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Partnership for the Development of Next Generation Simulation Tools to Evaluate Cementitious Barriers and Materials Used in Nuclear Applications - 8388

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ABSTRACT

The US DOE has initiated a multidisciplinary cross cutting project to develop a reasonable and credible set of tools to predict the structural, hydraulic and chemical performance of cement barriers used in nuclear applications over extended time frames (e.g., >100 years for operating facilities and > 1000 years for waste management). A partnership that combines DOE, NRC, academia, private sector, and international expertise has been formed to accomplish the project objectives by integrating existing information and realizing advancements where necessary.

The set of simulation tools and data developed under this project will be used to evaluate and predict the behavior of cementitious barriers used in near surface engineered waste disposal systems, e.g., waste forms, containment structures, entombments and environmental remediation, including decontamination and decommissioning (D&D) activities. The simulation tools will also support analysis of structural concrete components of nuclear facilities (spent fuel pools, dry spent fuel storage units, and recycling facilities, e.g., fuel fabrication, separations processes). Simulation parameters will be obtained from prior literature and will be experimentally measured under this project, as necessary, to demonstrate application of the simulation tools for three

prototype applications (waste form in concrete vault, high level waste tank grouting, and spent fuel pool). Test methods and data needs to support use of the simulation tools for future applications will be defined.

This is a national issue that affects all 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. The problem is difficult because it requires projecting conditions and responses over extremely long times. Current performance assessment analyses show that engineered barriers are typically the primary control to prevent the release of radionuclides from nuclear facilities into the environment. In the absence of an adequate predictive tool, assessments cannot fully incorporate the effectiveness of the concrete barriers, and the inventory of radionuclides (especially the long-lived radionuclides) that may be safely disposed of in shallow land disposal and the predicted service life of operating nuclear facilities.

This project is 5 year effort focused on reducing uncertainties associated with current methodologies for assessing cementitious barrier performance and increasing the consistency and transparency of the assessment process. The results of this project will enable improved risk-informed, performance-based decision making, and supports several of the strategic initiatives in the DOE-EM Engineering & Technology Roadmap.

INTRODUCTION

The USDOE identified durability of engineered barriers for radioactive waste treatment and disposal as an area for future technology in 2006. A program to develop scope to address this need was initiated in 2006. A workshop was held in December 2006 to define DOE needs, the state of the art, and the state of practice by DOE-EM [1, 2]. The outcome of the workshop was the formation of a multidisciplinary team, the Cementitious Barriers Partnership (CBP) in early 2007. The CBP consists of members from government (DOE, NRC, and NIST), academia (CRESP/Vanderbilt), and international partners (ECN, SIMCO). The objective of the CBP is to identify and develop tools necessary to address performance of cementitious materials in the near surface low-level waste disposal environment. The partners and organizational structure for this project are shown in Figure 1.

A project plan for a three phase effort over five years was finalized in October 2007. The scope for Phase I (six months) includes documenting background information, identifying reference cases, and testing existing software. Phase I will also provide input on test bed objectives and design. Phase II (three years) involves development of simulation tool models, integrating framework, and the user interface in addition to work on uncertainty reduction, and targeted experiments. Phase III (two years) involves additional work on uncertainty reduction, refinement of simulation tools, and validation of the tools.

BACKGROUND

The Department of Energy Order 435.1-1 requires Performance Assessments (PAs) to be prepared for DOE low-level radioactive waste disposal facilities. The order specifies that a PA should provide reasonable assurance that a low-level waste (LLW) disposal facility will comply with the performance objectives in the Order. According to the Order, calculations of releases from a facility and resultant potential doses should address a 1,000-year period after the facility closes. Cementitious barriers are used or planned for disposal of low level waste disposal at

Idaho Operations Office, Office of River Protection, Richland Operations Office, Savannah River Site, and the West Valley Demonstration Project. Consequently, an in-depth evaluation of mechanisms and uncertainty associated with concrete containments, grout fills, and waste forms performance over long times is required to support complex-wide DOE waste disposal activities.

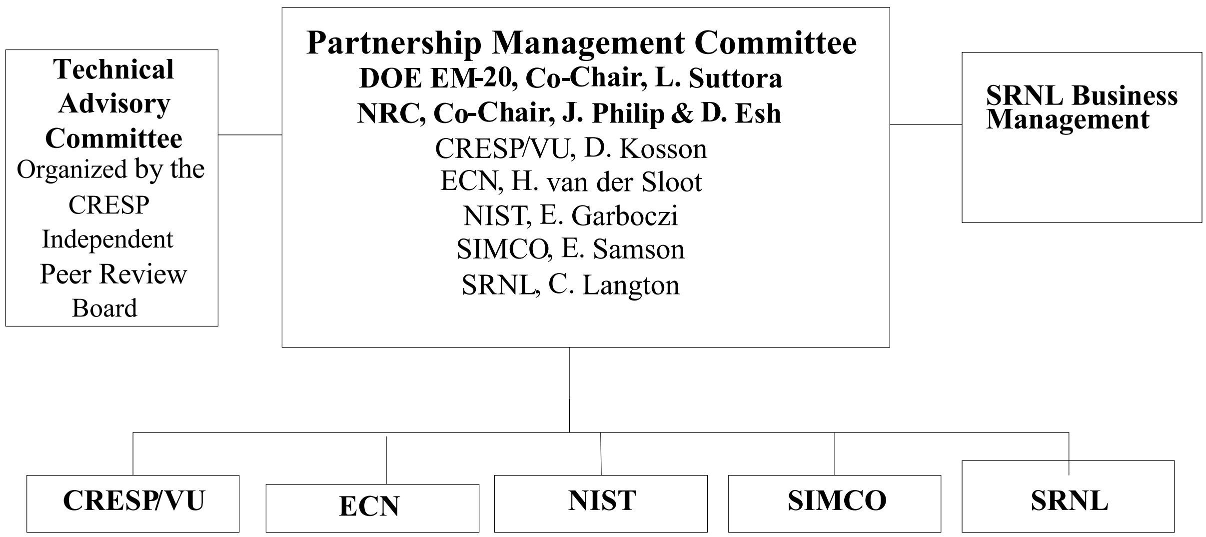

Figure 1. Partnership Organization Chart

Currently, DOE performance assessments for LLW disposal assume that concrete barriers used to control migration of radionuclides into the environment physically degrade to soil-like material spontaneously after 100 to 500 years. The current assumption of a step change from concrete to soil at 100-500 years does not reflect reality and this impacts the calculated release of radionuclides. In addition, bulk properties which are used in the current approach probably do not reflect actual conditions.

Within the PA process, degradation applies solely to the hydraulic properties (permeability) and the degraded cementitious barrier is assumed to maintain its concrete chemical properties. These chemical properties are known to change over time as a function of the water flux (water moving through the barrier).

Cementitious barriers include not only containment structures but also waste forms. Evolution of waste forms and the interaction between waste forms and concrete containments over time has not been extensively studied. Consequently, a high degree of uncertainty is included in the current PA analyses. At the present time, methodology for assessing these uncertainties is not available due to lack of data and models.

Current performance assessment analyses show that engineered barriers are typically the primary control to prevent the release of radionuclides from nuclear facilities into the environment. In the absence of an adequate predictive tool, assessments cannot fully incorporate the effectiveness of the concrete barriers. This limits the inventory of radionuclides (especially the long-lived radionuclides) which can be safely disposed of in shallow land disposal and the predicted service life of operating nuclear facilities. Characterizing the properties and reducing the uncertainty in understanding the behavior of cementitious barriers is necessary to adequately evaluate and improve system designs. A transparent and defensible understanding will allow performance assessments to incorporate realistic behavior of the cementitious barriers as part of engineered and natural systems used to protect human health and the environment. This will enable risk-informed performance-based decisions.

This is a national issue that affects all 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. The problem is difficult because it requires projecting conditions and responses over extremely long times. Uncertainty reductions require coupling multi-scale and multi-physics processes, including physical-chemical evolution and transport phenomena applied to heterogeneous materials with changing boundary conditions. Principal uncertainties need to be characterized, quantified and effectively communicated.

TECHNICAL APPROACH AND DISCUSSION

The CBP identified several areas for advancing the current level of knowledge and practice. One area addresses development of computational architecture to incorporate science-based modeling of the cementitious barriers into an integrated structure that can provide a consistent user interface while accommodating changes in the underlying science, software, and hardware that comprise the overall system model. Other areas include the development of: 1) science-based models that accommodate evolution, coupling, and integration of existing models and 2) experimental programs to (i) reduce uncertainty in the conceptual model of controlling processes and transformation mechanisms, (ii) measure model parameters where literature support is insufficient, and (iii) validate and quantify uncertainties with respect to the integrated approach (Figure 1). Methodology to quantify and reduce uncertainty as consequence of model and data improvements will be incorporated into the simulation tools and overall project. A flow chart for integrating process and mechanism-based modeling with experimentation and uncertainty analysis is illustrated in Figure 2.

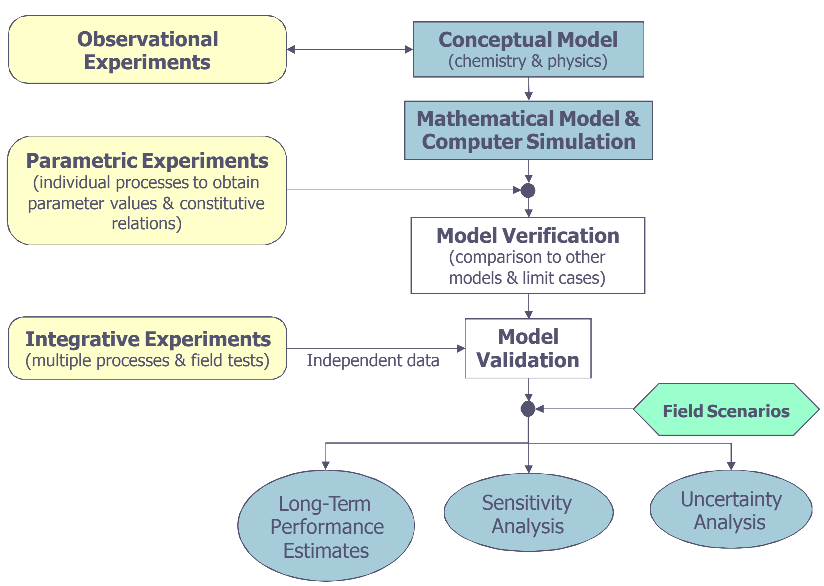

Figure 2. CBP Process and Mechanism-based Modeling and Experimentation.
(Integration of experiments with model development with prototype scenarios occurs throughout the project to reduce uncertainty.)

The fundamental purpose of the architecture, about which a science-based cementitious barriers modeling capability is built, is to provide the most productive problem solving environment possible for both developers and users. This problem solving environment is part of a larger system analysis concept that extends from a graphical user interface (GUI) on an end-user's desktop to tools that capture or implement functionality and behaviors that developers might require. These tools might include security, data provenance, fault tolerance, integration of remote services, and so on.

This architecture fits within the software development concept of a thin client exploiting a rich networked capability. The design will ensure that the architecture is the most enduring aspect of the overall suite of computational capabilities, since it will allow all of its constituent parts to evolve as both hardware and software capabilities evolve over the lifetime of the project. At the same time, the integrating nature of the architecture means that it needs to be designed and implemented correctly the first time, since it will be difficult to change after initial deployment.

The architecture is intended to put effective simulation and monitoring tools into the hands of engineers, operators, managers and regulators to meet the diverse goals of predicting the impact of barrier performance. These tools will incorporate detailed science-based simulations of all components, full process models, and go far beyond incremental improvements to the current analyses and result in significantly improved designs. The intended end-to-end modeling incorporating full-system uncertainty and risk analysis will enable faster design evaluation that can couple from basic science into engineering design and will provide the potential for breakthrough advances in design, performance, cost, and risk.

CBP project is divided into four efforts which are listed below:

1. Develop a platform and structure for integrating the modules required to meet the objectives.
2. Identify, modify or develop phenomenological modules for predicting the required properties and behaviors.
3. Identify and develop an experimental program that complements the computational development of the two efforts above.
4. Develop and integrate an uncertainty methodology that will incorporate the quantitative accuracy of the computational models and project their coupled behavior forward in time with a definable uncertainty.

Each effort will have an individual QA/QC plan and documentation. Model validation will be coordinated with the results of focused experiments and with a parallel task to develop test beds.

A diagram of the architectural concept is shown in Figure 3. Integrating functions, which are listed below, represent the implementation of the architectural concept into a computational framework:

- A central system software architecture that glues the individual components together,
- Data representations so that modules can readily exchange information,
- Process simulation and uncertainty evaluation modules (simulation, experiment, engineering, etc.) with clearly defined information documentation and exchange protocols, and
- Interfaces to the larger world, especially for users and information exchange with external models used in performance assessments.

The remainder of this section will discuss the assimilation of various types of integrating functions into an overall architecture to produce a cementitious barriers model that not only satisfies the requirements of a variety of users, but also accommodates the evolutionary developments that will certainly take place over the lifetime of the project.

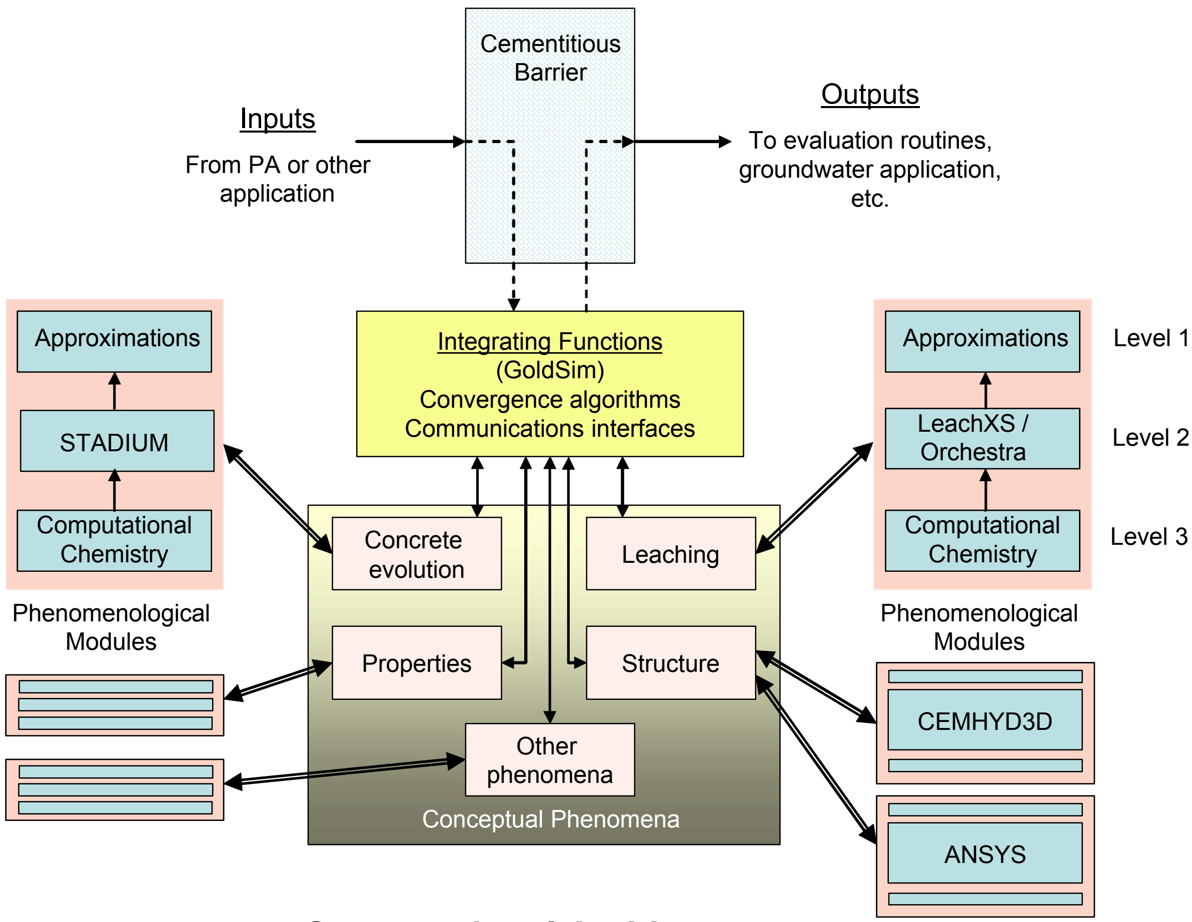

Figure 3. CBP Computational Architecture. (Unlabelled stacks in lower left represent data resources and additional algorithms not yet identified.)

Computational Structure

The overall computational approach is composed of two fundamental functions: (i) a collection of individual modules, each focused on a particular phenomenon that likely affects and is affected by the other modules, and (ii) an integrating framework or backbone through which the individual modules communicate with each other and via which an outside application – perhaps a user interface or an interface to another application – communicates with the cementitious barrier model. As mentioned above, the integrating framework remains consistent throughout the lifetime of the project but is designed to allow the individual modules to evolve over time and to accommodate those changes seamlessly from the user perspective.

A modular approach will be used to develop the set of integrated simulation tools that will predict the hydraulic properties and chemical stability of the radionuclides and cement matrix phases, release fluxes of constituents in response to variable boundary conditions (infiltrating water flux, chemical corrodents known to impact cementitious materials, and events that impact the integrity of the entire structure) over relevant time periods. The purpose of the integrating framework is to embrace this evolutionary behavior and, to the extent possible, avoid reworking of the computational model.

The level of engineering detail needed to execute the tools will be flexible and based on the requirements of the analysis (e.g., scoping assessments, engineering approximations, detailed evaluations). The simulation tools will be developed based on existing capabilities and software, including STADIUM, LeachXS, CEMHYD3D, GoldSim and ANSYS.[1] The objective is to use these modules to ultimately predict the degradation of user-identified cementitious materials used as a barrier due to chemical and physical properties and environmental stresses. Additional modules will likely be added as the science and understanding of cementitious barriers advances.

IMPACT / EXPECTED RESULTS

The resulting set of simulation tools will be used to support:

- DOE and NRC Performance Assessments
- Design of new nuclear facilities and engineered barrier systems
- Development of monitoring and maintenance approaches for extended service life
- Evaluation of existing and new structures
- Development and interpretation of laboratory and field measurements for modeling system calibration and verification/validation.
- Development and updating of NRC guidance documents
- Decommissioning decision making
- Informing stakeholders regarding realistic scenarios and uncertainty

The enhanced cementitious barrier modeling are expected to lead to a more informed assessment of the effectiveness of a variety of near surface waste management and decommissioning options. With more accurate, realistic predictions of performance, additional credit may be taken for containment by these barriers allowing for the possibility of more contaminants with higher radioactivity permitted as part of disposition. The service life predictions for containments are expected to be improved by re-evaluating and reducing conservatism of certain performance assumptions.

The results of this project are expected to support improved risk-informed, performance-based decision making. Additional benefits include: more efficient use of materials and designs, shorter analysis time because of integration of components, shorter review time because of improved transparency, and reduced potential for human error through integration of process steps.

CONCLUSIONS

In 2007 the USDOE formed the Cementitious Barriers Partnership to identify scope for a multidisciplinary cross cutting project to develop a reasonable and credible set of tools to predict the structural, hydraulic and chemical performance of cement barriers used in nuclear applications over extended time frames (e.g., >100 years for operating facilities and > 1000 years

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[1] Certain commercial equipment and/or materials are identified in this report in order to adequately specify the experimental procedure. In no case does such identification imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the equipment and/or materials used are necessarily the best available for the purpose.

for waste management). A project plan was developed which supports several of the strategic initiatives identified as part of the DOE-EM Engineering & Technology Roadmap. Work on the five year project is expected to begin in the second quarter of FY08.

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