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Cementitious Barriers Partnership Accomplishments and Relevance to the DOE Complex

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ABSTRACT

The Cementitious Barriers Partnership (CBP) was initiated to reduce risk and uncertainties in the performance assessments that directly impact U.S. Department of Energy (DOE) environmental cleanup and closure programs. The CBP is supported by the DOE Office of Environmental Management (DOE-EM) and has been specifically addressing the following critical EM program needs: (i) the long-term performance of cementitious barriers and materials in nuclear waste disposal facilities and (ii) increased understanding of contaminant transport behavior within cementitious barrier systems to support the development and deployment of adequate closure technologies. To accomplish this, the CBP has two initiatives: 1) an experimental initiative to increase understanding of changes in cementitious materials over long times (> 1000 years) over changing conditions and 2) a modeling initiative to enhance and integrate a set of computational tools validated by laboratory and field experimental data to improve understanding and prediction of the long-term performance of cementitious barriers and waste forms used in nuclear applications.

In FY10, the CBP developed the initial phase of an integrated modeling tool that would serve as a screening tool which could help in making decisions concerning disposal and tank closure. The CBP experimental programs are underway to validate this tool and provide increased understanding of how CM changes over time and under changing conditions. These initial CBP products that will eventually be enhanced are anticipated to reduce the uncertainties of current methodologies for assessing cementitious barrier performance and increase the consistency and transparency of the DOE assessment process. These tools have application to low activity waste forms, high level waste tank closure, D&D and entombment of major nuclear facilities, landfill waste acceptance criteria, and in-situ grouting and immobilization of vadose zone contamination.

This paper summarizes the recent work provided by the CBP to support DOE operations and regulatory compliance and the accomplishments over the past 2 years. Impacts of this work include: 1) a forum for DOE-NRC technical exchange, 2) material characterization to support PA predictions, 3) reducing uncertainty in PA predictions, 4) establishing base case performance to improve PA predictions, and 5) improving understanding and quantification of moisture and contaminant transport used in PAs. Additional CBP accomplishments include: sponsorship of a national test bed workshop to obtain collaboration in establishing the path forward in obtaining actual data to support future predictions on cementitious barrier performance evaluations, and participation in an International Atomic Energy Agency (IAEA) Cooperative Research Project on the use of cementitious barriers for low-level radioactive waste treatment and disposal.

INTRODUCTION

Cementitious barriers are employed to achieve long-term performance for waste disposal units especially in areas of moderate to high rainfall and shallow to moderate ground water tables (Figure 1). Cementitious barriers are also employed in nuclear processing and nuclear energy facilities where current issues are service life extension of existing facilities and performance-based design for future facilities. The National Academies identified developing improved understanding of the long-term ability of cementitious materials to isolate wastes as a high priority gap. Savannah River Site legacy waste operations and closure projects, Hanford Tank Farm closure projects, Saltstone Disposal Facility, Idaho clean-up projects, Oak Ridge remediation and decommissioning, and the West Valley Demonstration Project are examples of end users for technology developed by the CBP.



Figure 1: Engineered Cementitious Barriers at SRS

Evaluations of historic performance assessments (PAs) show that engineered barriers are needed to prevent radionuclide releases into the environment from near-surface nuclear facilities. In the absence of adequate predictive tools, assessments cannot fully incorporate the effectiveness of cement barriers used in containment and/or as part of the waste zone. This limits both the inventory of radionuclides that may be safely disposed of in shallow land disposal and the predicted service life of operating nuclear facilities. The efficacy of cementitious materials as barriers to the release of contaminants affects all disposal sites that use cementitious waste forms and concrete and grout structures, those that are undergoing D&D activities and service life determination of existing radioactive waste facilities, as well as the design of future public and private nuclear facilities.

The Cementitious Barriers Partnership (CBP) was initiated for two primary reasons:

- ◀ To reduce risk and uncertainties in the performance assessments that directly impact U.S. Department of Energy (DOE) environmental cleanup and closure programs.
- ◀ To address the National Research Council of the National Academies recommendations to DOE to address the science and technology gap that long-term ability of cementitious materials to isolate wastes is not demonstrated.

The CBP is a multidisciplinary partnership of DOE, NRC, academia, private sector, and international expertise sponsored by the US DOE Office of Environmental Management. Since knowledge on long-term performance of cementitious barriers needs to be advanced, the CBP is developing a set of computational tools, laboratory and field experimental data, test methods and guidance documents to improve understanding and prediction of the long-term performance of cementitious barriers and waste forms used in nuclear applications. The partners were selected for their existing tools that can enable evaluation of the performance of cementitious barriers but realizing advancements can be made to reduce uncertainties and improve understanding.

The CBP tools have already been proven to reduce the uncertainties of current methodologies for assessing cementitious barrier performance and increase the consistency and transparency of the assessment process. CBP results are being used and anticipated by performance assessment developers and regulatory reviewers as providing key scientific and technical foundations for resolving near-term issues and evaluating future options.

Objectives & Goals

The CBP project is a five-year effort to develop the tools, data bases and resources necessary to evaluate the long-term performance of cementitious barriers to increase the consistency and transparency of the assessment process. This paper describes the CBP's five year goals, how it has met its key early year milestones and how its completed work promises to allow the completion of its full mission. This document also provides clear evidence that as CBP work is completed, it is being immediately made part of the decision making and compliance-response processes that have typically delayed nuclear waste management in the past. The CBP is doing so as the direct result of the combination of technical design clarity, organizational formats and a carefully orchestrated and diverse membership. This document further explains how the tools CBP is developing are not "academic science projects" but rather they emerge as part of a coherent plan to resolve the wide-range of application issues posed by predicting long-term performance of complex engineered waste management barriers.

The CBP five year effort is divided into three phases as shown in Table 1. Phase I scope is complete and Phase II scope is in progress and is about 65% complete into the 3-year program. Initiation of Phase III will begin during FY2011 and is a 2 year program. Overlapping time periods are used to support efforts in Phases I and II, and Phases II and III to achieve project efficiencies. The goal of the multi-institution CBP, after two years of solid progress, is to within the next 3 years provide the key modeling tools and data that provide a technical basis for regulatory acceptance of the performance assessment of DOE facilities, as well as, private nuclear facilities.

Table 1: CBP 5-Year, 3 Phased Scope

Phase	Work to Be Completed	% Complete
I	Phase I included documenting background information, identifying reference cases, testing existing software, and providing input on test bed objectives and design.	100% Complete
II	Phase II includes development/enhancement of simulation tool models, integrating framework, and the user interface in addition to work on uncertainty reduction, and targeted validation experiments.	65% Complete
III	Phase III involves additional work on uncertainty reduction, refinement of simulation tools, and validation of the tools and improved cementitious material data bases.	5% Complete

Technical Approach

The CBP goal is being accomplished through the development of a set of computational tools, experimental data, test methods and peer-reviewed expert guidance that improves the understanding and prediction of the long-term structural, hydraulic, and chemical performance of cementitious barriers and waste forms used in nuclear applications. The following aging and degradation phenomena have been identified as key determinants in the long-term performance of cementitious materials and mechanism-based simulation of these phenomena serve as the foundation for reducing uncertainty in long-term performance: (i) sulfate attack, (ii) chloride corrosion, (iii) carbonation, (iv) primary constituent leaching, (v) oxidation, (vi) crack formation, and (vii) contaminant leaching. Modules for each of these phenomena form the building blocks for tools that provide scenario-based simulations and assessments. Simulation tools currently are being provided as modules for GoldSim-based integration to improve the accuracy and credibility of performance assessments and regulatory evaluation of performance assessments.

The CBP program incorporates both experimental and modeling tasks addressing phenomena occurring at multiple scales from microstructural to field. Activities include 1) hydraulic properties characterization and modeling, 2) matrix phase characterization, evolution, and modeling, 3) contaminant characterization leaching and modeling, 4) model integration, 5) uncertainty characterization and quantification, 6) test beds, and 7) simulation support. Outcomes include test methods, data and data compilations, scenario-specific conceptual models, performance assessment guidance, and computational modeling tools.

The CBP has defined a set of reference cases to provide 1) a common set of system configurations to illustrate the methods and tools developed by the CBP, 2) a common basis for evaluating methodologies for uncertainty characterization, 3) a common set of cases to develop a sufficient set of parameters and changes in parameters as a function of time and changing conditions, 4) a basis for experiments and model validation, and 5) a basis for improving conceptual models and reducing model uncertainties. The reference cases are: 1) a cementitious low activity waste form in a reinforced concrete disposal vault, 2) a concrete vault containing a steel waste tank filled with grout (closed high-level waste tank), and 3) a spent nuclear fuel basin during operation. Additional cases of grouting, decommissioning (D&D) and entombment of a nuclear material processing facility (e.g., canyons) and in-situ grouting of vadose contamination are under development. Each case provides a different set of desired performance characteristics and interfaces between materials and with the environment. Examples of concretes, grout fills, and a cementitious waste form have been identified for the relevant reference case configurations.

“CROSS-CUTTING” INTEGRATION WITH OTHER DOE PROGRAMS

The CBP key technical focus areas are listed in Figure 2 and have far-reaching impacts on other DOE programs that are also tasked to address similar concerns as shown in Table 2. The fact that the CBP and other DOE Programs have “cross-cutting” focus areas highlights the need for a centralized program for cementitious material expertise to promote synergy and add consistency, transparency and prevent redundancy. The following specific needs of various DOE programs are also applicable for benefiting from the implementation of the CBP tools:

- ◀ Cement waste forms as the matrix for defined nuclear waste streams,
- ◀ Cement barriers used to close or entomb contaminated structures (tanks and reactors),
- ◀ Encapsulation methodologies used to achieve containment systems for near surface waste disposal,
- ◀ Disposition pathways for contaminated cementitious structures in decontamination and decommissioning activities,
- ◀ Cementitious structures in newly designed public and private nuclear facilities,
- ◀ Extension of the service life of concrete materials used in existing nuclear facilities, and future facilities.

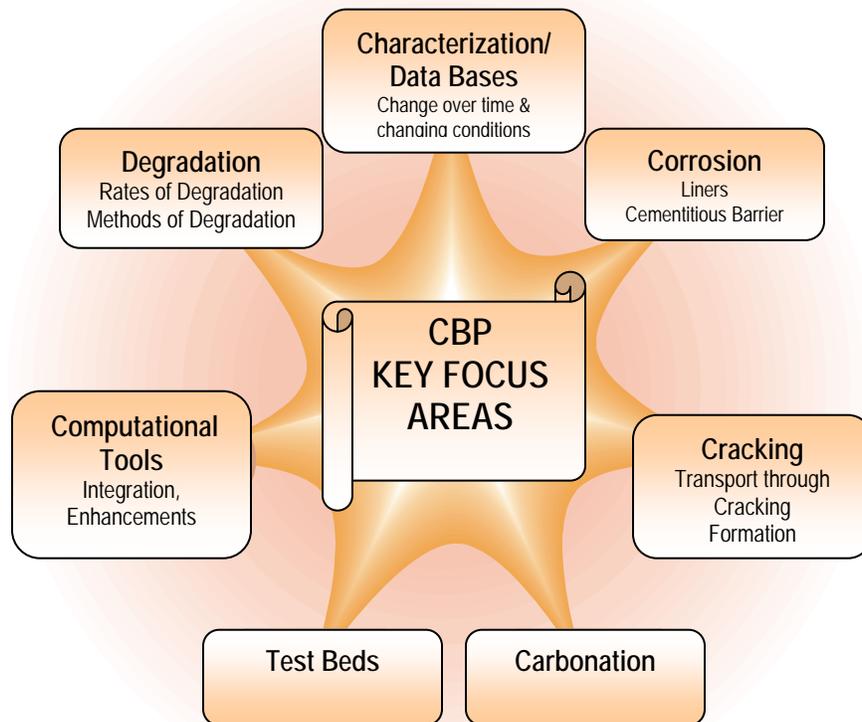


Figure 2: CBP Key Technical Focus Areas

Table 2: “CBP Cross-Cutting” Focus Areas Contrasted with Needs of Other DOE Programs

CBP Focus Area	ASCEM	HLW Tank Closure	LLW Waste Forms	D&D
Modeling Tools	X	X	X	
Test Beds		X	X	X
Characterization/ Data Bases	X	X	X	
Degradation	X	X	X	X
Corrosion	X	X	X	X
Carbonation	X	X		X
Cracking	X	X	X	X

Integration with ASCEM

Starting in FY 2011, CBP simulation codes will also be provided to ASCEM as source term modules for engineered barrier systems in the ASCEM high performance computing platform. Use of more realistic and accurate tools for estimating the impact of these phenomena will improve waste management system designs and reduce orders-of-magnitude in over-conservatism, thus allowing extended service life of structures and improved waste acceptance criteria for near-surface disposal. CBP methodologies and results are providing a readily transferable template for the evaluation of new waste forms currently being considered by DOE-EM (e.g., fluidized bed steam reforming wastes, secondary wastes at various DOE sites, hot isostatic press materials, and separated aluminum streams).

CBP software tools will offer a specialized capability to predict physical and chemical properties of cementitious materials through time and space, and the transport/leaching of contaminant species from cementitious waste forms and through concrete barriers. CBP is focused on phenomena occurring in the near-field, such as coming out of the liquid waste tank barriers shown in Figure 3, whereas, ASCEM will focus on the far-field fate and transport of contaminants. The software modules developed by CBP will become modules within the ASCEM system model for source zone material properties and/or contaminant flux.

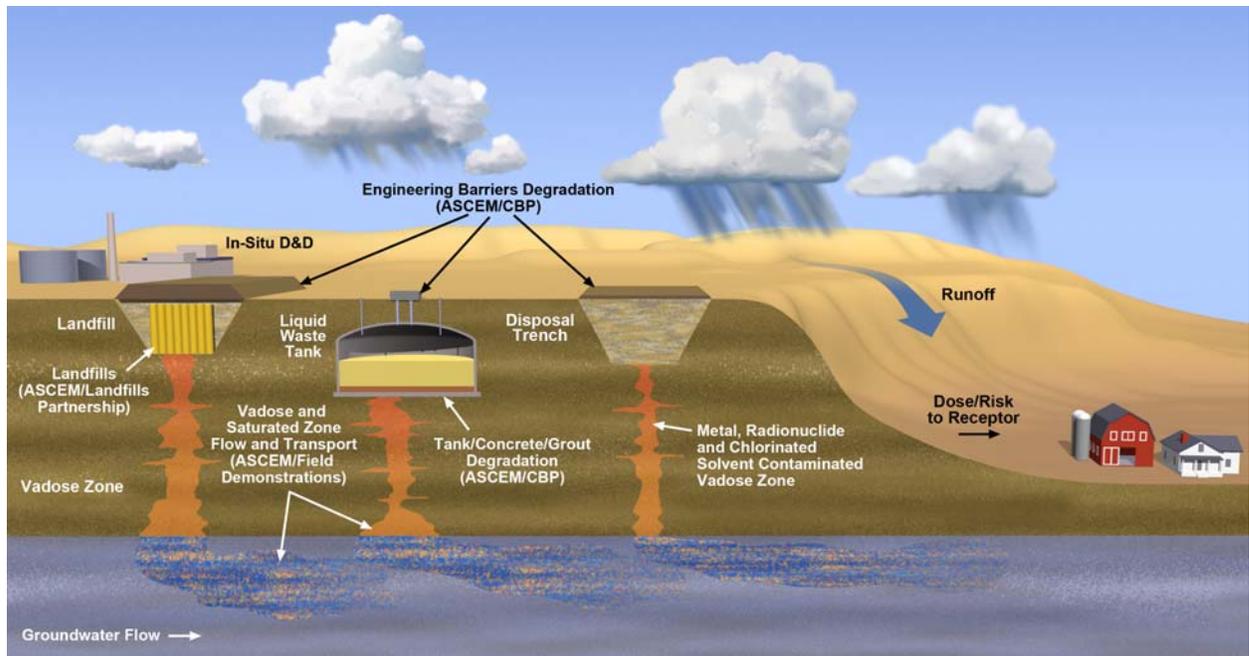


Figure 3: CBP focuses on near-field providing source terms from cementitious barriers/waste forms to the ASCEM High Computing Modeling System focusing on phenomena in the far-field.

ACCOMPLISHMENTS

Since its founding in 2008, the Cementitious Barriers Partnership has produced an enviable record of results documented in many reports, some of which are available at www.cementbarriers.org. The CBP has performed an extensive literature review of the characteristics of cementitious materials known to date. It has hosted several workshops concerning cementitious materials. The relevance to DOE EM mission and programs is briefly discussed in this section, as well as, a detailed listing of accomplishments and modeling tools.

Relevance to the DOE EM Mission and Programs

Specific instances where CBP has shown relevance to the DOE mission and programs include:

- (i) Providing a Forum for DOE-NRC Technical Exchange: The CBP is a successful forum for technical exchanges between DOE and NRC in which issues, needs, and solutions to both 1) legacy waste disposal problems (performance assessments) and 2) next generation waste disposal needs are discussed and resolved. For example, a part of the CBP scope is in response to NRC's perspective on material characterization, data gaps (structure performance, condition, and aging effects), degradation mechanisms and rates, and incorporation of uncertainty into the performance evaluation. The CBP is currently addressing an NRC request 1) to include probabilistic uncertainty

analyses as part of source term calculations in performance assessments, and 2) to develop a performance evaluation screening tool that uses a GoldSim® platform for both DOE and NRC.

- (ii) Providing Material Characterization to Support PA Predictions: A CBP partner, SIMCO Technologies, Inc., provided material characterization (parameters / data) for reference case concretes, grouts, and waste forms for several SRS PAs that currently use the PORFLOW® code to model moisture flow and radionuclide transport over the relevant assessment periods (i.e., 100 years for operating facilities and > 1000 years for disposal facilities). SRNS operations funded these studies and the CBP is funding incorporation of these results in the CBP material property data base, which will be available to the DOE complex. CBP scope also includes determining parameters for aged and degraded materials. Aging and degradation studies are currently in progress by the CBP partners. Several additional surrogate materials are also included in a CBP developed database of characteristics for relevant materials (Figure 4).



Figure 4: Cementitious Material Surrogates used for Property Testing

- (iii) Reducing Uncertainty in PA Predictions: To address NRC and other stakeholder requests to incorporate additional uncertainty analyses in the SRS PAs, the CBP has combined (integrated) GoldSim® probabilistic features with the STADIUM® reactive transport model in a computational tool for the uncertainty analysis of the PORFLOW® code used at SRS. A parallel effort is well underway to integrate GoldSim® uncertainty with output from LeachXS™/ORCHESTRA to support the SRS PAs, with initial demonstration cases completed. This methodology for evaluating uncertainty can directly or indirectly support the ASCEM effort and NRC screening evaluations of waste disposal site performance. A Vanderbilt University PhD thesis, completed in July of 2010, has made foundational advances in the area of uncertainty. Results from SIMCO, another CBP partner, resolved that sulfate attack is not a credible failure mechanism for salt-based wastefoms.

- (iv) Establishing Base Case Performance to Improve PA Predictions: NIST, a CBP partner, is chartered with developing the THAMES hydration-microstructural development model that is needed to enhance earlier NIST models. THAMES is being developed to address the CBP need to dramatically improve predictions of the microstructure of aging cementitious materials, i.e., base case evaluations, and thus functions as a computational microprobe tool for cementitious materials.
- (v) Advancing Understanding and Quantification of Moisture and Contaminant Transport for Engineered Barriers in PAs: Programs to evaluate the effects of cracks on transport of moisture, gas and contaminants through dual porosity materials / structures (cracked concrete) have been initiated at SRNL and CRESPI/VU. Vanderbilt University, SRNL with postdoctoral support from the University of South Carolina are currently working on physical property – microstructural relationships.

Detailed List of Accomplishments

The CBP has accomplished much despite the reduced funding in its two years of operation. This section highlights a few of the significant CBP accomplishments:

- (i) Established the Baseline for Identifying R&D Needs Applicable to LLW Disposal Sites (Ref. CBP-TR- 2009-001) – The CBP issued a state-of-the-art report on cementitious barrier aging, deterioration, reactive transport modeling, uncertainty analysis.
- (ii) Documented the Use of and Need for Cementitious Barriers (CB) in the DOE Complex (Ref. CBP-TR- 2009-002) – Cementitious barriers are employed to extend the performance for waste disposal units especially in areas of moderate to high rainfall and shallow to moderate ground water tables. The CBP issued a report that documented the need for these barriers in the DOE Complex.
- (iii) Provided a Roadmap for Development Work to Enhance Software that Models Aspects of Cementitious Barrier Performance (Ref. CBP-TR-2009-003) – The CBP issued a report in which the objective was to describe: 1) the current status of the candidate software, and 2) the computational concept for the CBP integrating platform in order to provide a roadmap for the development work in future tasks.
- (iv) Sponsored a Test Bed Workshop to Provide Data to Validate Performance Modeling (Ref. CBP-TR-2010-004, draft) – The CBP sponsored a test bed workshop in July 2009 in Salt Lake City, Utah for cementitious materials. The workshop served as a forum to discuss needs, experience and design related to test beds. A report that summarizes the workshop and lays out plans to obtain future data from test beds to support and validate performance modeling is currently in draft.
- (v) Established a Representative Set of Cementitious Materials that are Applicable to the DOE Complex (Ref. CBP-TR-2010-006) – The CBP issued a report that defined a set of reference cases to provide the following functions: (i) a common

- set of system configurations to illustrate the methods and tools developed by the CBP, (ii) a common basis for evaluating methodology for uncertainty characterization, (iii) a common set of cases to develop a complete set of parameter and changes in parameters as a function of time and changing conditions, and (iv) a basis for experiments and model validation, and (v) a basis for improving conceptual models and reducing model uncertainties. These reference cases include the following two reference disposal units and a reference storage unit: (i) a cementitious low activity waste form in a reinforced concrete disposal vault, (ii) a concrete vault containing a steel high-level waste tank filled with grout (closed high-level waste tank), and (iii) a spent nuclear fuel basin during operation. Each case provides a different set of desired performance characteristics and interfaces between materials and with the environment. Examples of concretes, grout fills and a cementitious waste form are identified for the relevant reference case configurations.
- (vi) Developed a Dynamic-link Library (DLL) to link external codes (e.g., STADIUM and LeachXS/ORCHESTRA) to the GoldSim integration program (Ref. CBP-TR-2010-009-2, Rev. 0) – The overall concept behind this development is to use GoldSim as top level modeling software with interfaces to external codes for specific calculations. The DLL that performs the linking function is designed to take a list of code inputs from GoldSim, create an input file for the external application, run the external code, and return a list of outputs read from files created by the external application back to GoldSim. GoldSim is the probabilistic modeling software preferred by the DOE-EM Performance Assessment community.
 - (vii) Demonstrated the Capabilities of Partner Software on Prototype Case for CBP (Ref. CBP-TR- 2010-007, C1-C3) – Each of the CBP partners demonstrated their software on CBP reference cases documented in CBP-TR-2010-006 and using material and conditions associated with a salt-based waste form. Each of the partners documented their respective software capabilities in a separate report which provided meaningful and useful ways to simplify the problem and assist engineers and scientists doing the performance assessment of the waste disposal facilities.
 - (viii) Provided PA Support Work on Cementitious Material Degradation (CBP-TR-2010-013-01). The CBP has provided an enhanced understanding of sulfate attack on concrete barriers of salt-based waste forms and conveyed key technical insights to site contractors for incorporation into the PA maintenance program.

These reports are available at www.cementbarriers.org

CONCLUSIONS

The CBP has made a significant impact in reducing risk and uncertainties in the performance assessments that directly impact U.S. Department of Energy (DOE) environmental cleanup and closure programs. The CBP has developed the initial phase of an integrated modeling tool that would serve as a screening tool. The initial CBP products are anticipated to reduce the uncertainties of current methodologies for assessing cementitious barrier performance and increasing the consistency and transparency of the DOE assessment process. This CBP integrated tool will predict the hydraulic properties and chemical stability of the radionuclides and cement matrix phases and release fluxes of constituents, in response to variable boundary conditions. The CBP is reducing the uncertainty by coupling multi-scale and multi-physics processes, including physical-chemical evolution and transport phenomena applied to heterogeneous materials with changing boundary conditions. The CBP is characterizing, quantifying and effectively communicating the principal uncertainties. In addition, the CBP experimental program has been designed to provide test data to support chemical and physical degradation mechanisms for cementitious barriers. These tools have application to low activity waste forms, high level waste tank closure, D&D and entombment of major nuclear facilities, landfill waste acceptance criteria, and in-situ grouting and immobilization of vadose zone contamination.

The CBP, in its 2 year existence, has already provided: 1) a forum for DOE-NRC technical exchange, 2) material characterization to support PA predictions, 3) uncertainty reduction in PA predictions, 4) base case performance to improve PA predictions, and 5) improvement in understanding and quantification of moisture and contaminant transport used in PAs. Additional CBP accomplishments include: sponsorship of a national test bed workshop to obtain collaboration in establishing the path forward in obtaining actual data to support future predictions on cementitious barrier performance evaluations, and participation in an International Atomic Energy Agency (IAEA) Cooperative Research Project on the use of cementitious barriers for low-level radioactive waste treatment and disposal.