Cementitious Barriers Partnership
Project Overview

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Cementitious Barriers Partnership

CBP Training
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CBP
Cementitious Barriers Partnership

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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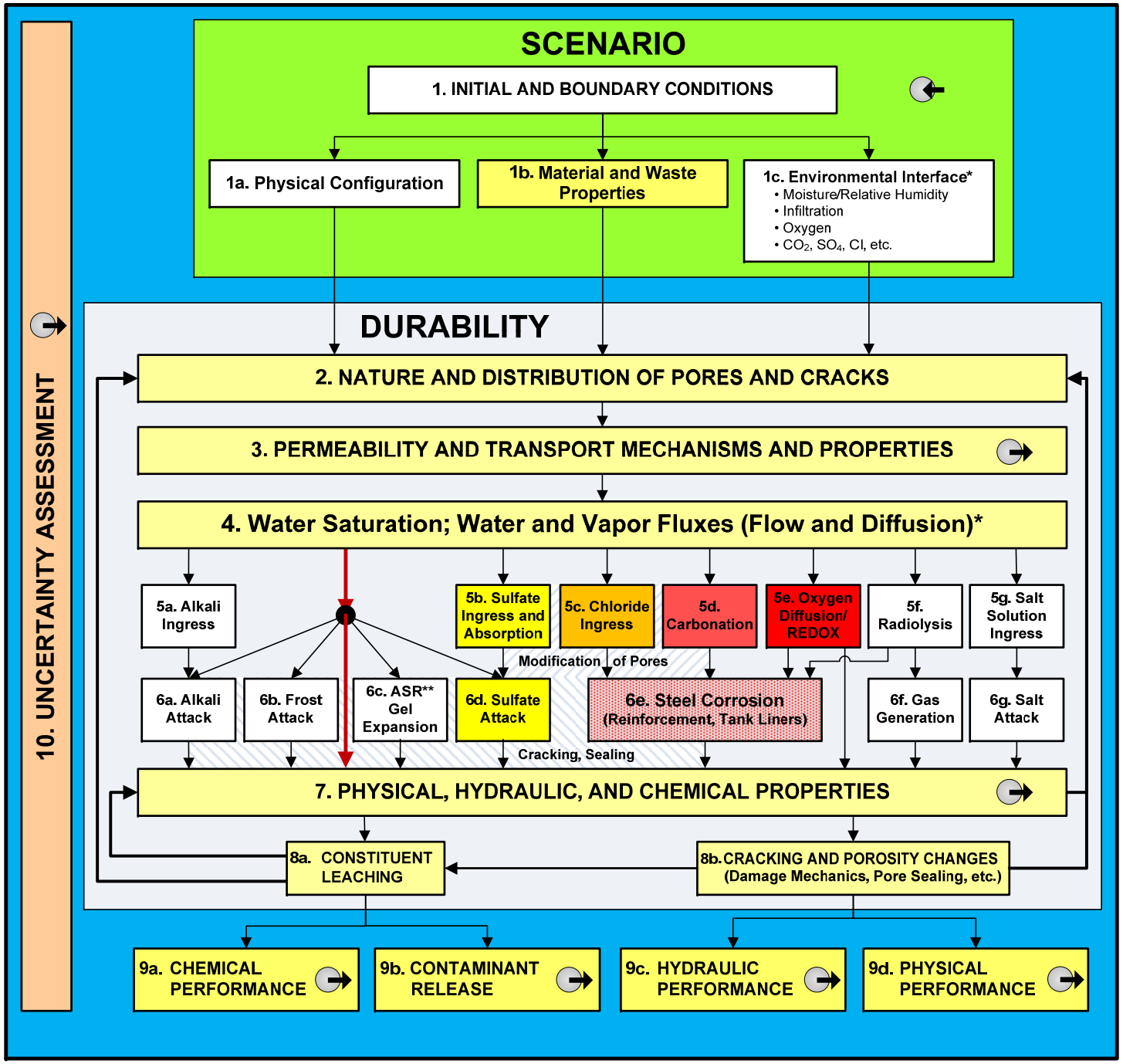
DOE-EM Project Manager: Pramod Mallick

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

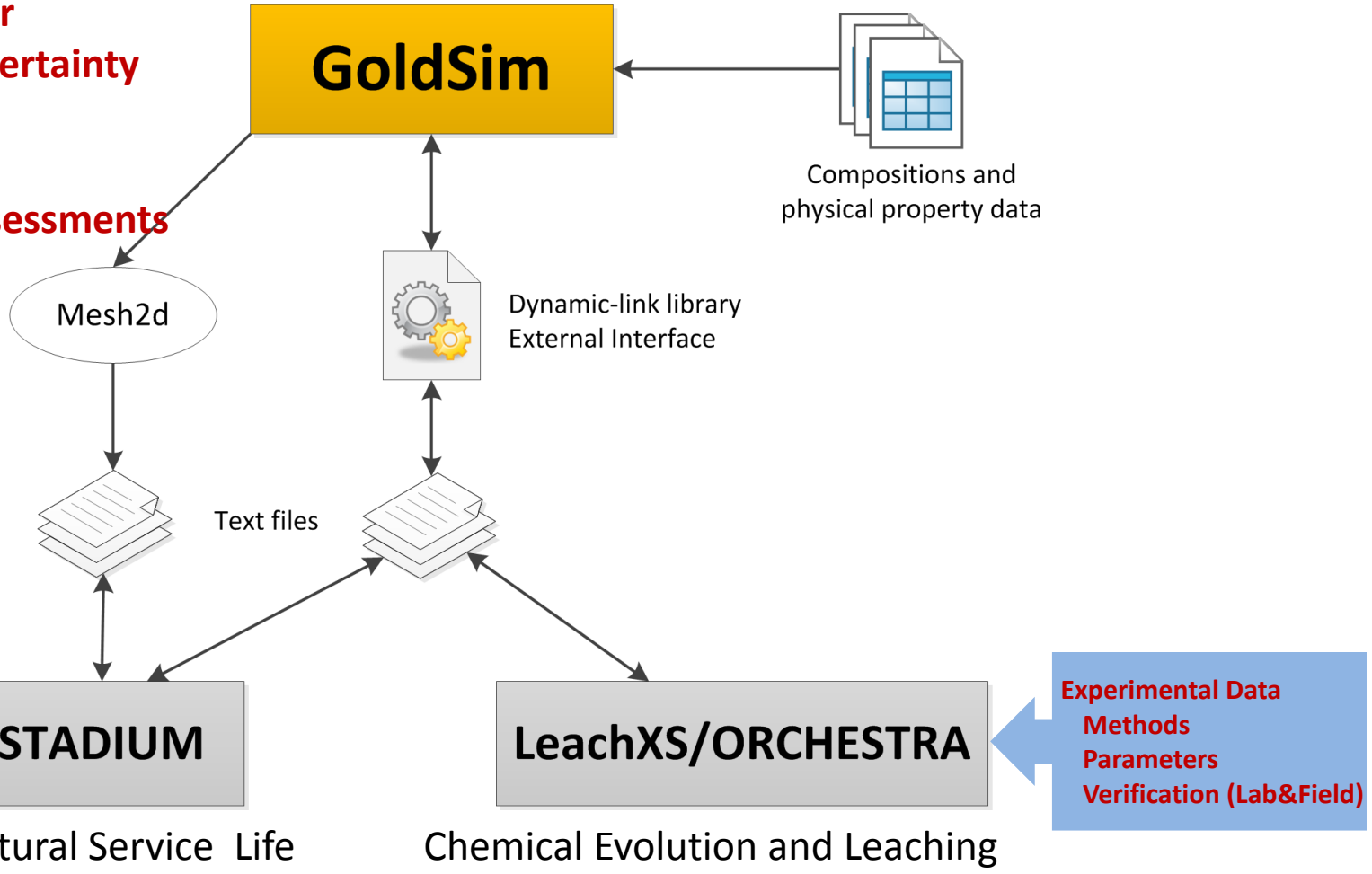
CBP Partner Codes and Integration

- **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

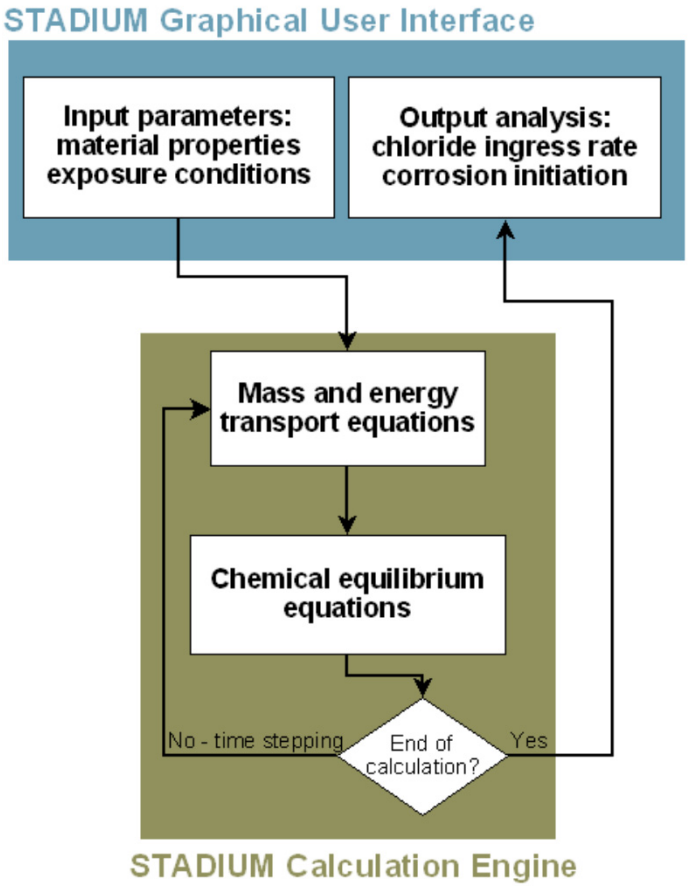


Key Advances Included in CBP Toolbox Version 2.0 – LeachXS/ORCHESTRA

- 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

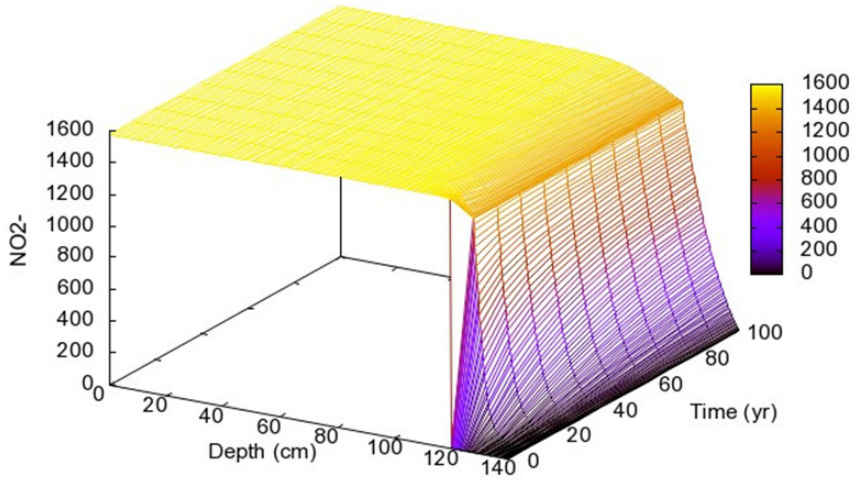
Key Advances Included in CBP Toolbox Version 2.0 – STADIUM

- 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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