Cementitious Barriers Partnership

C. Langton[1], D. Kosson[2] and H. Burns[1]

[1]Savannah River National Laboratory

[2]Vanderbilt University & CRESP

EM-30 Technical Exchange

17 November 2010

www.em.doe.gov

Cementitious Barriers in Waste Management

CERCLA Disposal Cell

Disposal Engineered Trench

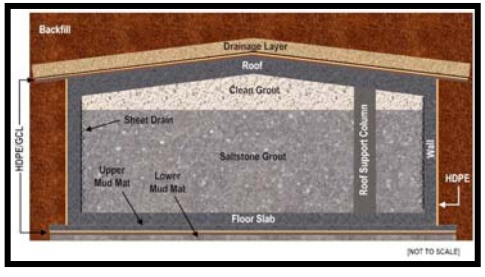
LAW Disposal in Vaults

LLW Disposal Grouted in Vault

D&D

Large Facility Closure

Tank Integrity & Closure



Saltstone Vault Disposal

Cementitious Engineered Barriers

- Used to enhance environmental performance of waste disposal units
  - Mobile, short- and long-lived radionuclides
  - Humid and possibly semi arid sites
  - Shallow to moderately deep aquifers
- Legacy waste, facilities, and environmental clean-ups
  - **Tank Closures** (SRS and Hanford)
    - Salt waste (SRS)
    - HLW tank closure (SRS, Idaho, Hanford)
  - **D&D, In-Situ Decommissioning** (Reactors, Canyons)
  - **CERCLA Remediation:** (Soil and Groundwater Remediation)

Cementitious Barrier Performance Needs

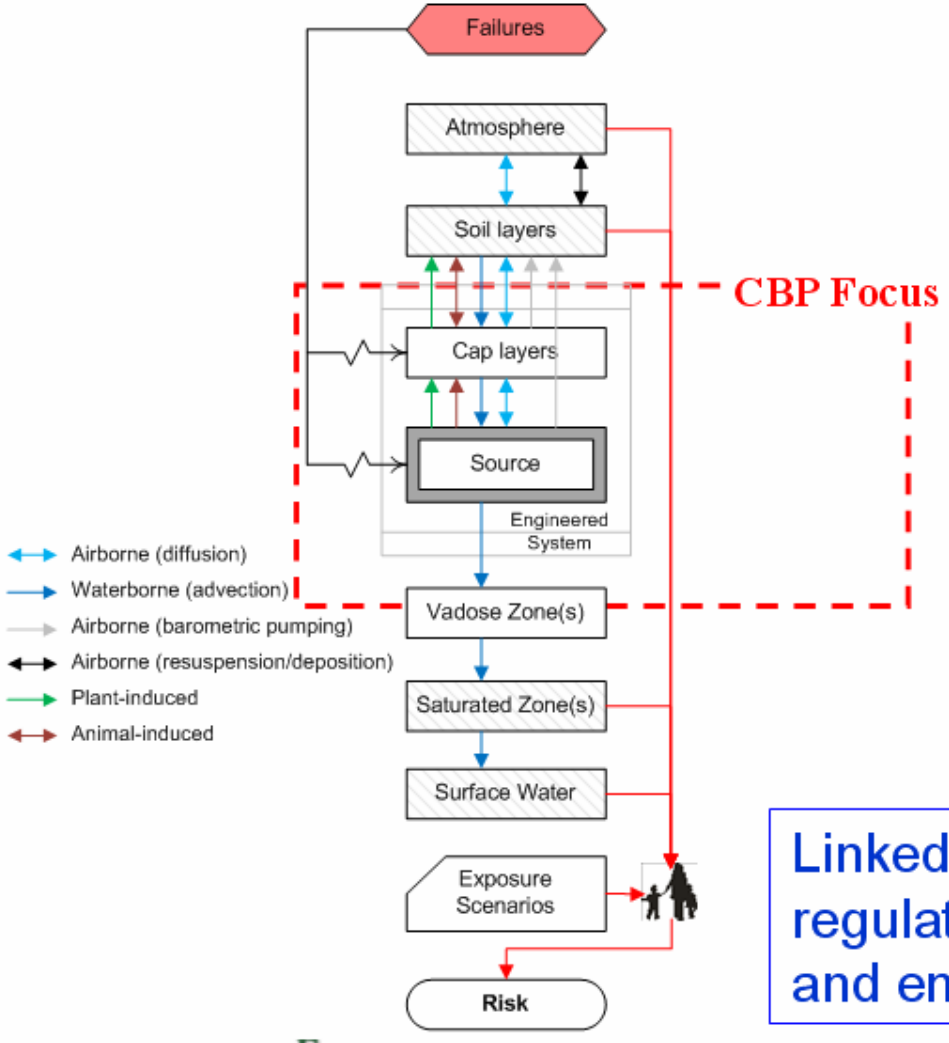
- Engineered Barrier Performance is incorporated into
  - DOE Performance Assessments
  - CERCLA Risk Documents (EPA, DOE, States and public)
- Engineered Barrier Performance is needed for
  - Management of existing waste disposal facilities
  - New waste disposal site selection decisions and facility designs
  - New waste treatment flow sheets
  - Next generation DOE and Commercial nuclear facility design and licensing (DOE and NRC)

CBP 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., >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

Regulatory Credibility is Essential

CBP Focus: Engineered Barriers & Source Terms



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.

Linked with current PAs, regulatory evaluation tools (GoldSim®) and emerging DOE tools (ASCEM)

Technical Strategy / Approach

- **Coordinated experimental and computational program**
  - Focus on key aging mechanisms effecting performance
    Sulfate attack, Carbonation, Oxidation, Leaching, Cracking
  - Conceptual model improvement – mechanistic basis for radionuclide mobility and material durability
  - Uncertainty Assessment – Bayesian/Stochastic methodologies

- **Experimental program**
  - Define test methods and parameter measurements
  - Model validation – Exposure testing & test beds

- **Modeling program**
  - Long term extrapolation of performance based on field scenarios
  - Hydraulic, chemical and mineralogical changes (time, conditions)
  - Radionuclide retention and release

Technical Strategy / Approach

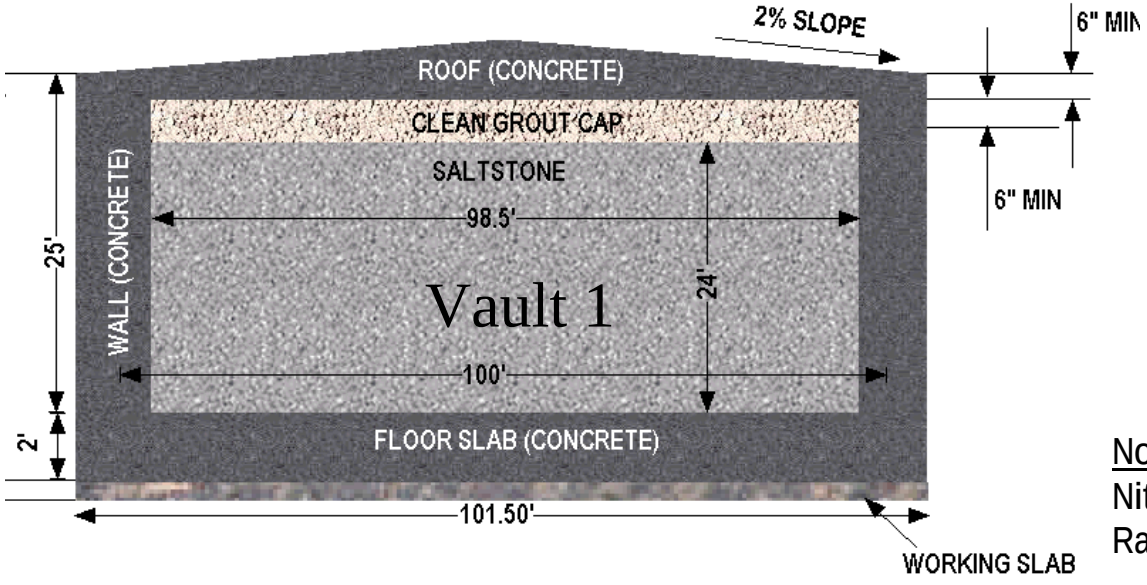
- **Reference Cases – provide basis for comparison and demonstration of tools under development**
  - Cementitious waste form in concrete vault with cap
  - High level waste tank integrity & closure
  - Nuclear processing facilities closure/ D&D (e.g., reactors & canyons)
  - Grouted vadose zone contamination
  - Spent fuel pool
- **Reference Materials** – surrogate LAW cementitious waste form, reducing grout, reinforced concrete
- **Extension/enhancement of existing tools –**
  - STADIUM (service life & durability)
  - LeachXS/Orchestra (leaching & chemical evolution)
  - CEMHYD3D/Thames (transport properties)
  - GoldSim – Integration & uncertainty assessment platform

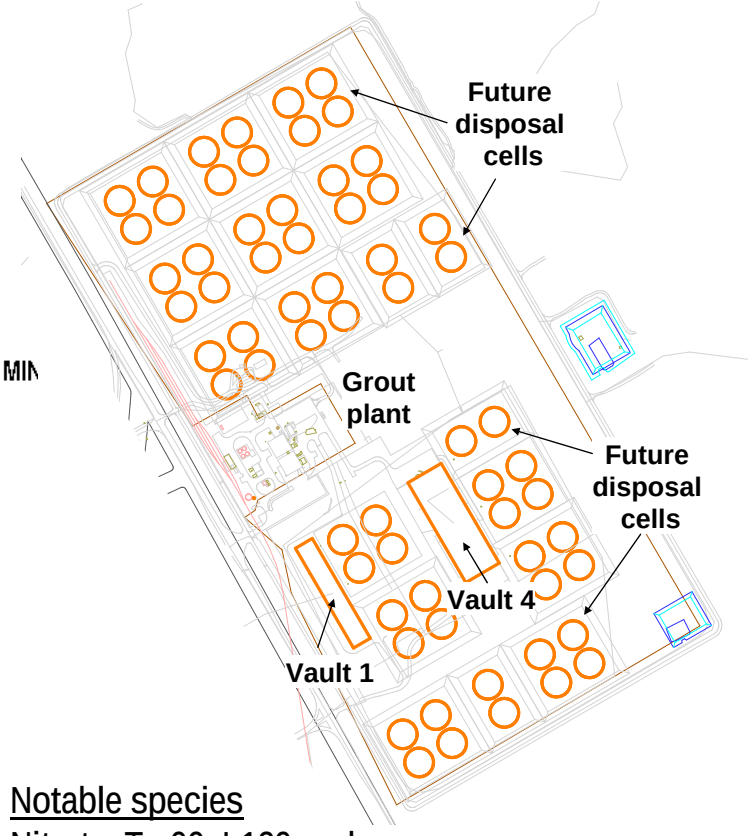
Partnership Members

- **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 & Transport Properties
- **SIMCO**
  - STADIUM – Physical & Hydraulic Performance
- **Energy Research Centre of the Netherlands**
  - LeachXS/ORCHESTRA – Chemical Performance & Constituent Release
- **Vanderbilt University/CRESP**
  - Chemical Performance & Constituent Release (experimental)
  - Uncertainty Analysis Framework
  - Model Integration

Contaminant Retention in Cementitious Materials: Savannah River - Saltstone Disposal Facility

- Salt liquid waste mixed with dry grout to form "Saltstone"
- Blast furnace slag in Saltstone grout and vault concrete to create reducing conditions





Notable species

Nitrate, Tc-99, I-129 and Ra-226 ingrowth from Th-230

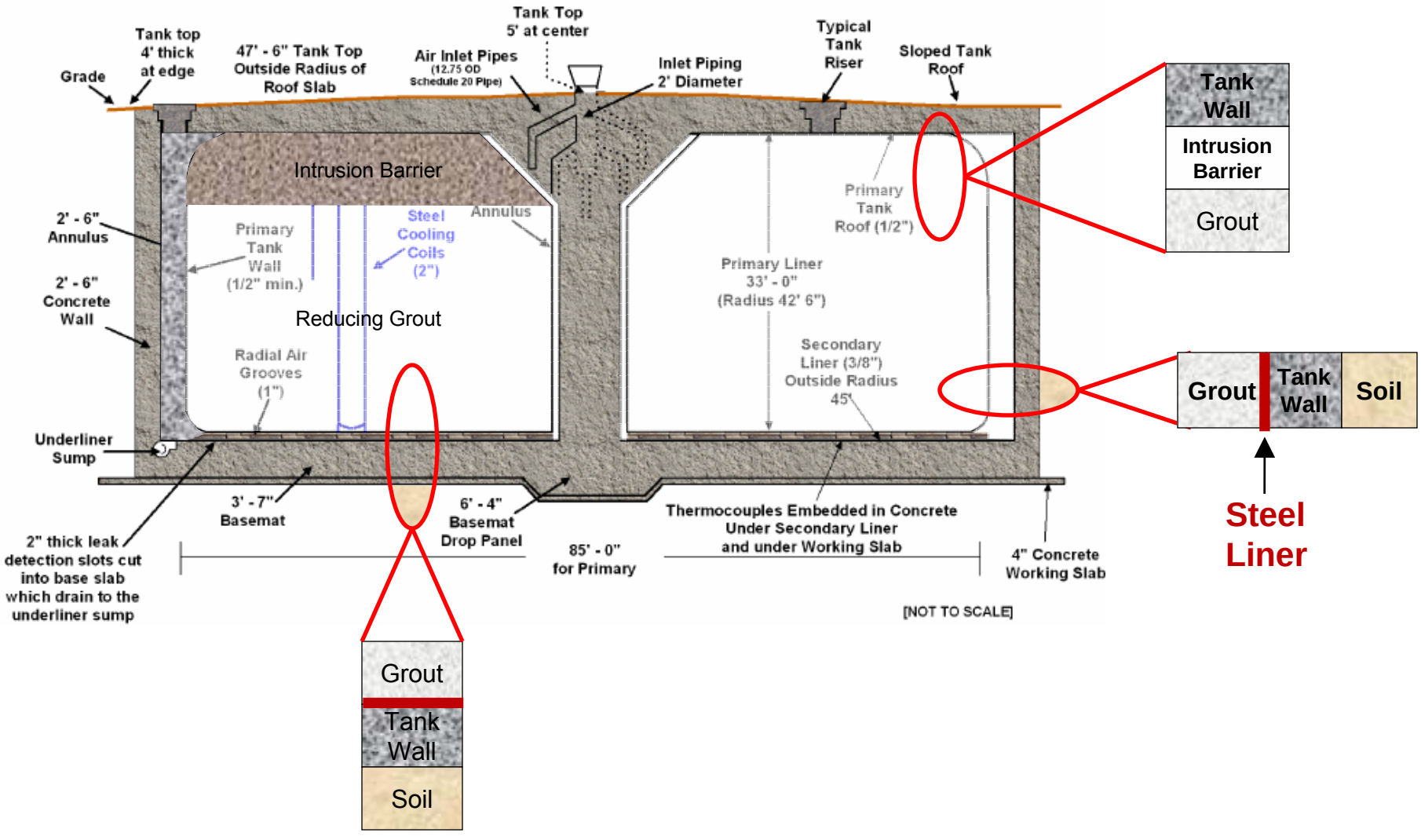
Environmental Management

safety ❖ performance ❖ cleanup ❖ closure

www.em.doe.gov

Presented by Greg Flach, SNRL
Performance Assessment Community of Practice

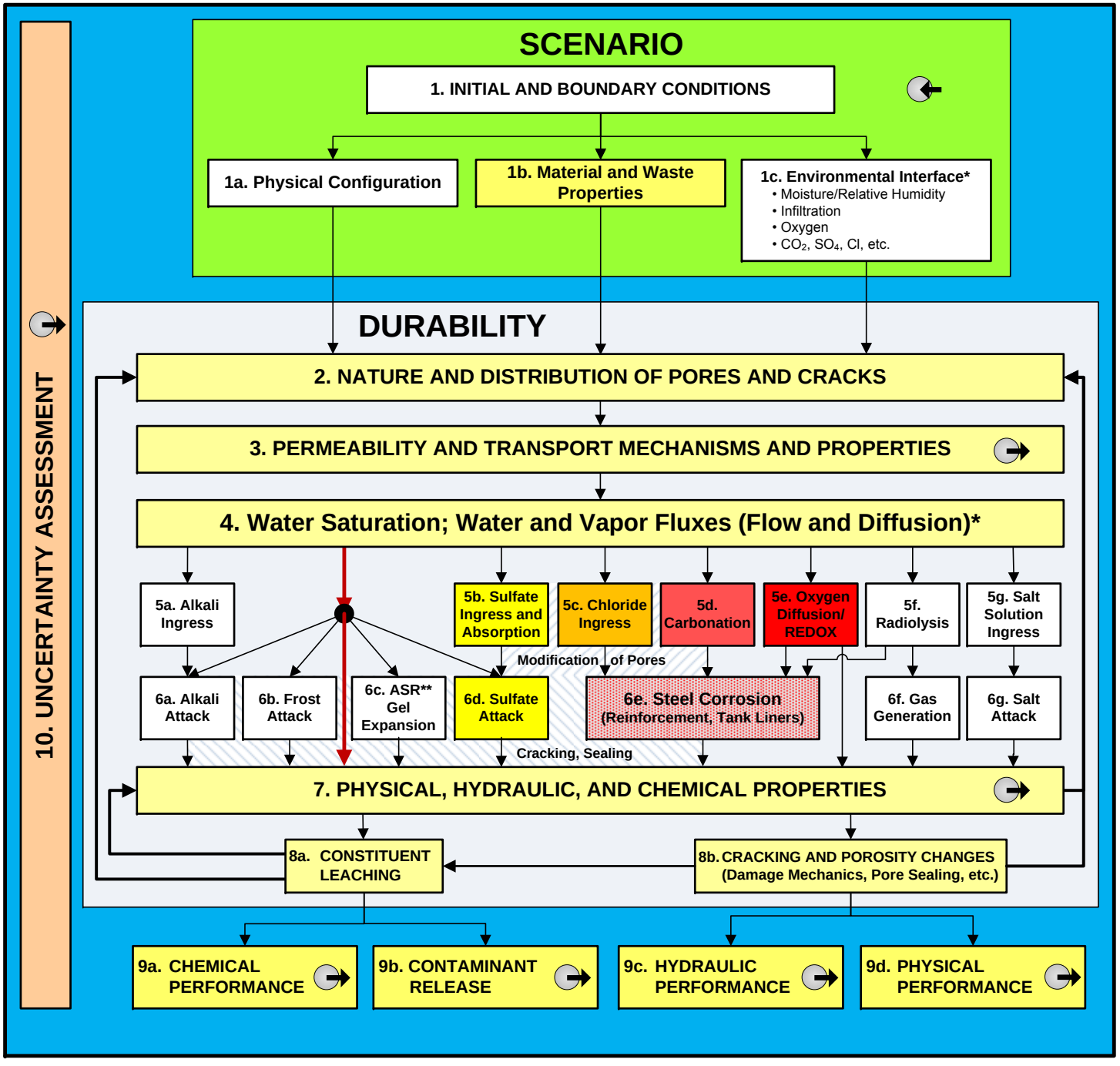
Type IIIA Tank – Conceptual Closure Model



Print

Close

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



Print

Close

CBP Example Problem
Salt Waste Disposal System Integrity

➢ Potential concerns

- **Sulfate** from waste form may degrade vault concrete
- **Oxygen** ingress may accelerate Tc-99 release

➢ Knowledge Gaps

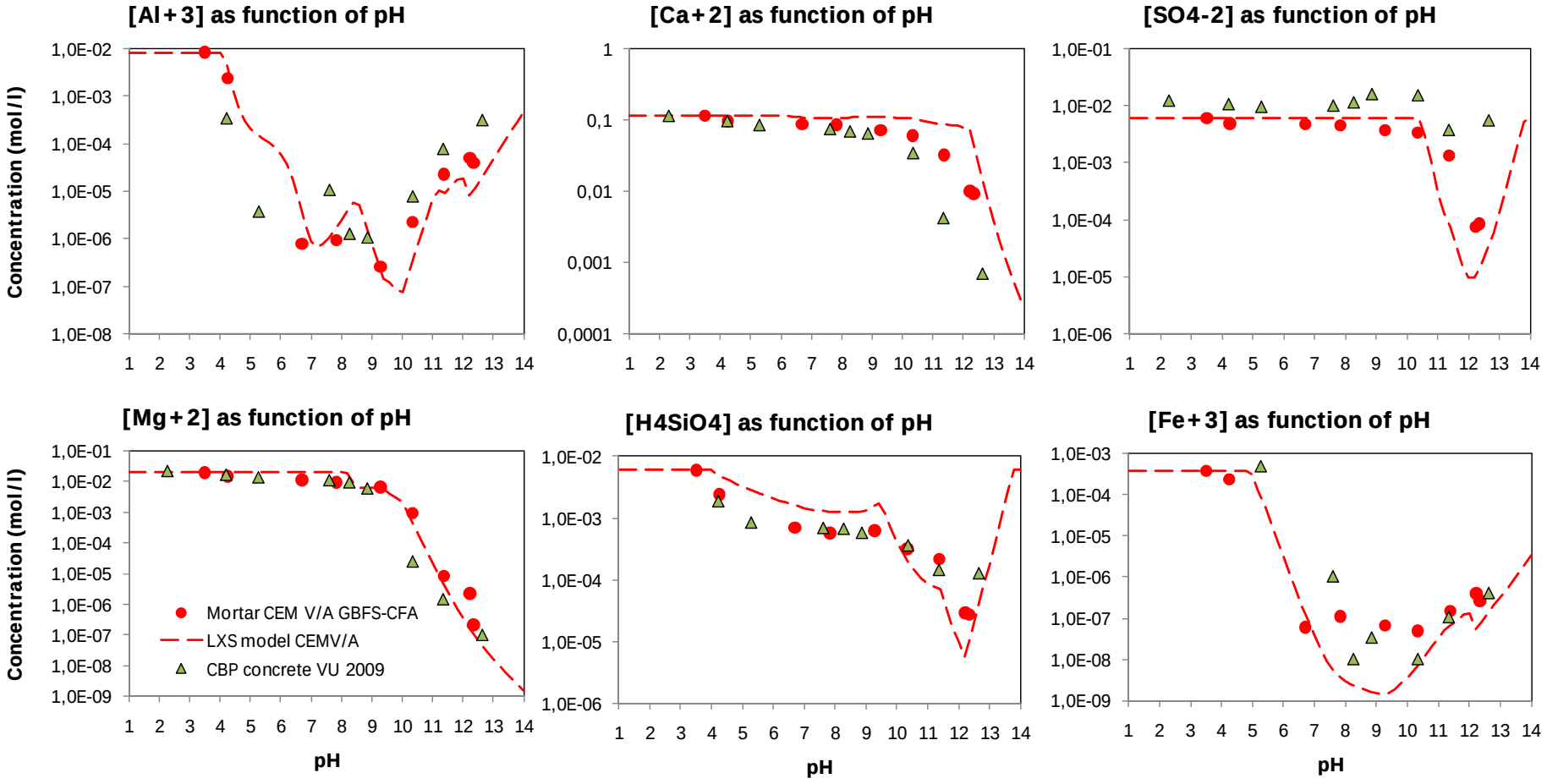
- Current concrete formulations are complex and exposure scenarios are not typical of usual environmental conditions
  - Portland cement/slag cement/fly ash and modifiers to create reducing and low permeability concrete
  - Complex chemical interface (with waste form)
- Rates of degradation and threshold sulfate concentrations unknown
- Mechanistic model needed to evaluate specific design scenarios
- Experimental data needed for model calibration & validation

CBP Example Problem
Salt Waste Disposal System Integrity

➢ Approach

- Define & validate thermodynamic model for vault concrete
- Define conceptual model
- Adapt reactive transport model and couple with damage mechanics - captures impact of change in material structure on transport phenomena
- Gather & augment experimental data for model parameterization and validation
- Model scenarios & assess uncertainty

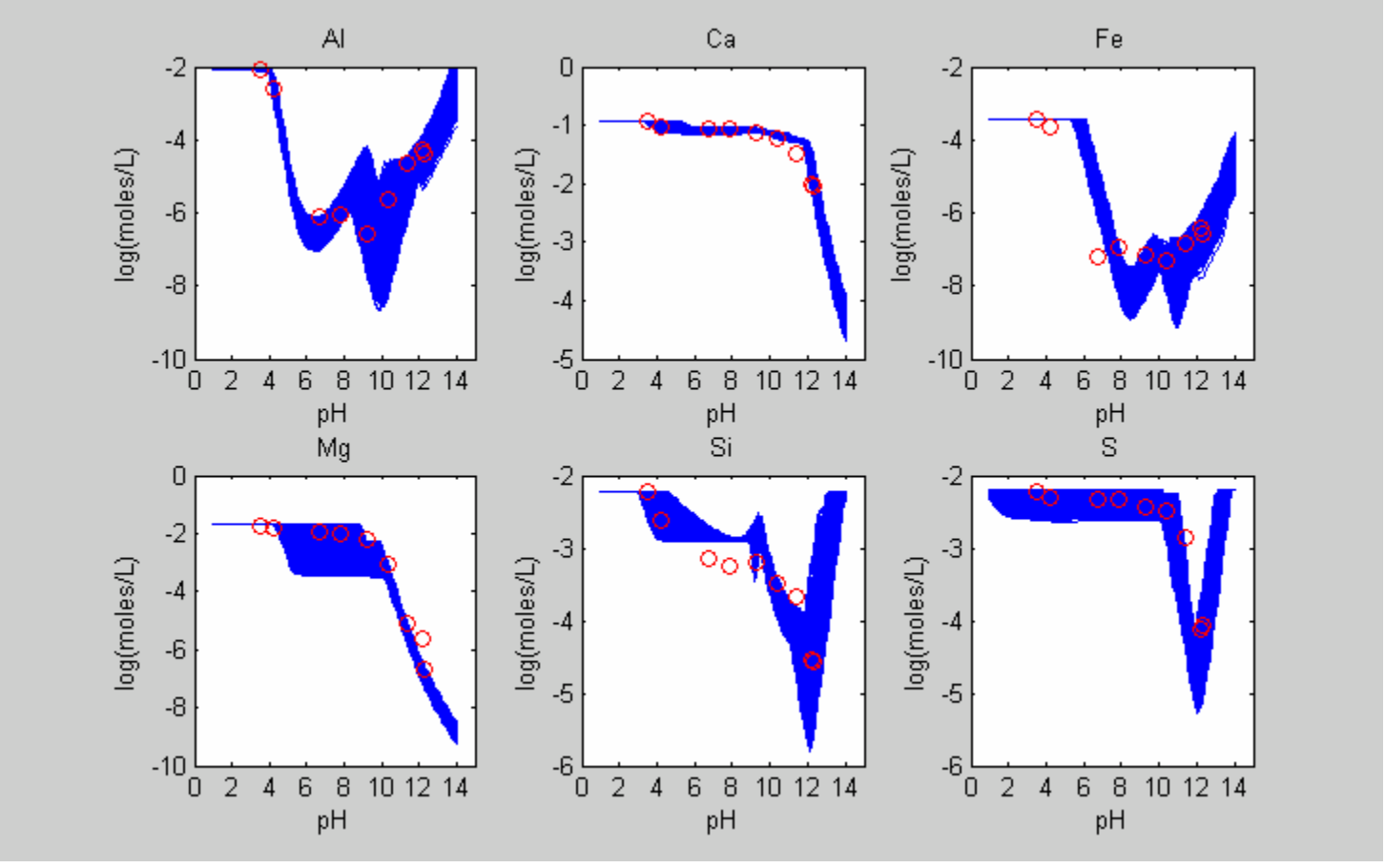
Comparison of Cement Data and Thermodynamic Model Predictions



Environmental Management
safety ❖ performance ❖ cleanup ❖ closure

Experimental data from USEPA draft Method 1313

Data Uncertainty – Calibration of Thermodynamic Model Parameters



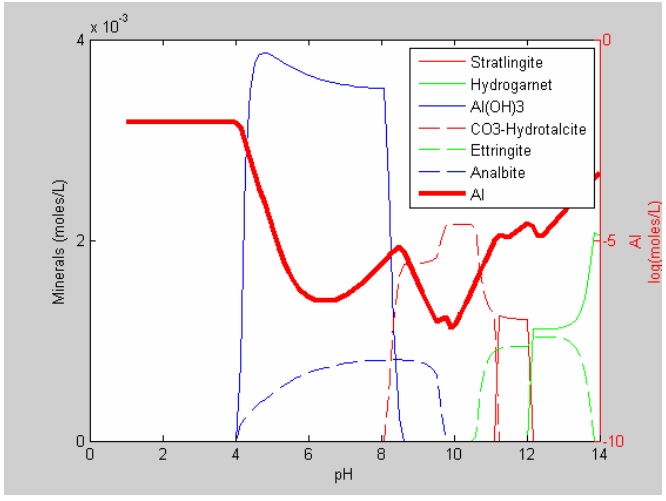
Data and Model uncertainty considered

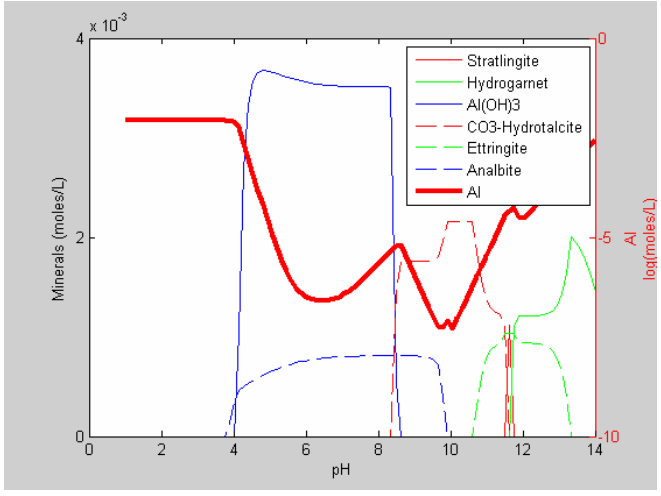
Uncertainty Reduction in Thermodynamic Model Parameters

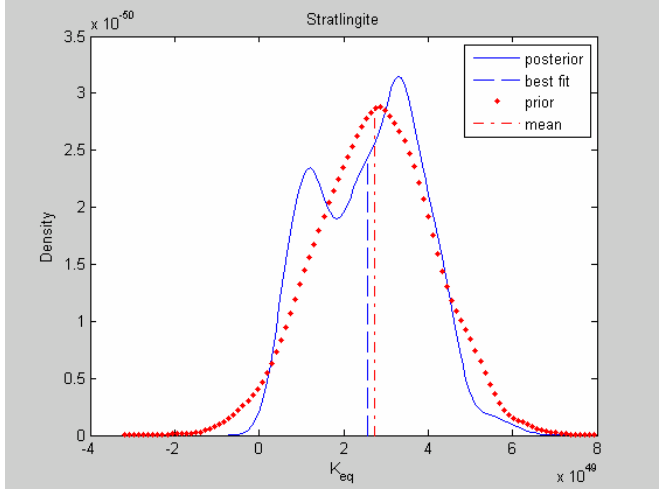
Prior

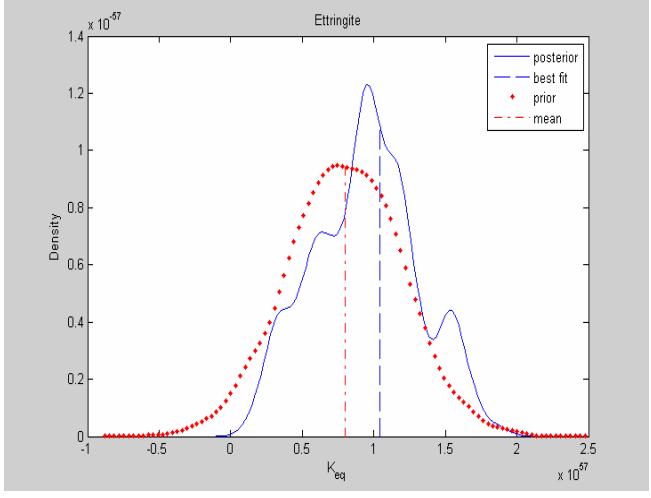
Best Fit

Al







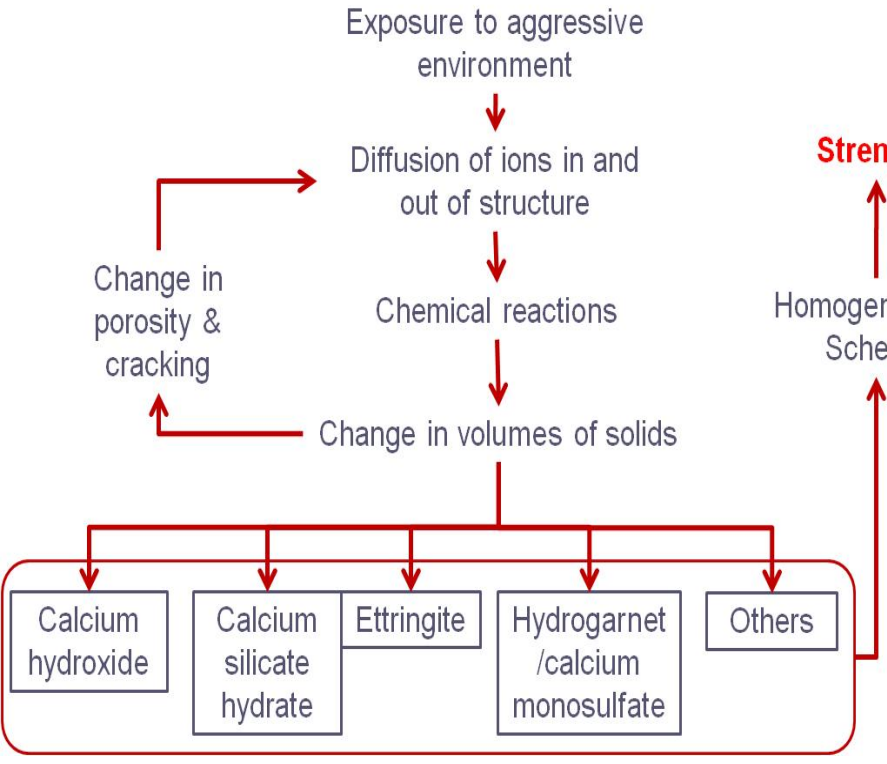


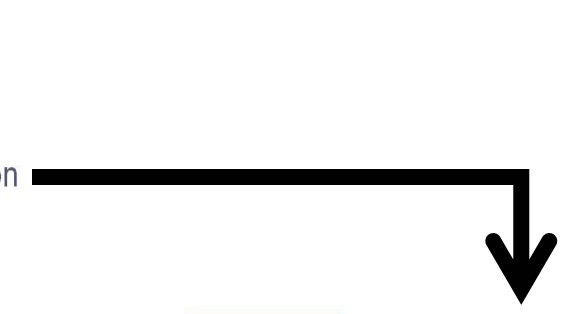
Most prominent changes: Stratlingite, hydrogarnet and ettringite

Print

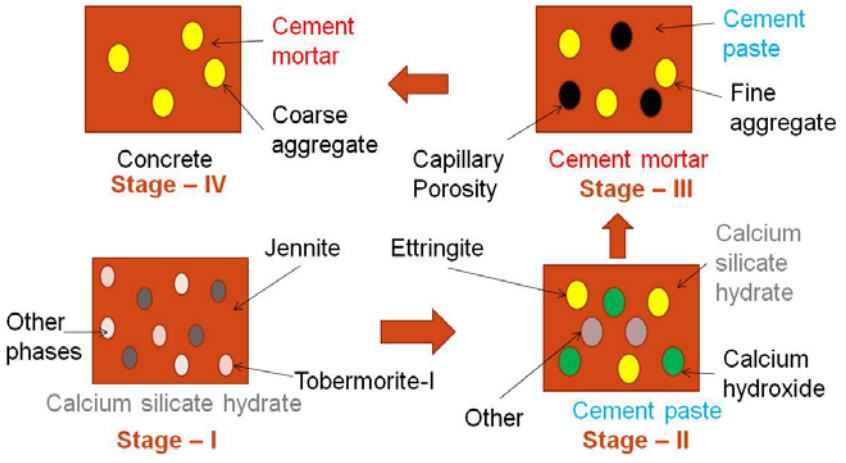
Close

Change in Mechanical Properties due to Chemical Reactions





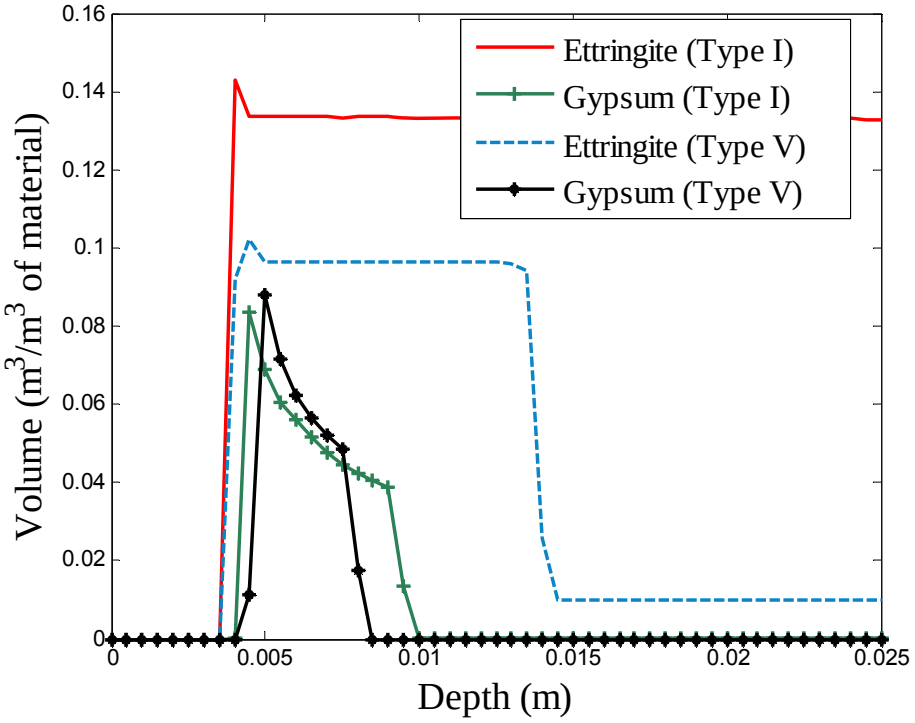
- Elastic moduli of solid phases obtained from the literature



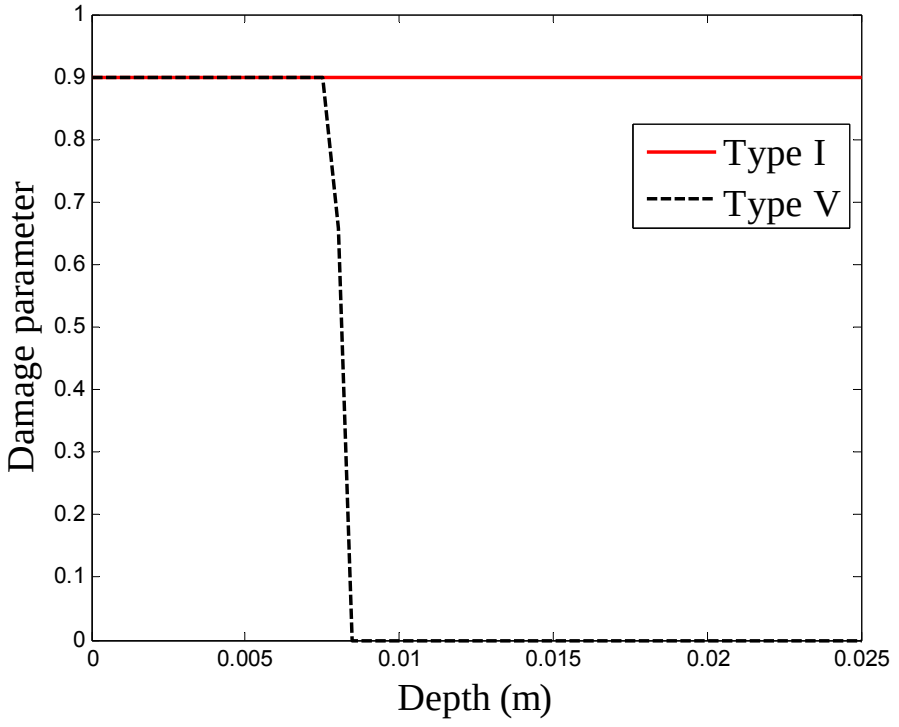
18

Influence of Cement Type on Damage

Ettringite and Gypsum Profiles

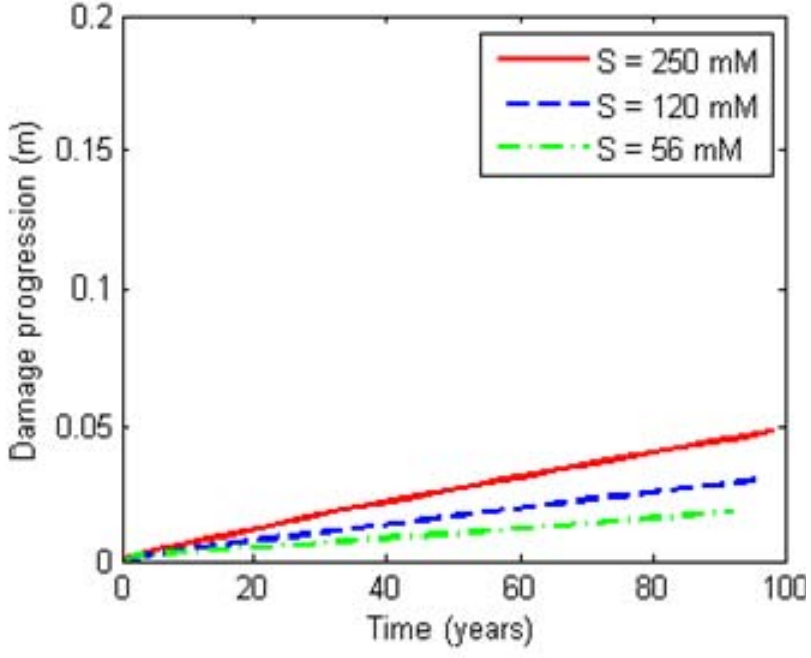


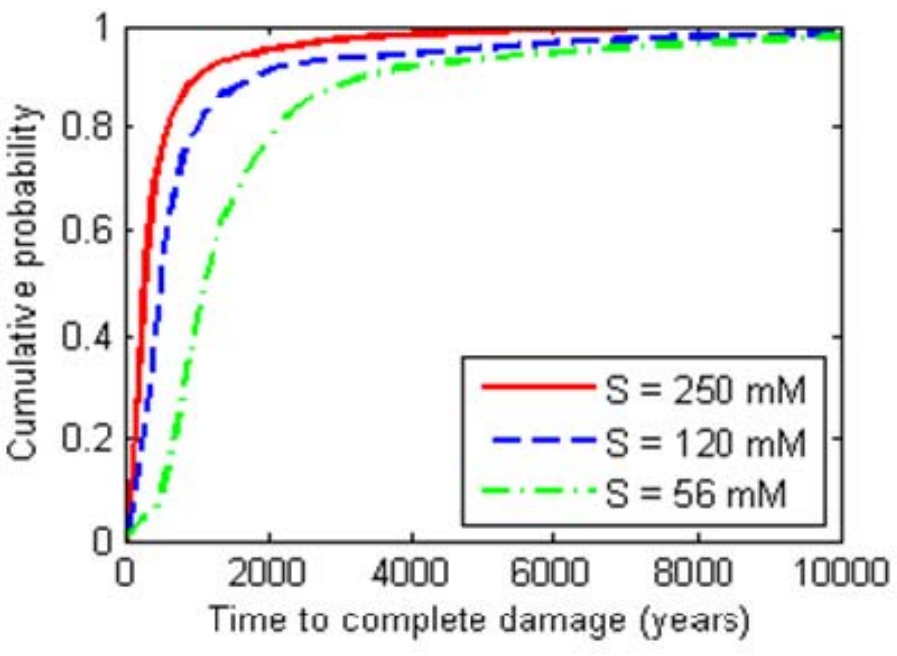
Damage Fronts



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

Sensitivity Analysis – Effects of Sulfate Concentration on Damage Progression in Example Concrete





CBP Example Problem
Salt Waste Disposal System Integrity

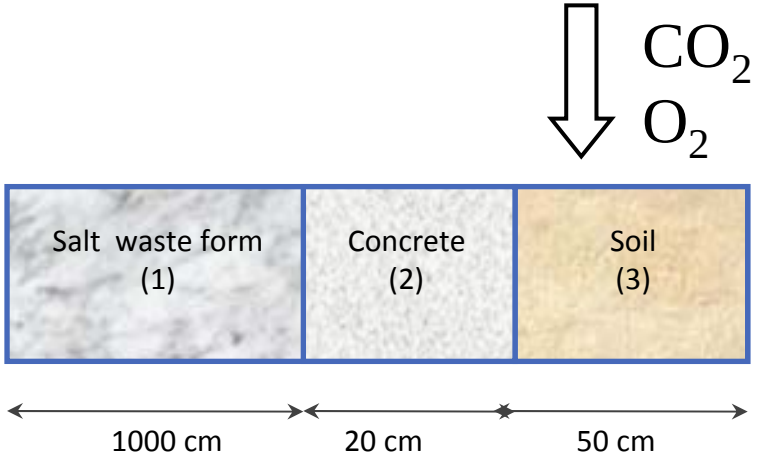
➢ Summary of Results for Sulfate

- 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
- Models and data assembled can be used for evaluation of a range of materials and scenarios

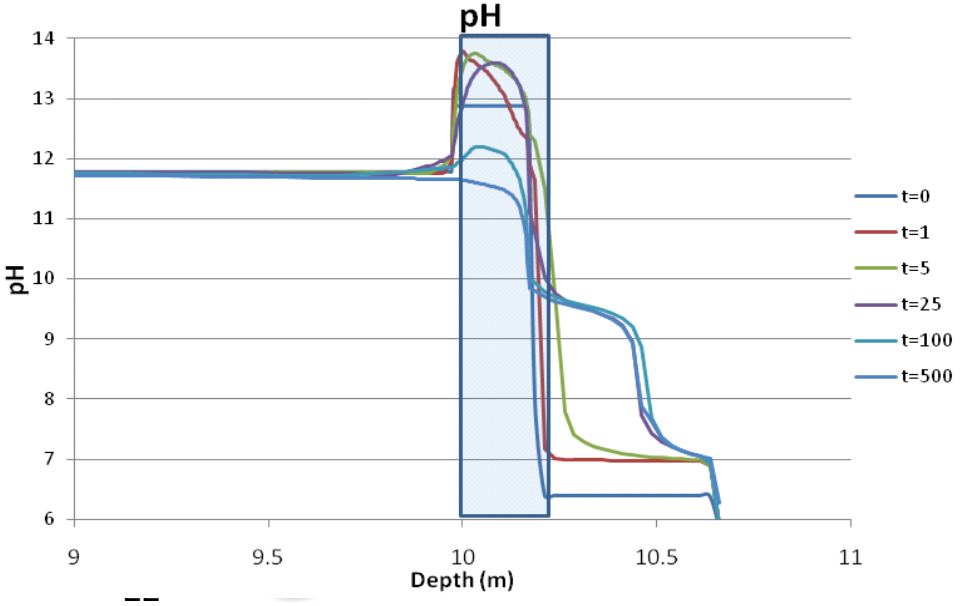
➢ Impact

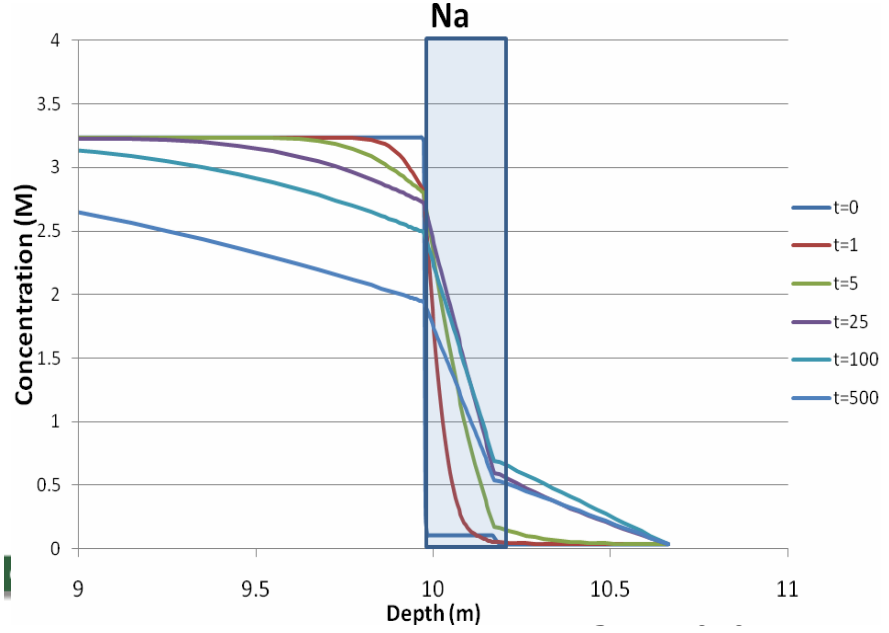
- Allows selection of design parameters and materials to insure long-term durability and meeting performance goals
- Results can be integrated into existing performance assessment fate and transport models

CO_2 and O_2 Ingress Challenge
3-Layer Reference Scenario

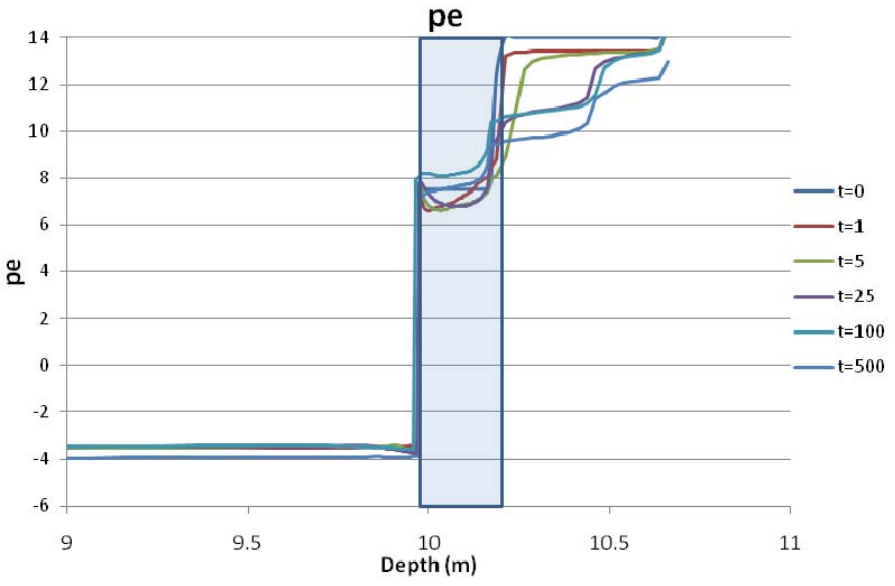


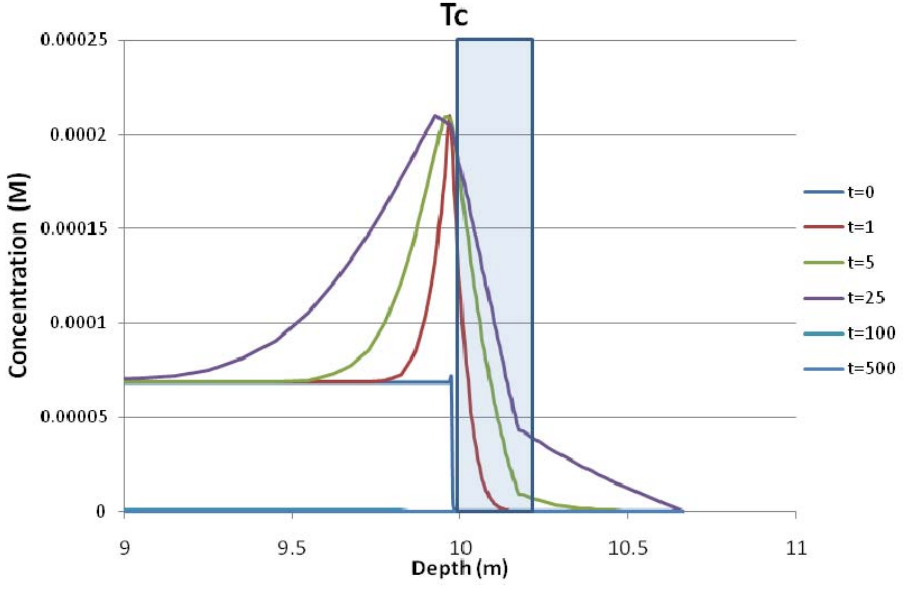
- 3-Layer, 1-D diffusion model for reactive substances
- CO_2 and O_2 influx in soil layer proportional to partial pressure difference air-soil.





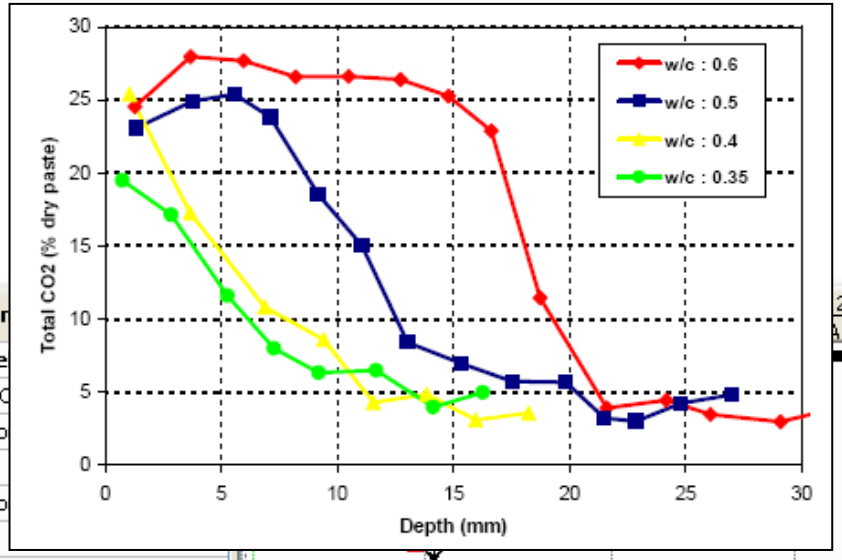
Effect of O_2 Ingress on Redox Gradient Evolution & Tc-99 Release





CO_2 Ingress & Carbonation modeling

SIMCO Experimental results for validation



	Nar
1	⊟CBP Task 10 - Mode
2	Litterature review - C
3	Effect of pore solutio
4	Reporting
5	Effect of pore solutio
6	Reporting
7	Implementation of secondary species
8	Reporting
9	Development of 1st version of damage model
10	Carbonation modeling

model + test

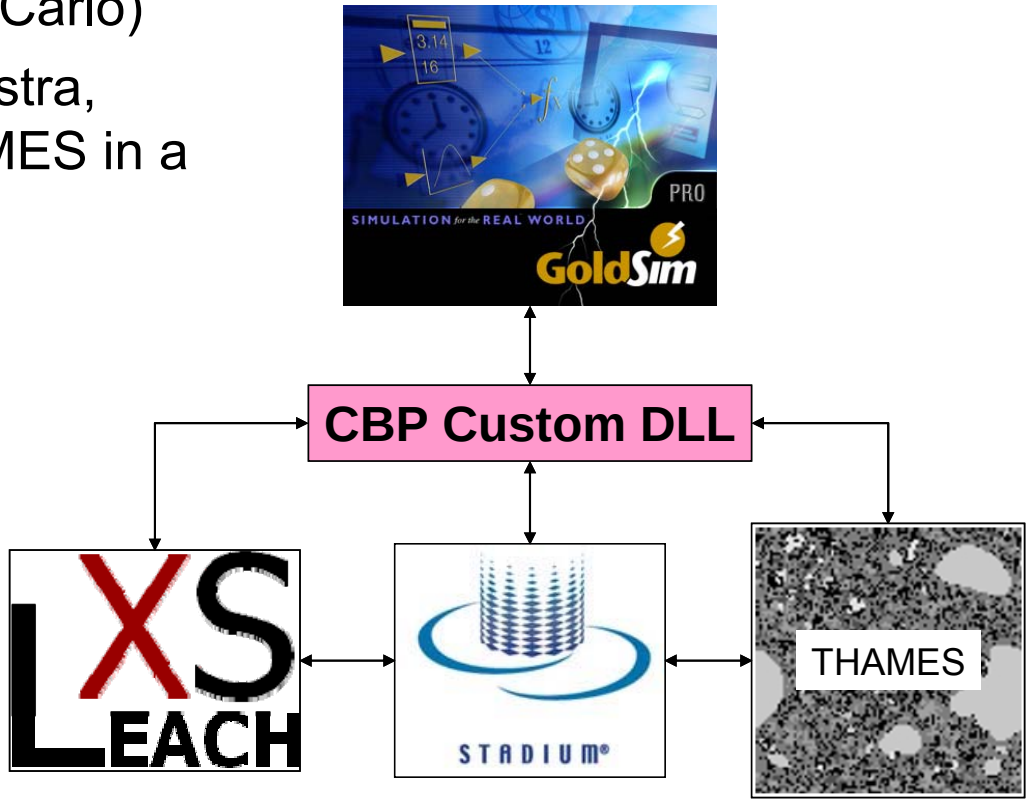
2, 2011 | Half 1, 2012 | Half 2, 2012

SrResEng
SrResEng
ResEngSci-A[50%]
SrResEng
SrResEng;ResEngSci-A
SrResEng
ResEngSci-A[50%]
SrResEng;ResEngSci-A[50%]
ResEngSci-A[50%];SrResEng[50%]
SrResEng;ResEngSci-A

All CBP Partners ProvideUnique Data Sources

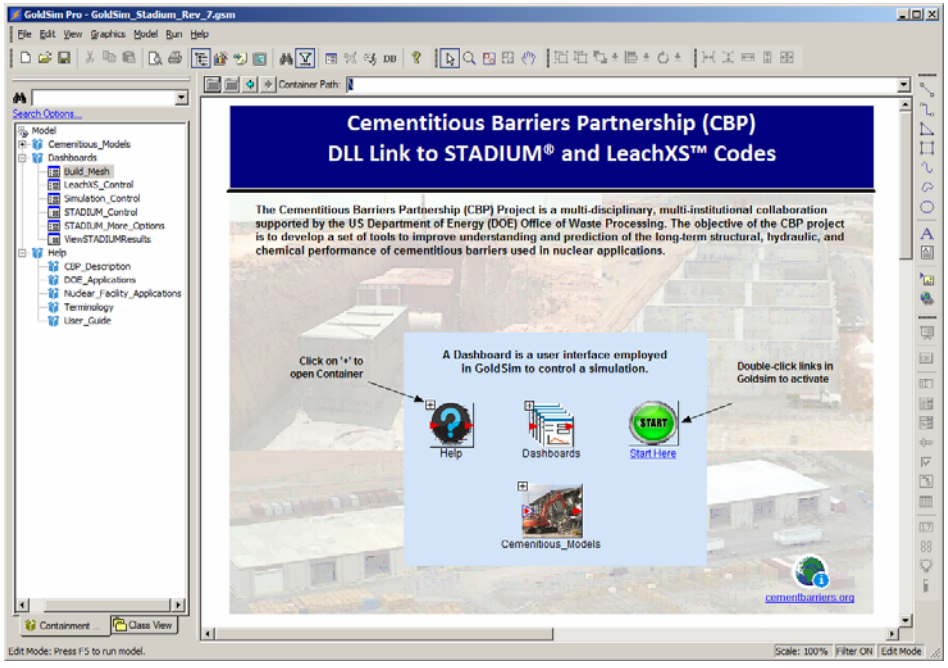
CBP Partner Code Integration

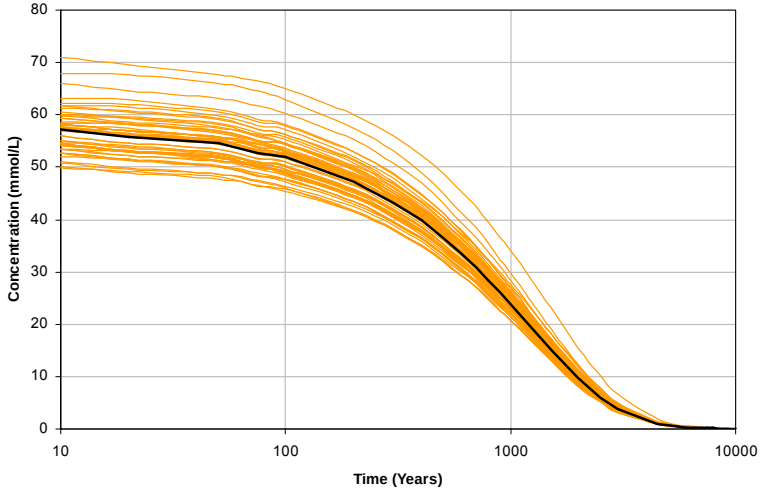
- Software integration objectives:
  - Provide a common unified interface to CBP partner codes through a GoldSim GUI
  - Provide a wrapper for probabilistic uncertainty/sensitivity analysis (e.g. Monte Carlo)
  - Couple LeachXS/Orchestra, STADIUM and THAMES in a synergistic manner
  - Connect to broader systems-level environmental assessment models



CBP Partner Code Integration

- GoldSim graphical user interface to STADIUM and LeachXS/Orchestra
- Implement sub-models for different scenarios
- Demonstration of user interface for deterministic and Monte Carlo analyses
- Integrates with current platforms and system models used by NRC and PA developers





Environmental Management
safety ❖ performance ❖ cleanup ❖ closure

CBP Next Steps

- **Integration of CBP models into GoldSim Platform**
  - Capability demonstrated during FY 2010
  - First licensing (sulfate attack in GoldSim) expected during FY 2011
- **Extension of CBP Models and Data to Other Phenomena**
  - Oxidation front analysis demonstrated during FY 2010
  - Carbonation ingress analysis planned for FY 2011 (e.g., tank integrity & closure scenario)
  - Impact on constituent and radionuclide release (leaching, K_ds) initiated during FY 2010
  - Impact of cracking scenarios to be initiated during FY 2011
  - Database for evaluation of cementitious materials to be released in FY 2011
- **Test Beds and Exposure Testing for Model Confirmation**

Acknowledgements

D. Esh, M. Furman, J. Phillip, US NRC

K. Brown, S. Mahadevan, A. Garrabrants, J. Arnold, S. Sarkar, CRESP, Vanderbilt U.

H. Van der Sloot, J.C.L. Meeussen, R. Comans, ECN (NL)

E. Garboczi, K. Snyder, J. Bullard, P. Stutzman, NIST

E. Samson, J. Marchand, SIMCO, Inc. (CA)

G. Flach, R. Seitz, S. Marra, H. Burns, SRNL

DOE-EM Project Manager: Pramod Mallick

CBP Project Support Provided by EM-30

Contact Information

SRNL : Christine Langton (803) 725-5806

Heather Burns (803) 725-2607

CRESP: David Kosson (615) 337-5889

www.cementbarriers.org