and other users at two-day workshops at NIST, Savannah River, and Hanford for training and evaluation using important degradation scenarios, including sulfate ingress/attack and carbonation of cementitious materials. The first day of the training session consisted of a series of presentations (available at [3]) including:

- Performance Assessment Challenges and Model Abstraction
- STADIUM® Software Overview – Durability and Service Life of Concrete Structures
- Leaching Assessment and USEPA Development of the Leaching Environmental Assessment Framework (LEAF)
- Materials Testing and Data Management with LeachXS™ Software
- Technical Basis for Models: Leaching, Sulfate Attack and Carbonation Models
- Introduction to Geochemical Speciation and Scenario Modeling with LeachXS™
- Introduction to the GoldSim Dashboard Interface and Software Communication Bridge

The second day included a series of hands-on training sessions that included:

- Data Management with LeachXS™
- Development of a Geochemical Speciation Model
- Scenario Modeling
- Using the GoldSim Dashboard Interface and CBP Software Communication Bridge
    - Running LeachXS™/ORCHESTRA and STADIUM® from GoldSim
    - Probabilistic Simulations with CBP Models in GoldSim
    - Scenario/Simulation Customization
    - Integrating CBP Models into Larger GoldSim Simulations

MODELING AND SIMULATION TOOLS

The CBP Software Toolbox is a suite of software used to simulate reactive transport in cementitious materials under the influence of selected, important degradation phenomena. The primary software components are LeachXS™/ORCHESTRA, STADIUM® and a GoldSim interface for probabilistic analysis of selected degradation scenarios. The current version supports analysis of leaching, external sulfate attack, including damage mechanics, and carbonation.

LeachXS™/ORCHESTRA and Leaching Environmental Assessment Framework (LEAF)

The Leaching eXpert System (LeachXS™) [4] is an extensive material property and leaching measurements database (Fig. 2) with emphasis on cementitious materials used in USDOE facilities, such as Saltstone (Savannah River), Cast Stone (Hanford), tank closure grouts and barrier concretes [5,6]. Geochemical speciation and chemical reaction/transport modeling are seamlessly integrated into LeachXS™ using the Objects Representing CHEmical Speciation and TRAnsport (ORCHESTRA) code [7].

LeachXS™ functions in the context of reference scenarios that can be simulated along with user-defined changes in materials, material properties and boundary conditions, for each scenario. Reference scenarios include those applicable to laboratory testing and parameter definition (e.g., liquid-solid equilibrium partitioning, percolation column leaching, monolith leaching) and field prediction scenarios. Current field prediction scenarios include (i) monolith leaching under saturated or unsaturated conditions, and with or without oxygen and carbon dioxide ingress and reaction, (ii) sulfate ingress, reaction and damage coupled with major and trace constituent leaching, (iii) diffusion and reaction of multi-layer materials and materials interfaces under saturated and unsaturated conditions, with and without oxygen and carbon dioxide ingress and reaction. Several percolation scenarios will be added during Spring 2013, including dual porosity and flow through cracks with diffusion to/from crack surfaces. Predefined contacting fluids include deionized water, Hanford infiltration, Savannah River infiltration and sea water; the chemistry of individual fluids can also be modified by the user. Predefined geochemical speciation models are available for ordinary Portland cements and concretes, cement and concrete typical of waste management vault construction (i.e., with fly ash and granulated blast furnace slag admixtures) and high-level waste (HLW) tank closure grouts. Multiple thermodynamic databases are available for use for evaluating major and trace constituents and radionuclides. Tools are also included for user development and refinement of geochemical speciation models for individual materials.

Fig. 2. Leaching eXpert System (LeachXS™) (above) with Available Scenarios (below)

One of the foundations of the CBP is an emphasis on integrating modeling and corresponding experimental results. All materials in the environment are typically exposed to water and thus leaching whereby constituents in the solid material (in this case, concrete) are released into the contacting water under a common set of chemical phenomena (e.g., mineral dissolution, desorption, and complexation) and transport (Fig. 3).

The USEPA Leaching Environmental Assessment Framework (LEAF) test methods and assessment methodology [4] provide an integrated and consistent framework for the evaluation of inorganic constituent and radionuclide leaching from wastes and secondary materials [8]. The test methods are also applicable to soils remediation and evaluation of alternative waste forms and treatment process effectiveness.

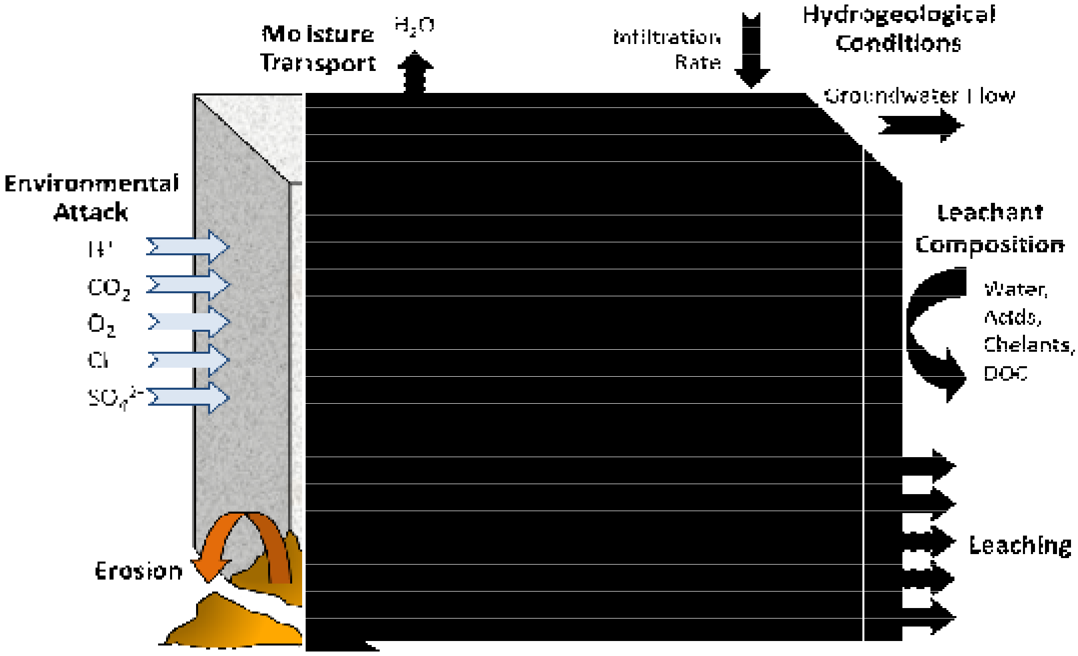


Fig. 3. Physical and Chemical Factors Influencing Leaching [9]

The USEPA LEAF tests have been included in "Test Methods for Evaluating Solid Waste, Physical/Chemical Methods" (SW-846). Material leaching characterization under the LEAF protocol consists of testing using one or more of the following four methods:

- **Method 1313**: Liquid-Solid Partitioning (LSP) as a Function of Eluate pH Using a Parallel Batch Extraction Procedure
- **Method 1314**: Liquid-Solid Partitioning (LSP) as a Function of Liquid-to-Solid Ratio Using an Up-Flow Percolation Column Procedure
- **Method 1315**: Mass Transfer Rates in Monolithic and Compacted Granular Materials Using a Semi-dynamic Tank Leaching Procedure

- **Method 1316**: Liquid-Solid Partitioning (LSP) as a Function of Liquid-to-Solid Ratio Using a Parallel Batch Extraction Procedure

Software for Transport and Degradation in Unsaturated Materials (STADIUM®)

SIMCO Technologies, Inc. developed the Software for Transport and Degradation in Unsaturated Materials (STADIUM®) numerical model to predict the transport of ions and liquids in reactive porous media including degradation of unsaturated concrete structures exposed to chemically aggressive environments [6,10]. STADIUM® has been used to estimate the service life of concrete structures (e.g., roads, bridges, marine, and parking structures) under attack from chloride and sulfate ions. STADIUM® predictions have been confirmed through laboratory test results and field exposure observations. Furthermore, STADIUM® is the only acceptable concrete structure service life prediction software specified by the U.S. government (Unified Facilities Guide Specification 03-31-29, dated August 2012).

STADIUM® calculations are STADIUM® calculations are based on a Sequential Non-Iterative Approach (SNIA) that separates mass transport and chemical reactions [10,11]:

- The transport module accounts for coupled transport of ions and water by solving the Poisson-extended Nernst-Planck system of equations; the latter account for electrical coupling between the ionic species in solution and chemical activity effects. Water content and saturation are calculated using a model based on capillary pressure and accounts for the contribution of vapor and liquid water. Time-dependent boundary conditions can be considered, making possible to simulate wetting and drying cycles.
- After each transport step, the chemical equilibrium module equilibrates concentrations at each node with the phases present. Solid phases may form when species penetrate into the pores of the material or dissolve upon leaching of species in the environment. Variation in solid phases can lead to local variations in porosity that affects the local transport properties of the material (accounted for in the transport module). Dissolution/precipitation and solid solution formation are considered.

STADIUM® and LeachXS™/ORCHESTRA have been used to support Savannah River performance assessments [12]. For example, predictions of external sulfate attack in the Saltstone Disposal Facility (SDF) performance assessment (PA) were based on one-layer STADIUM® simulations of reactive transport using surrogate concrete formulations. The formation of ettringite (an expansive mineral phase) was assumed to coincide with physical damage (e.g., cracking) that impacts the hydraulic conductivity and diffusion coefficient of the cementitious barrier. Additional multi-layer STADIUM® runs have made that have further informed the SDF PA. Additional phenomena important to USDOE PAs are being incorporated into the STADIUM® model (as supported by experimental results) including cracking (sulfate attack) and carbonation / corrosion.

GoldSim Dashboard Interface and CBP Software Communication Bridge

The CBP GoldSim Dashboard Interface (Fig. 4) uses a custom Dynamic-link library (DLL) developed by the CBP [13] to link GoldSim to the STADIUM® and LeachXS™/ORCHESTRA codes. Information exchange with GoldSim occurs through native STADIUM® and LeachXS™/ORCHESTRA input and output text files. The custom DLL receives a list of code inputs from GoldSim, populates these values in one or more input file templates for the external code, runs the external code, retrieves a list of values from output file(s), and returns results to GoldSim for analysis. The specific instructions for communicating with a given code are contained in a "DLL instructions" text file (editable by the user) that is read by the DLL at run-time. Data placement into code input templates and retrieval from code output can be uniquely specified in the DLL instructions file through a variety of options. A row (record) may identified by number, a text label or numeric value within a tolerance in a designated field, or the presence of a string anywhere within the record. Similarly, column location can be specified by column (field) number, or text header or numerical value within a tolerance in a designated row. The intersection of row and column defines the appropriate location. Data may be separated by commas, tabs, or whitespace. The DLL generates a record of input and output values passed through the routine and also manages directories and files for probabilistic runs. Although developed for CBP use, the DLL functionality is generic and can be used to link GoldSim to a wide variety of external codes by composing the appropriate DLL instructions files.

In the CBP ToolBox application, the LeachXS™/ORCHESTRA and STADIUM® codes are called from the GoldSim Dashboard Interface to simulate reactive transport and important degradation phenomena in cementitious materials for selected performance assessment scenarios [14,15]. Each of these codes was originally intended to be run deterministically in a standalone fashion; the GoldSim interface allows the user to vary selected input parameters for predetermined scenarios and run either program probabilistically or perform sensitivity analyses using built-in GoldSim functionality. The GoldSim interface also supports linking CBP scenarios with broader GoldSim simulations including performance assessments.

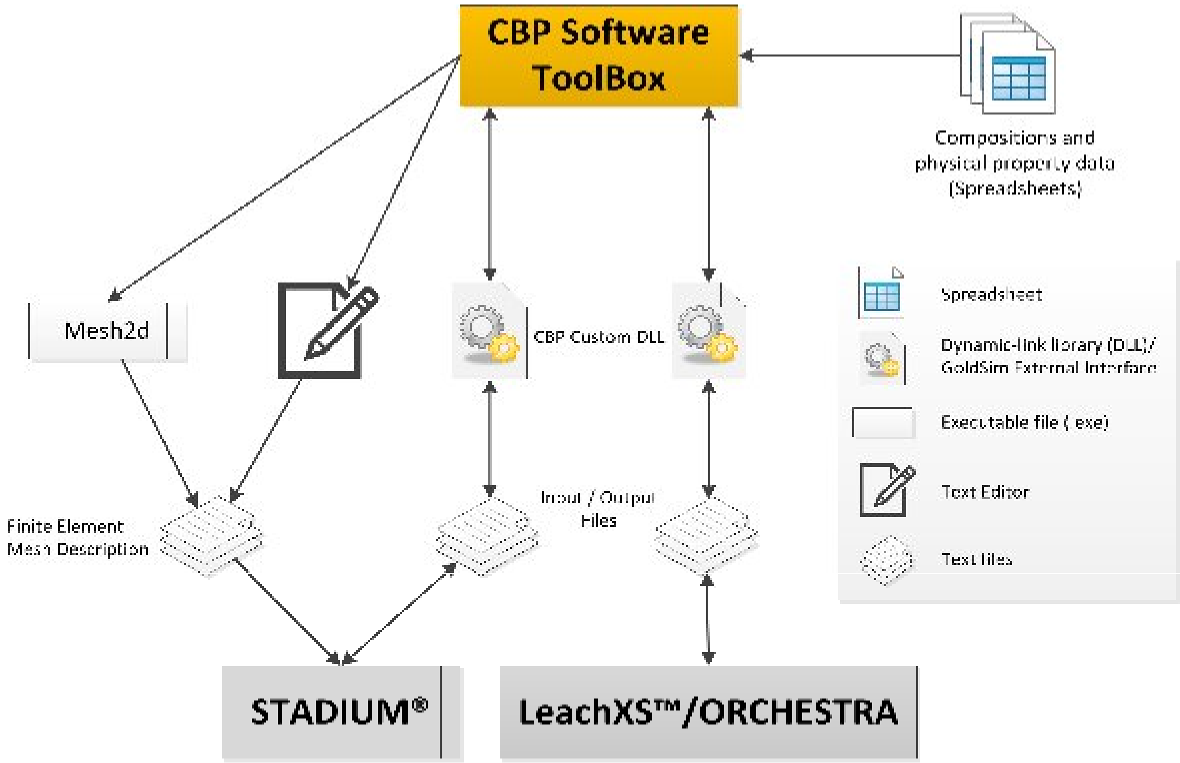


Fig. 4. Schematic Representation of CBP Code Integration Framework [14]

THE DEGRADATION SCENARIOS MODELED IN THE TOOLBOX

Constituent leaching and two important cement degradation phenomena, namely sulfate attack and concrete carbonation, can currently be simulated using the CBP Software ToolBox. These phenomena have the potential to impact current USDOE waste management processes, and an improved ability to characterize and predict the performance of the cement barriers and waste forms used would help inform the performance assessments associated with these practices. Otherwise, assumptions meant to provide conservative predictions must be used in performance assessments and may reduce tank waste options, increase the amount of waste that must be retrieved from HLW tanks or reduce the amount of waste that can be placed in disposal sites in which cementitious materials are used.

For the current CBP Software ToolBox, the available scenarios (Fig. 5) can be summarized as one-dimensional transport through a series of porous layers, at least one of which is composed of a cementitious material. The STADIUM® model as configured for the CBP ToolBox can be used to predict one-dimensional sulfate ingress (and presumed damage) for either a two- or three layer model. The LeachXS™/ORCHESTRA model can be used to predict sulfate attack and corresponding damage (based on continuum mechanics) for a concrete vault exposed to a leachate solution containing a high sulfate ion concentration (representing the waste form). LeachXS™/ORCHESTRA can also be used to predict the carbonation front movement for a single-layer case representing a tank integrity scenario and carbonation and oxidation coupled with leaching of major constituents and radionuclides from waste forms.

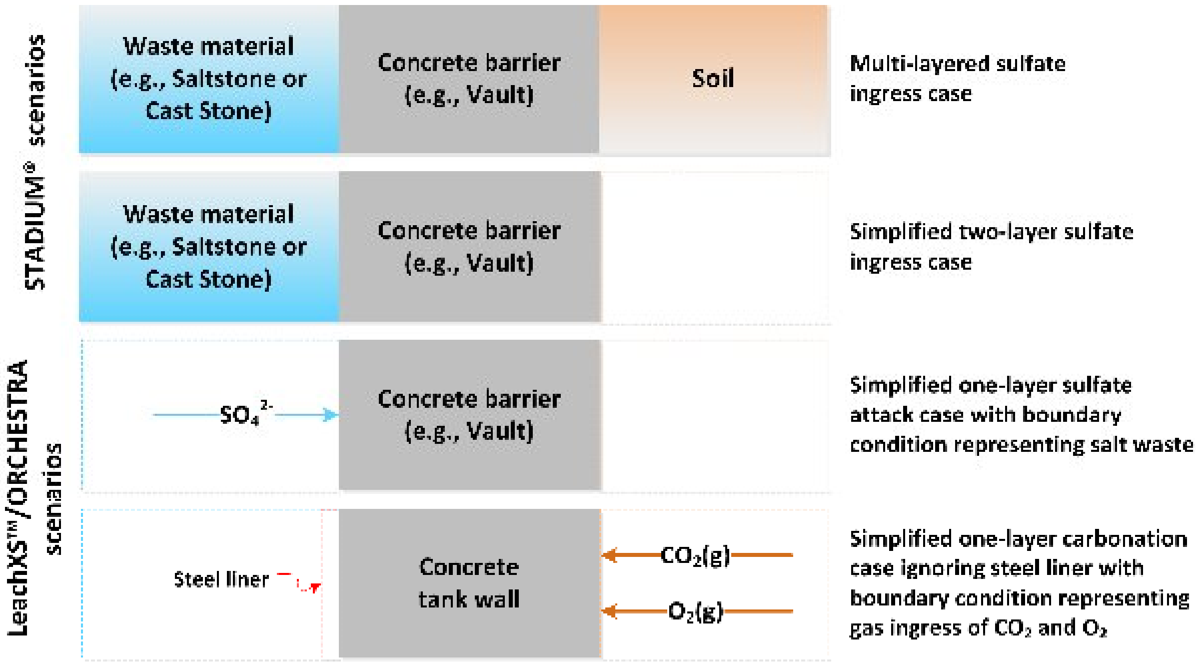


Fig. 5. Representation of CBP Software ToolBox Demonstration Cases

Modeling of External Sulfate Ingress and Attack

External sulfate attack is due to ingress of sulfates in an external solution (e.g., leaching from a high sulfate salt waste) into the concrete barrier pore solution. The sulfate reacts with the cement hydration products that can result in the formation of expansive mineral phases (e.g., gypsum and ettringite) that can fill the pore spaces and eventually cause cracking and loss of strength. The transport properties of the resulting cracked concrete are altered and can promote increased constituent release and migration from the concrete barrier.

Either STADIUM® or LeachXS™/ORCHESTRA can be used to model the potential impact of high sulfate waste in contact with a concrete barrier. These models have been shown to qualitatively agree with experimental results generated by SIMCO Technologies, Inc. to validate their sulfate ingress predictions [16]. The two models have different capabilities that help complement each other. STADIUM® is typically used for service life prediction of large, concrete structures and is concerned with bulk species. LeachXS™/ORCHESTRA can be used to simulate different contaminant release situations including state-of-the-art experimental procedures (e.g., USEPA Methods 1313 - 1316) used to evaluate performance under well-defined conditions; LeachXS™/ORCHESTRA can simulate both bulk and trace species as well as transport. The chemical and physical model components in both models can be used as part of a larger scale release scenario supporting environmental impact assessments.

Carbonation Modeling

The penetration of gaseous carbon dioxide within partially saturated concrete can initiate a series of carbonation reactions with both dissolved ions and the hydrated cement paste. The carbonation process does not have a negative effect, *per se*, on the physical properties of the cement and can even result in reduced porosity (pore filling) and can help form a protective layer at the surface of the concrete. However, carbonation has been shown to increase leaching of some constituents by altering pH and can potentially have a detrimental effect on reinforced concrete structures by lowering pH to ca. 9 and depassivating embedded steel (e.g., rebar or steel liner) and accelerating corrosion that can result in cracking and increased contaminant release and transport. These are important processes related to HLW tank integrity and closure evaluations. The current CBP Software ToolBox currently provides a simplified LeachXS™/ORCHESTRA model (Fig. 5) of a HLW tank integrity scenario.

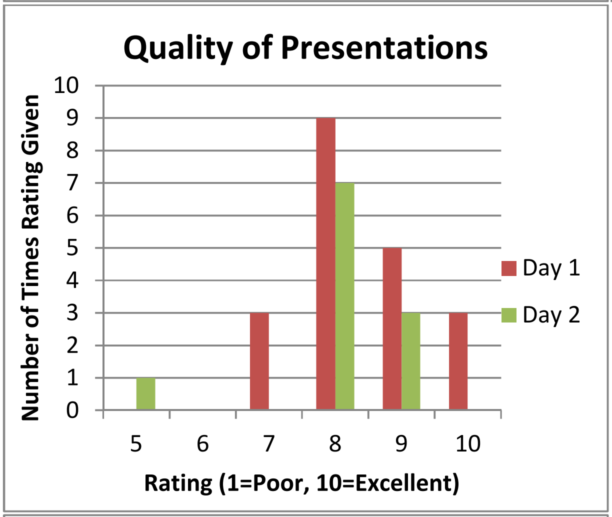
SUMMARY OF WORKSHOP RESULTS

CBP software tools were provided to USDOE and other users for training and evaluation based on a set of important degradation scenarios, including sulfate ingress/attack and carbonation of cementitious materials. On the first day of the workshop, the software components were described in a series of detailed presentations that area available on the CBP website [3], and the second day included hands-on tutorial exercises followed by discussions of enhancements desired by the participants.

Feedback from the training sessions help in April through June 2012 (Fig. 6) was generally positive. The CBP tools have been revised based on feedback obtained during the workshops, and workshop participants have access to the improved CBP Software ToolBox, including evaluation versions of STADIUM® and LeachXS™/ORCHESTRA, for a free-of-cost period. The CBP Software ToolBox has been released for USDOE use; those interested in the ToolBox, including the software components, can inquire via the CBP website [3].


Organization of the Workshop
Number of Times Rating Given
Rating (1=Poor, 10=Excellent)
Day 1
Day 2


Facilities
Number of Times Rating Given
Rating (1=Poor, 10=Excellent)
Day 1
Day 2


Quality of Presentations
Number of Times Rating Given
Rating (1=Poor, 10=Excellent)
Day 1
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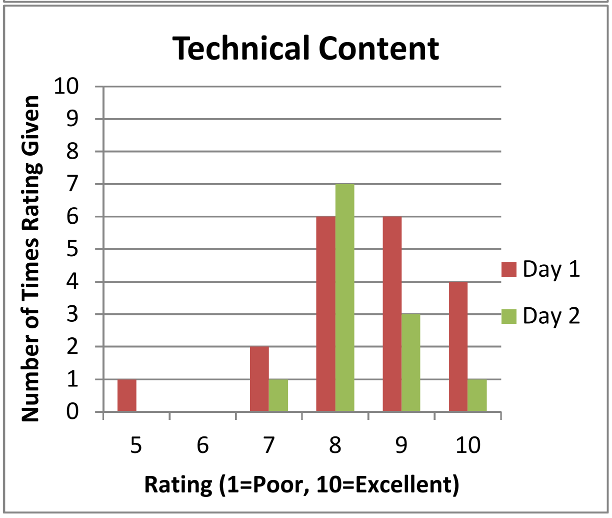
Technical Content
Number of Times Rating Given
Rating (1=Poor, 10=Excellent)
Day 1
Day 2

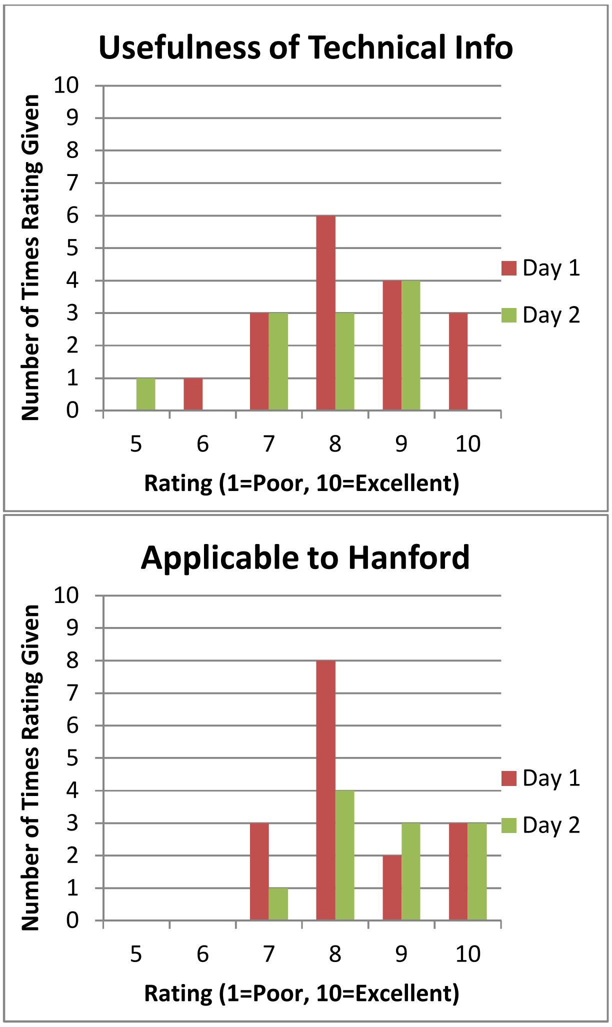

Fig. 6. Feedback from the Hanford Training Workshop (35 Attendees)

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