Cementitious Barriers Partnership

Project Overview

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CBP
Cementitious Barriers Partnership

Project Need

- Cementitious materials are used broadly by DOE-EM to accomplish its mission
  - Low activity waste forms (i.e., Saltstone at SRS)
  - HLW Tank Integrity (i.e., GAO report) and Tank closure requirements
  - Secondary waste treatment (i.e., ORP-WTP)
  - Used fuel storage – fuel pools and dry casks
  - Facility D&D and entombment
  - Alternative waste forms for near surface disposal (i.e., grouted waste forms)
  - Grouting for vadose zone remediation
- There is considerable technical debate over the physical and chemical performance and service life of cement materials in these applications because of the absence of modern, phenomenologically-based models and experimental methods that are mutually agreed upon by the technical and regulatory communities.
- CBP actively engages leaders in the scientific, regulatory and end-user communities to develop consensus models, test methods and data.

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 >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

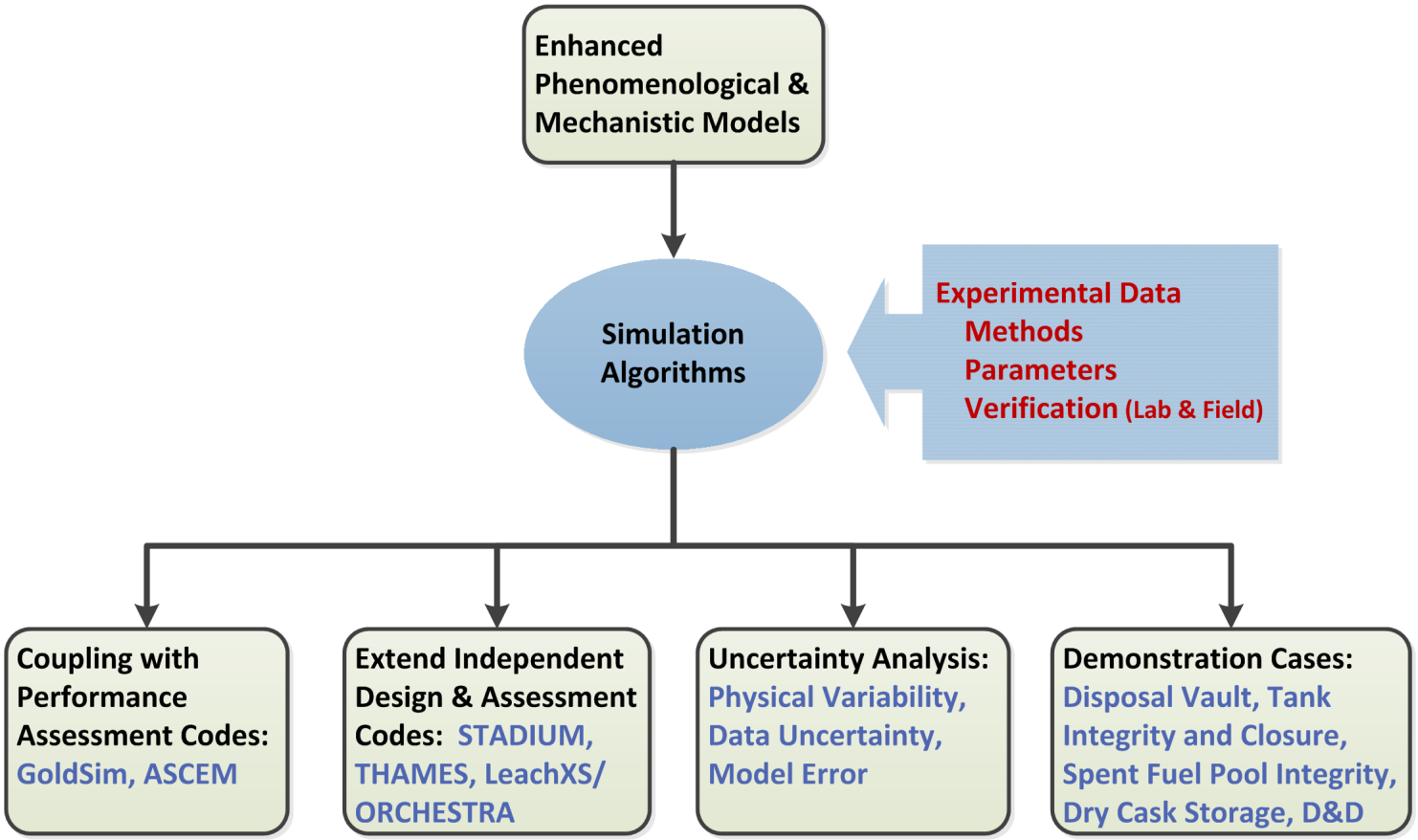
Partnership Members

- Department of Energy – Office of Environmental Management
  - Scenarios & Key Uncertainties
  - Primary end-user
- Nuclear Regulatory Commission
  - Scenarios & Key Uncertainties
  - Primary end-user
- Savannah River National Laboratory
  - PA Interface
  - Model Integration
  - Cracking Scenarios
  - Test Beds
- National Institute of Standards and Technology
  - THAMES – Microstructure Evolution & Properties
- SIMCO
  - STADIUM – Physical & Hydraulic Performance
- Energy Research Centre of the Netherlands (w/ Nuclear Research Group, Hans van der Sloot Consultancy)
  - LeachXS/ORCHESTRA – Chemical Performance & Constituent Release
- Vanderbilt University/CRESP
  - Chemical Performance & Constituent Release (experimental)
  - Uncertainty Analysis Framework
  - Model Integration

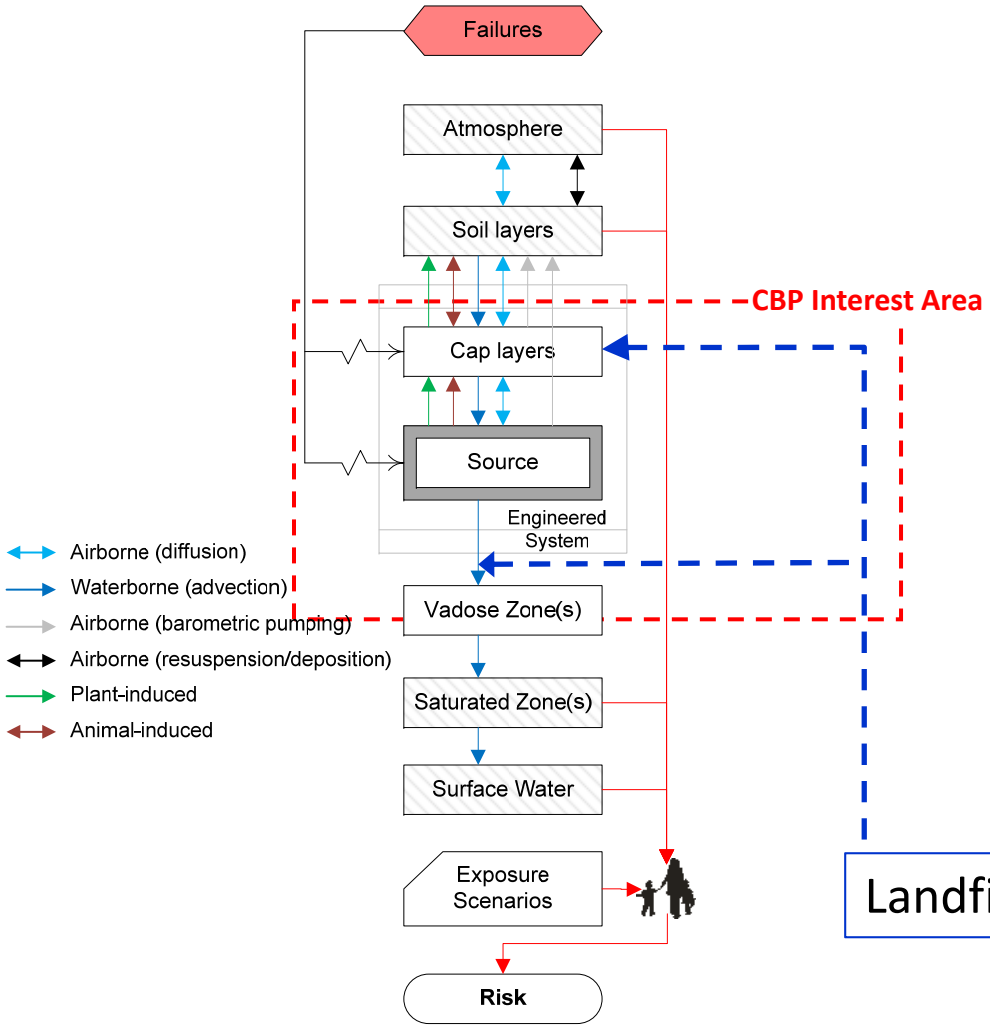
Technical Strategy / Approach

- **Reference Cases – provide basis for comparison and demonstration of tools under development**
  - Cementitious waste form in concrete disposal vault with cap
  - Grouted high level waste tank closure
  - Spent fuel pool
  - Nuclear processing facilities closure / D&D (e.g., canyons)
  - Grouted vadose zone contamination
  - Materials – surrogate LAW cementitious waste form, reducing grout, reinforced concrete (historical), reinforced concrete (future)
- **Extension/enhancement of existing tools –** CEMHYD3D/THAMES, STADIUM, LeachXS/ORCHESTRA, GoldSim PA framework
- **Coordinated experimental and computational program**
  - Conceptual model improvement
  - Define test methods and parameter measurements
  - Model validation

CBP Toolbox Development



Integration of CBP Tools with PAs



CBP Focus:

- Cementitious materials performance as part of engineered system and their interfaces with natural system
- To provide near field source term
- Uncertainty approach being developed to be broadly applicable to PA and design process.

Landfills Partnership (CRESP)

Key Aging Phenomena

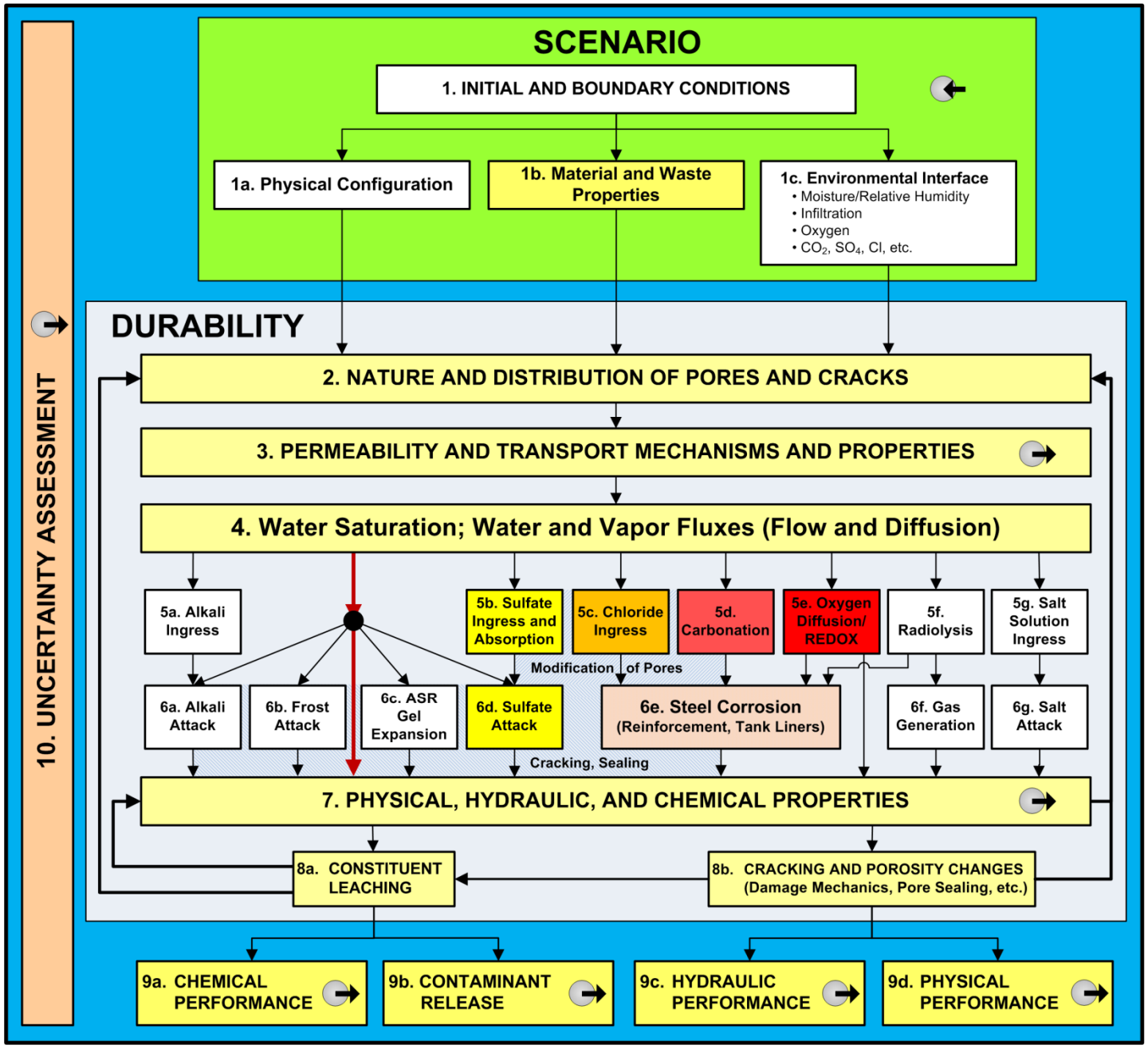
Phenomena

- Chloride ingress & corrosion
- Leaching
- Sulfate attack (2011)
- Carbonation (2012)
- Oxidation (2012)
- Cracking (2013)
- Pore structure relationships with mass transfer and hydraulic properties (?? NIST)

Integration with Conceptual Models

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

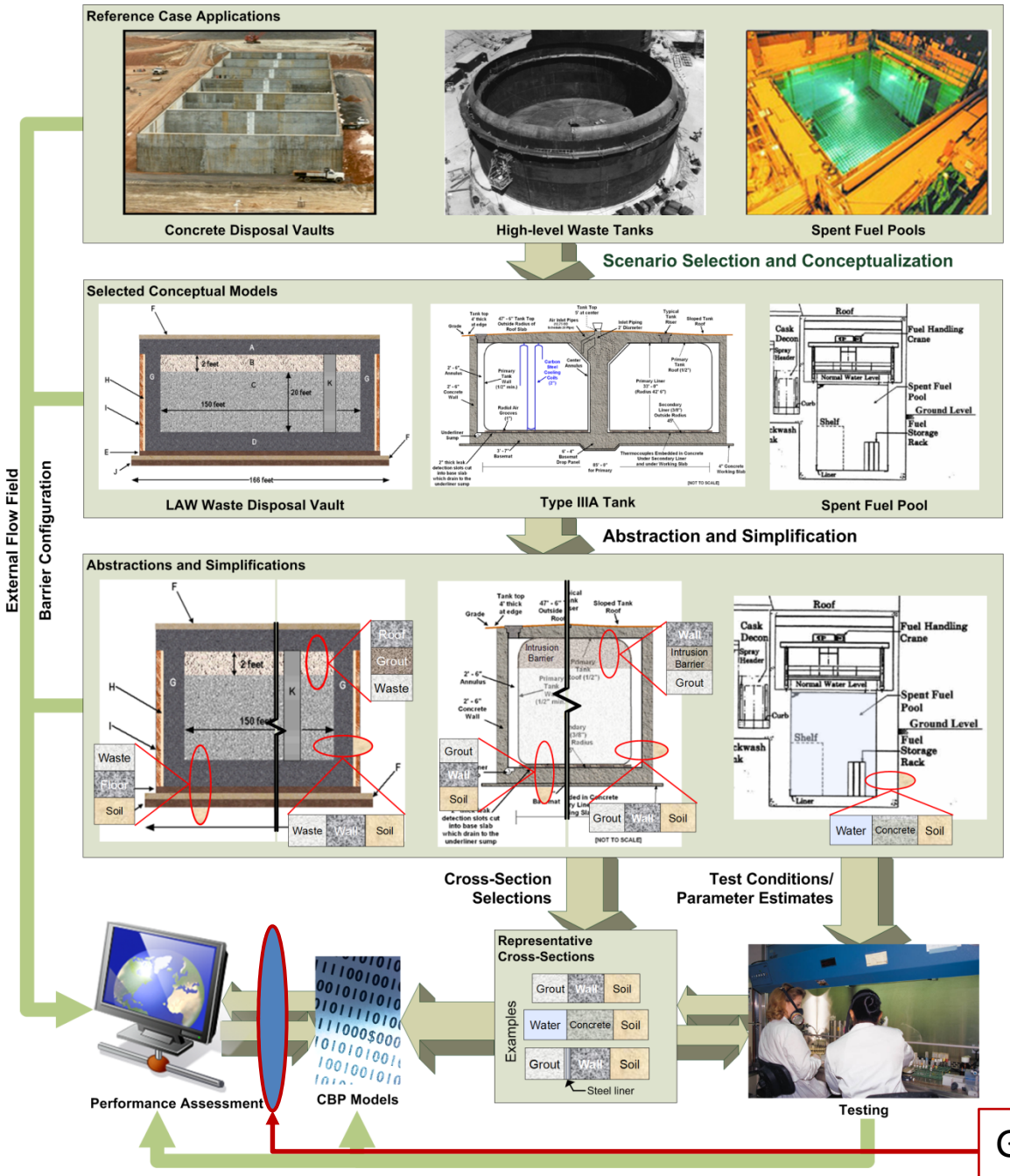
Specifications, Properties, and Phenomena for the Evaluation of Performance of Cementitious Barriers



FROM PA systems modeling

TO PA systems modeling

Linking Prototype Cases to Performance Models through System Abstraction



GoldSim & ASCEM

CBP Partner Codes and Integration

- **Partner Codes provide for scenario development, design evaluation and model parameterization**
  - ✓ **THAMES – Microstructure Evolution & Properties**
  - ✓ **STADIUM – Physical & Hydraulic Performance**
  - ✓ **LeachXS/ORCHESTRA – Chemical Performance & Constituent Release, also coupled with physical properties/damage evolution**
- **GoldSim Bridge (DLL) with STADIUM & LeachXS/ ORCHESTRA**
  - ✓ **Uses scenarios developed in Partner Codes**
  - ✓ **Monte Carlo simulations**
  - ✓ **Integration with GoldSim Performance Assessment Models**

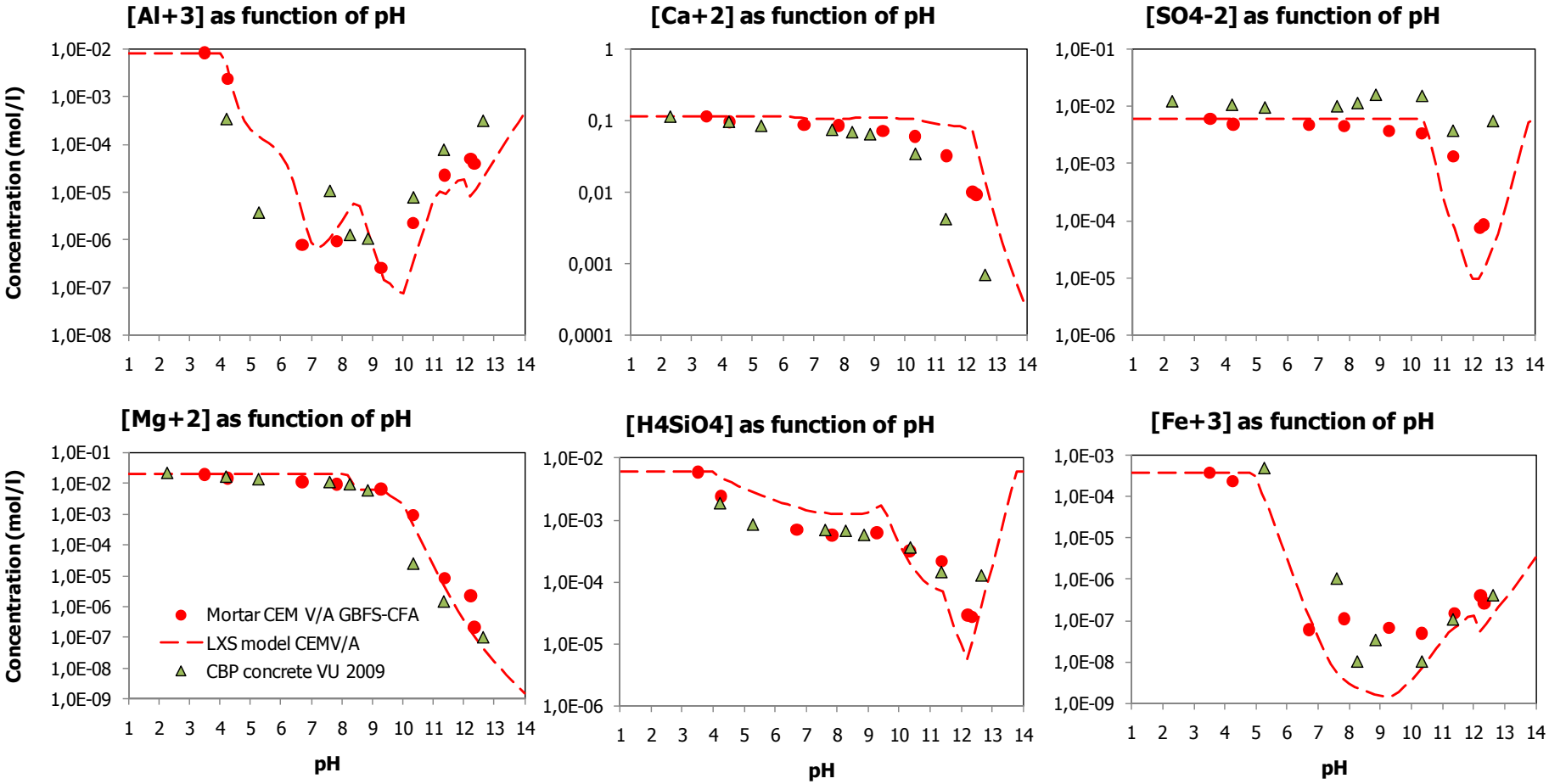
Development Path

1. Literature Review
2. Mechanistic Conceptual Model Development and Implementation
3. Calibration and Validation Data (experiments & measurements)
4. Model Testing & Demonstration Cases
5. Inclusion in software releases

Methods & Models

- Experimental methods for mass transfer properties and leaching
- Bayesian calibration of reactive transport parameters
- Mechanistic Models
  - Leaching
  - Sulfate attack
  - Chloride attack
  - Carbonation & Oxidation

Comparison of Cement Data and Thermodynamic Model Predictions



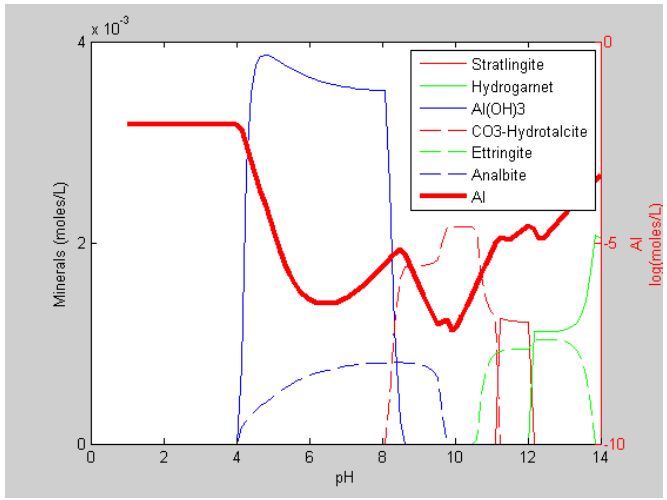
Experimental data from USEPA draft Method 1313

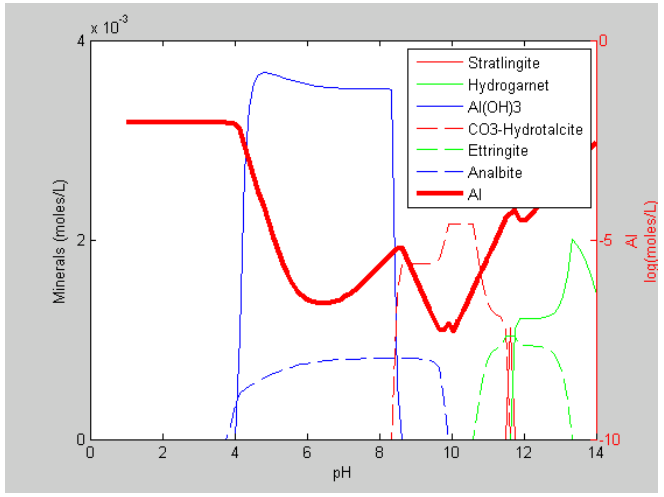
Uncertainty Reduction in Thermodynamic Model Parameters

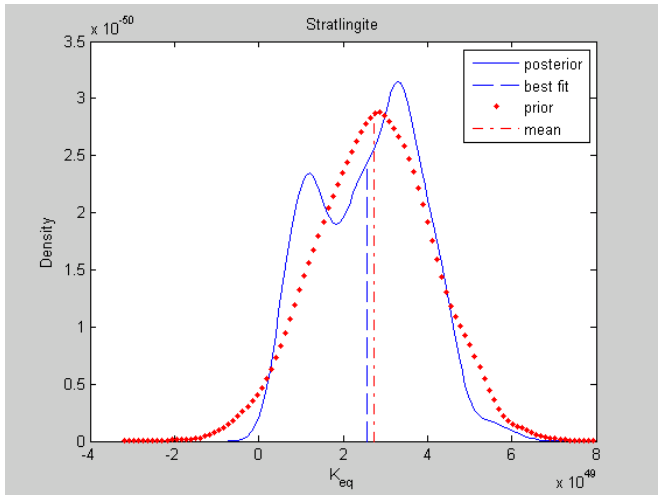
Prior

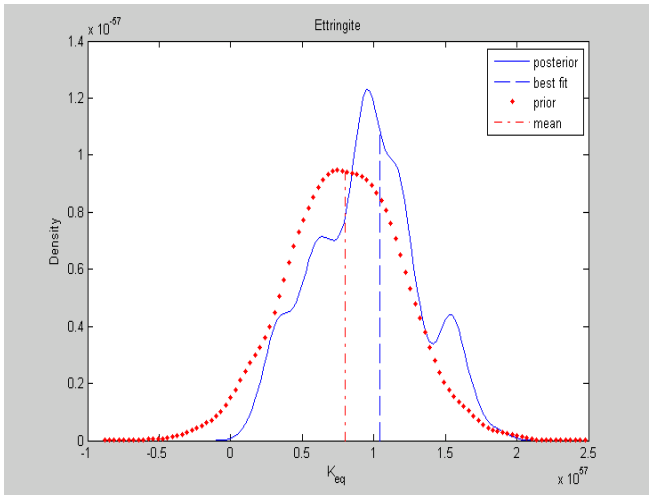
Best Fit

Al





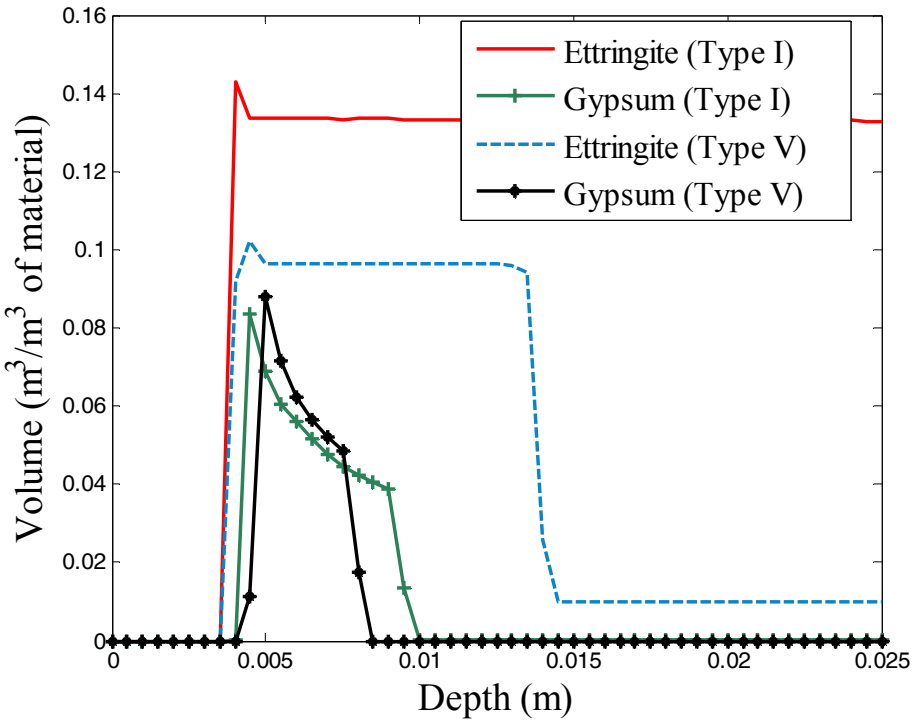




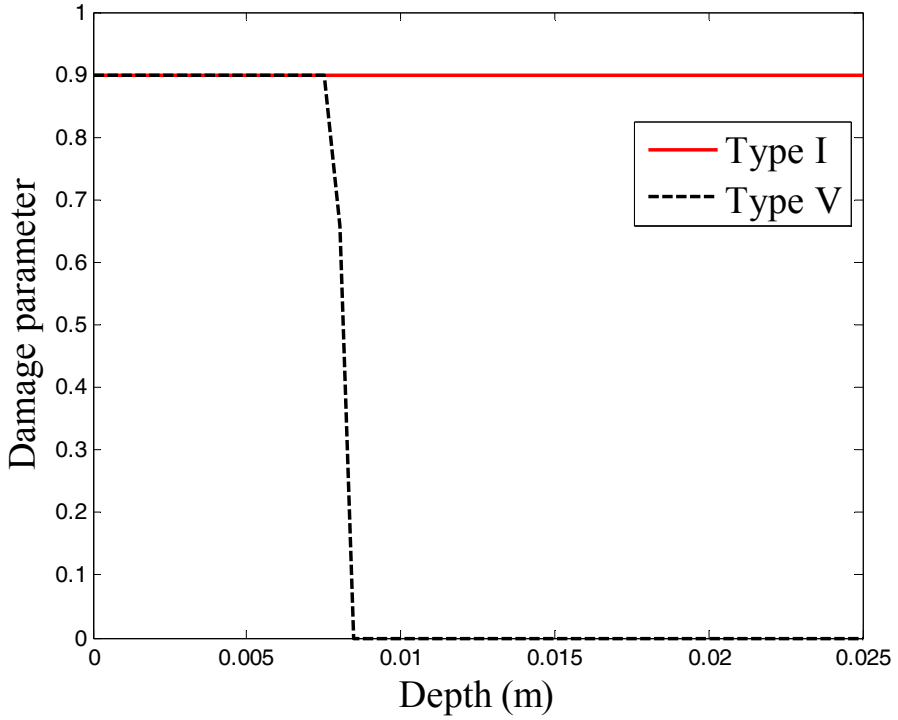
Most prominent changes: Stratlingite, hydrogarnet and ettringite

Influence of Cement Type on Damage

Ettringite and Gypsum Profiles



Damage Fronts



- Damage depends on both ettringite and gypsum formation; primary damage observed from ettringite for Type I and from gypsum for Type V cements.

CBP Example Problem
Salt Waste Disposal System Integrity

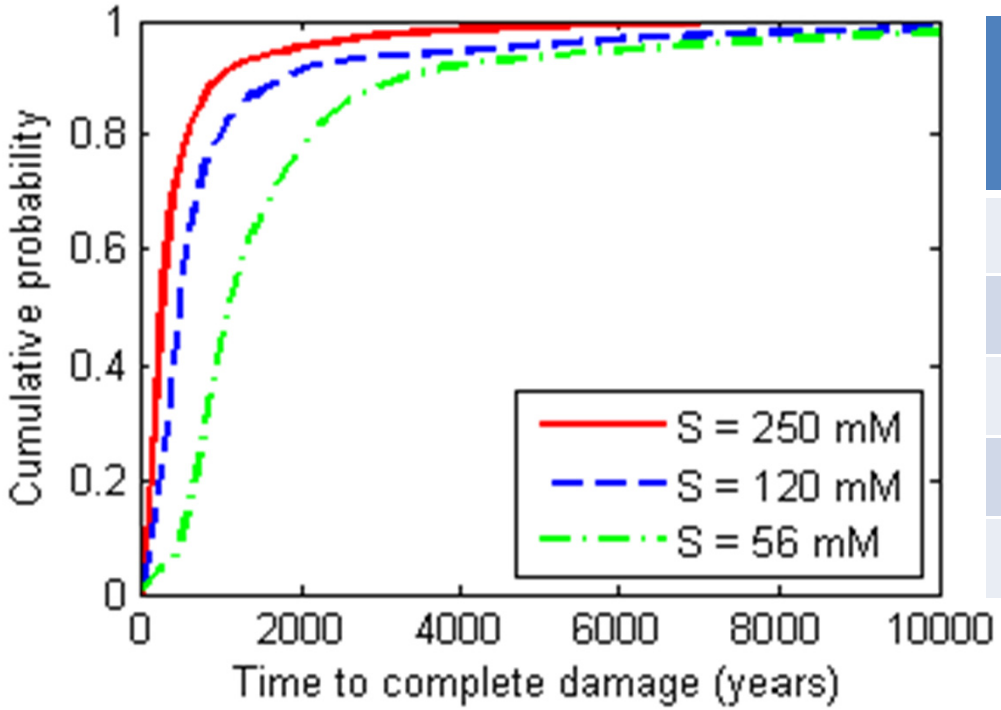
➢ Summary of Results for Sulfate Attack

- Ability to model sulfate attack and damage as a function of concrete type (cement type, physical properties) and external sulfate concentration
- Probabilistic analysis for model and parameter uncertainty
- Resulting models and parameters can be used for evaluation of a range of materials and scenarios

➢ Impact

- Allows selection of design parameters and materials to insure long-term durability and meeting performance goals
- Results can be integrated into existing performance assessment fate and transport models

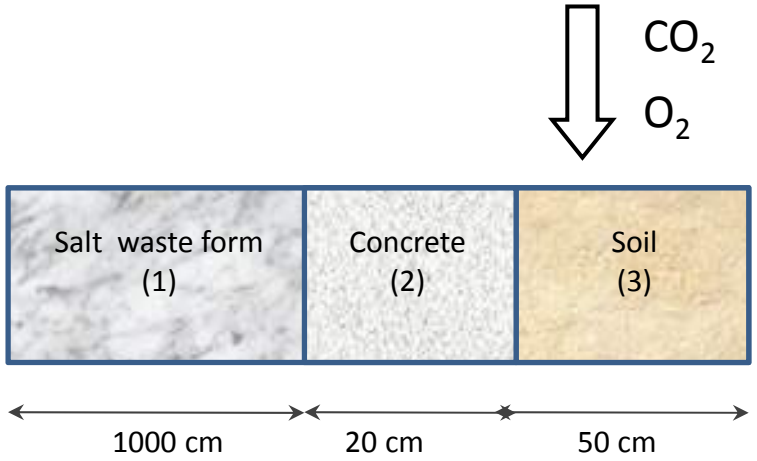
Sulfate Attack - Probability of Complete Damage (Example Case)



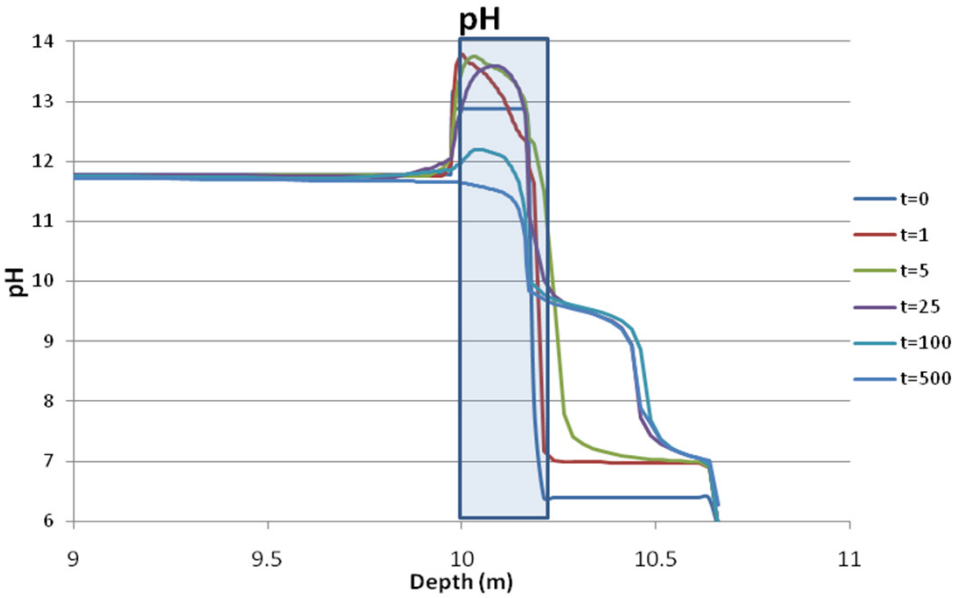
Percentiles	Time to complete damage (years)		
	Case 1 S = 250 mM	Case 2 S = 120 mM	Case 3 S = 56 mM
5th	78	109	338
25th	186	318	772
50th	285	508	1135
75th	513	835	1849
95th	1886	4354	6120

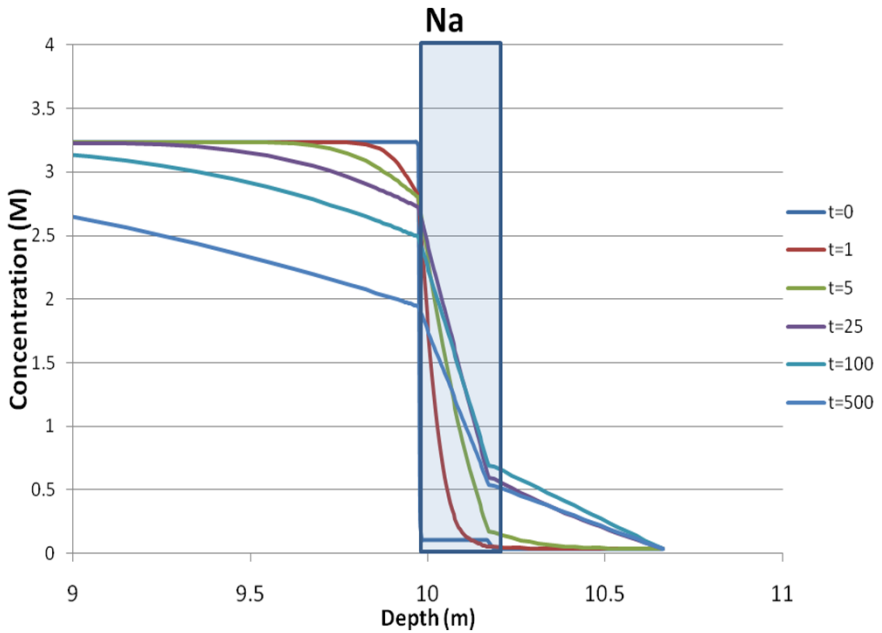
Complete damage (failure criteria): Time required for cracks to propagate through the entire structure

CO_2 and O_2 Ingress Challenge
3-Layer Reference Scenario



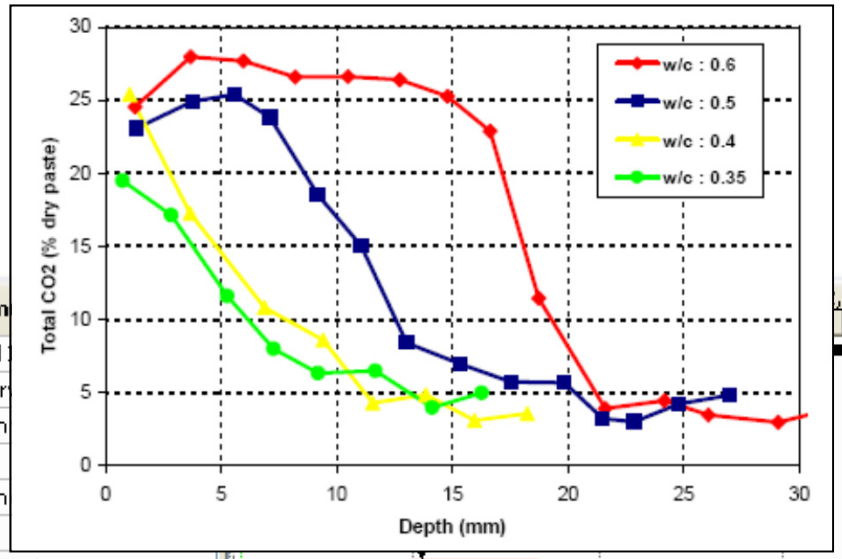
- 3-Layer, 1-D diffusion model for reactive substances
- CO_2 and O_2 influx in soil layer proportional to partial pressure difference air-soil.





CO_2 Ingress & Carbonation Modeling for Tank Integrity and Closure Scenarios

All CBP Partners Provide Unique Data Sources



Simco Tech., Inc. experimental results for validation

CBP Progress & Impact

- Developed coupling (DLL) of STADIUM and LeachXS/ORCHESTRA with GoldSim – Allows for regulator (NRC) and technical teams integration of CBP models with overall Performance Assessments, including uncertainty analysis (release 1st Q 2012)
- Understanding potential for sulfate attack during salt waste disposal – Facilitated resolution of NRC questions and provides a design basis for sulfate thresholds in waste forms (completed 2011)
- CBP models have capability to assist with addressing issues associated with potential leaching of residual Pu after tank closure (current concern)
- Extensive reference documentation developed providing technical basis and related information

CBP Progress & Impact

- Supporting ORP Secondary Waste treatment evaluation – provided experimental methods and basis for down selection of treatment technology (2011)
- Participation in inter-laboratory validation of new EPA Leaching Environmental Assessment Framework (LEAF) – provides technically defensible alternatives to TCLP for waste acceptance criteria consistent with DOE Performance Assessment approach
  (EPA Federal Register notice scheduled for 4th Q 2012)
- Data for evaluation of environmental impact of fly ash usage in cementitious materials (grout, concrete, etc.) – input into EPA regulatory process; provides technical basis for continued use of coal fly ash in DOE waste management
  (EPA report in Administrative Review, to be issued 3rd Q 2012)

CBP Plans for FY 2012

- Licensing and training on initial software releases – end-user group including NRC
- Further development and demonstration of models and experimental data to address HLW tank integrity and closure (e.g., external carbonation induced corrosion, engineered system aging and leaching of residual radionuclides after closure)
- ASCEM source term demonstration case (HLW tank closure example)
- Development and implementation of models and experimental data to further address cracking phenomena