Cementitious Barriers Partnership
Project Overview

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Cementitious Barriers Partnership

CBP Training
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Project Need

• Cementitious materials used broadly by DOE-EM to accomplish its mission.
  – **Low-Activity Waste (LAW) and Secondary Waste forms**
    (i.e., Saltstone at SRS, Cast Stone at ORP)
  – **High-Level Waste (HLW) Tank Integrity and Tank Closure requirements**
  – Nuclear power plant concrete structures (e.g., Seabrook Nuclear Power Plant)
  – Used nuclear fuel storage – fuel pools and dry casks (e.g., TMI-2)
  – Facility Decommissioning & Decontamination (D&D) and entombment (P-Reactor at SRS)
    – Alternative waste forms for near surface disposal (i.e., grouted waste forms)
    – **In-situ** grouting for vadose zone remediation

• Considerable technical debate over physical/chemical performance and service life of cement materials in nuclear applications because of absence of modern, phenomenologically-based models and experimental methods that are mutually agreed upon by technical and regulatory communities.
Primary Near-term Applications

- Hanford
  - Single shell tank integrity
  - C-Tank Farm – HLW tank closure assessment
  - Integrated Disposal Area Performance Assessment (PA)
  - Source term from Cast Stone (secondary waste, LAW supplemental treatment)
  - *In-situ* grouting performance

- Savannah River
  - Saltstone Performance
  - Disposal vaults and other concrete facilities

- Nuclear Energy
  - Dry cask storage performance
  - License extensions
Key Questions

• **Waste Forms and Disposal Systems**
  – What is the rate of release for radionuclides and contaminants under a range of scenarios?
  – What is the evolution of system pH?
  – What are the effects of cracking?
  – What is the rate and impact of aging processes (oxidation (Tc-99), carbonation, and leaching)?

• **Structural Systems Performance**
  – What is the service life?
  – What are the impacts of ingress of aggressive species (chloride, sulfate)?
Project Goal

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., up to and >100 years for operating facilities and >1000 years for waste management).

• Mechanistic / Phenomenological Basis
• Parameter Estimation and Measurement
• Boundary Conditions (physical, chemical interfaces)
• Uncertainty Characterization
Project Team Members

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*Project Leadership Team

DOE-EM Project Manager: Pramod Mallick
Technical Strategy / Approach

• **Reference Cases** — provide basis for comparison and demonstration of CBP tools
  – Cementitious waste form in concrete disposal vault with cap
  – Grouted high-level waste (HLW) tank closure
  – Used nuclear fuel pool, dray cask storage (future)
  – Nuclear processing facilities closure / D&D (e.g., canyons)
  – Grouted vadose zone contamination
  – Materials – surrogate low-activity waste (LAW) cementitious waste form, reducing grout, reinforced concrete (historical), reinforced concrete (future)

• **Extension/enhancement of existing tools** — CEMHYD3D/THAMES, STADIUM, LeachXS/ORCHESTRA, GoldSim Performance Assessment (PA) framework

• **Coordinated experimental and computational program**
  – Conceptual model improvement
  – Define test methods and parameter measurements
  – Model validation

→ **CBP Software ToolBox Version 2.0 Release (January 2014)**
Specifications, Properties, and Phenomena for the Evaluation of Performance of Cementitious Barriers
Key Aging Phenomena

Key Phenomena Addressed

- Chloride ingress and corrosion
- Leaching
- Sulfate attack (2011)
- Carbonation (2012)
- Oxidation (2012-2014)
- Cracking (2013-2014)
- Pore structure relationships with mass transfer and hydraulic properties (future)
- Alkali-silica reaction (ASR) (future)

Integration with Conceptual Models

- Coupled phenomena
- Saturated, unsaturated and variable saturation
- Liquid, vapor mass transfer
- System geometry and boundary conditions
CBP Partner Codes and Integration

• Partner Codes provide for scenario development, design evaluation and model parameterization
  ✓ STADIUM – Physical & Hydraulic Performance
  ✓ LeachXS/ORCHESTRA – Chemical Performance & Constituent Release, also coupled with physical properties/damage evolution
  ✓ THAMES – Microstructure Evolution & Properties*

• GoldSim Software ToolBox (CBP Custom DLL) with STADIUM and LeachXS/ORCHESTRA
  ✓ User scenarios developed in Partner Codes
  ✓ Monte Carlo simulations
  ✓ Integration with GoldSim Performance Assessment Models

*Further development on hold, pending available funding.
CBP Software ToolBox—Phase I

Provides tools for Monte Carlo uncertainty assessment and integration with Performance Assessments

- GoldSim
  - Compositions and physical property data
  - Dynamic-link library
  - External Interface

- Mesh2d

- Text files

- STADIUM
  - Structural Service Life

- LeachXS/ORCHESTRA
  - Chemical Evolution and Leaching

Experimental Data
- Methods
- Parameters
- Verification (Lab & Field)
Key Advances Included in CBP Toolbox Version 2.0 – LeachXS/ORCHESTRA

• Simulation basis for additional materials, solutions, water contact modes
  – CEM I (Portland cement), Vault concretes (VCO, VCT), Closure grout (BGM), Salt waste form (AWF)
  – DI water, Hanford infiltration, TCLP, sea water, user defined
  – Batch exchange, intermittent flow, continuous flow

• Additional Scenarios Defined
  – Laboratory cases – batch pH dependence (pE, LS), monolith, percolation column
  – Prediction cases – monolith (saturated, unsaturated, carbonation, sulfate attack), percolation (dual porosity), percolation (cracked materials)
  – Radionuclides using NEA thermodynamics database

• Data Sets
Key Advances Included in CBP Toolbox Version 2.0 – STADIUM

- Chloride Attack module added
- Improved mineral set in Sulfate and Chloride Attack modules
- Changes to allowable mesh size and input parameter values
Key Advances Included in CBP Toolbox Version 2.0 – GoldSim Interface

• Maximum nodes increased from 301 to 501
• GoldSim simulation time is now used to set the LeachXS/ORCHESTRA simulation time
• Improved error trapping and reporting within the DLL interface
• Enhanced graphics using Gnuplot to display model results
  – Plotting by node number in Version 1.0
  – Plotting by position in Version 2.0
  – Concentration vs. position and time (surface plots) available in Version 2.0
Workshop Objectives

• Provide introduction and demonstration to CPB Toolbox Version 2.0
  – LeachXS/ORCHESTRA
  – STADIUM
  – GoldSim Interface for Monte Carlo Simulations

• Selection and Technical Basis/Limitations for Specific Applications

• End-user input for development and application needs
We want your input!

Please send comments to:
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