Cementitious Barriers Partnership

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Environmental Management
safety ❖ performance ❖ cleanup ❖ closure

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**Hans van der Sloot Consultancy* after 1-1-2010

Examples of DOE- EM PA and PA-like Analysis Applications

CERCLA Disposal Cell

LLW Disposal Engineered Trench

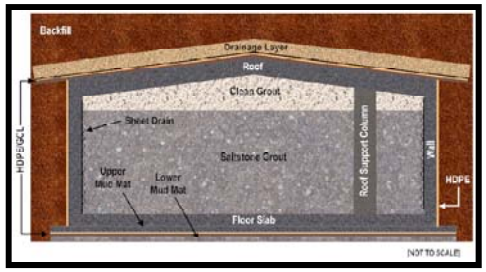
LLW Disposal in Vaults

LLW Disposal Grouted in Vault

D&D

Large Facility Closure

Tank Closure



Saltstone Vault Disposal

Environmental Management

safety ❖ performance ❖ cleanup ❖ closure

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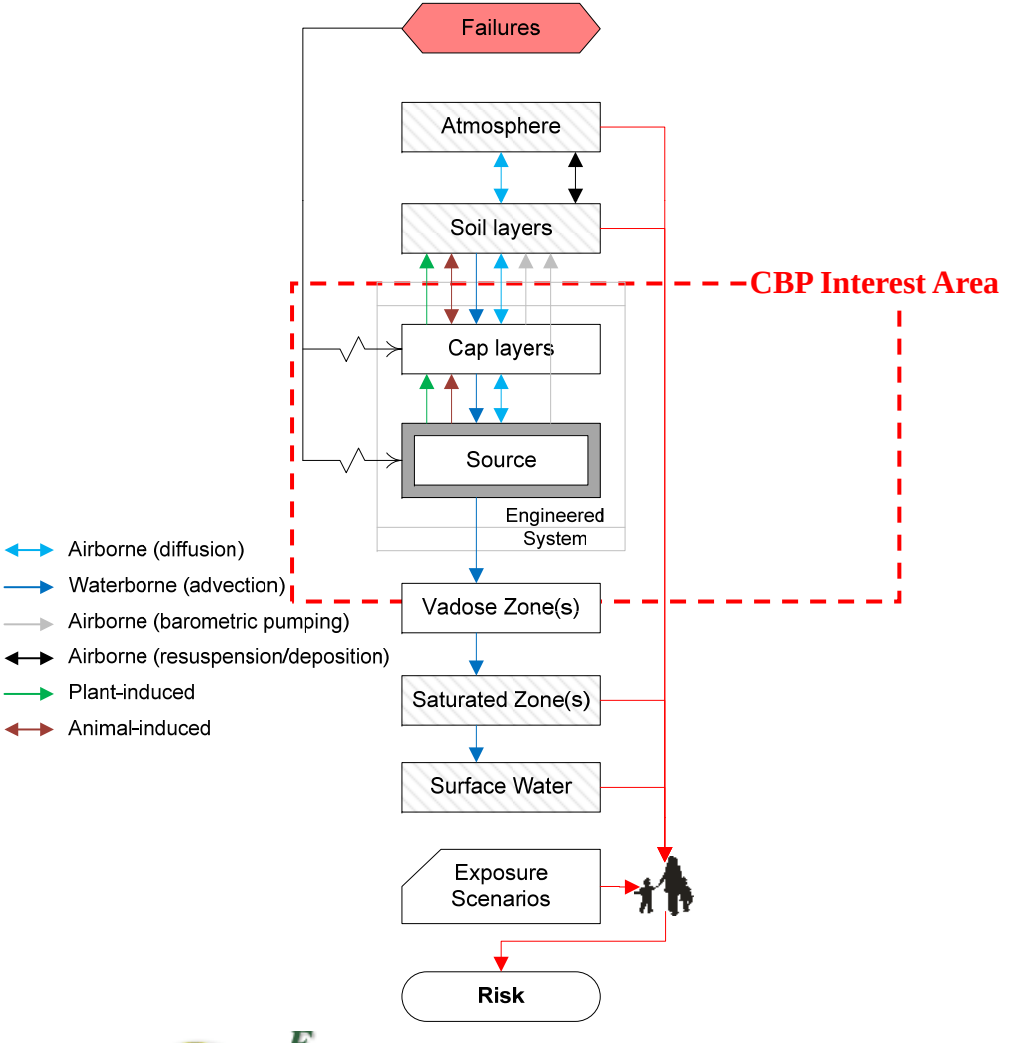
Presented by Martin J. Letourneau, DOE-EM Performance Assessment Community of Practice

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.

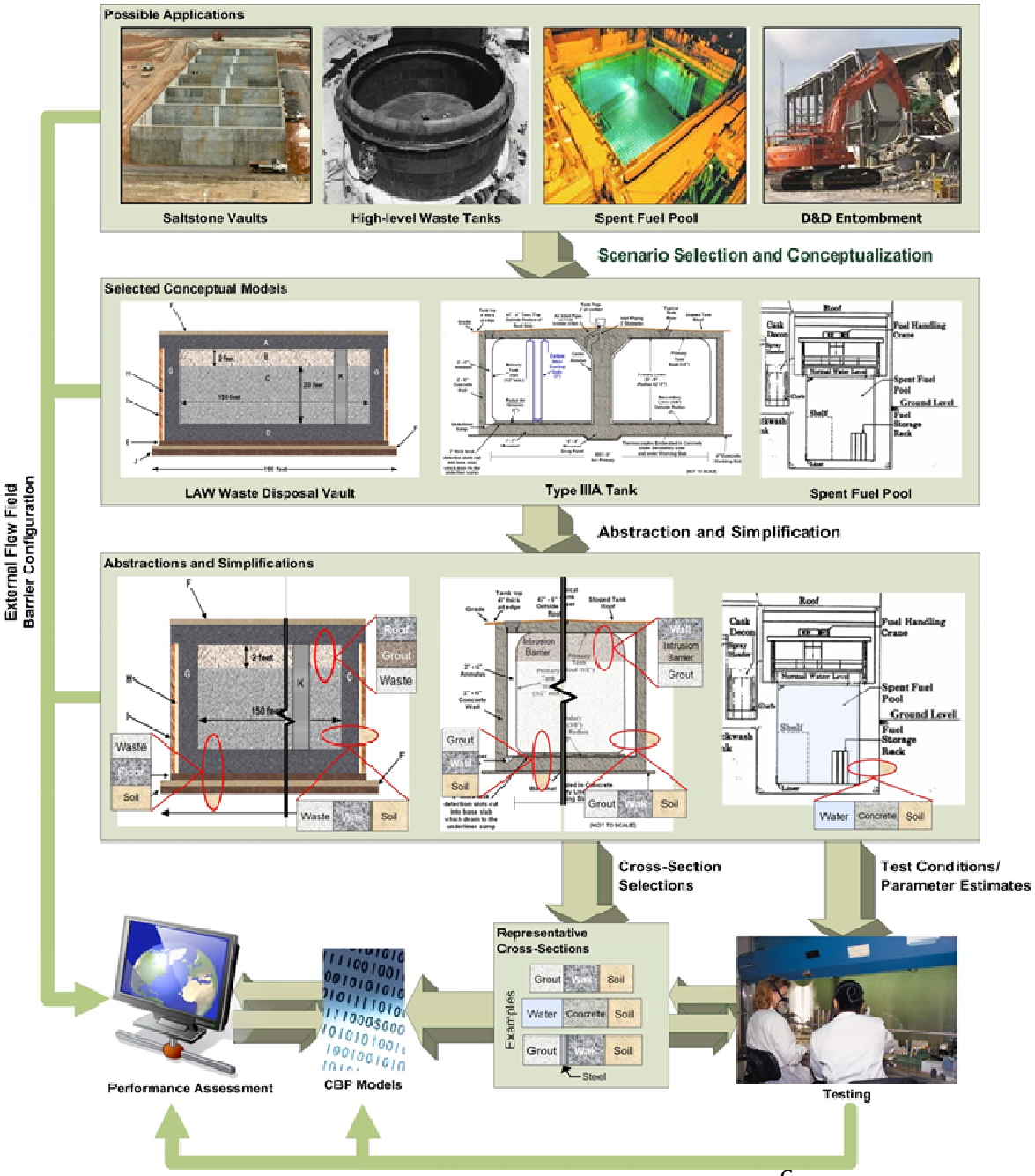
Project Goal

- 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

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
  - Spent fuel pool
  - Nuclear processing facilities closure (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

Linking Prototype Cases to Performance Models through System Abstraction



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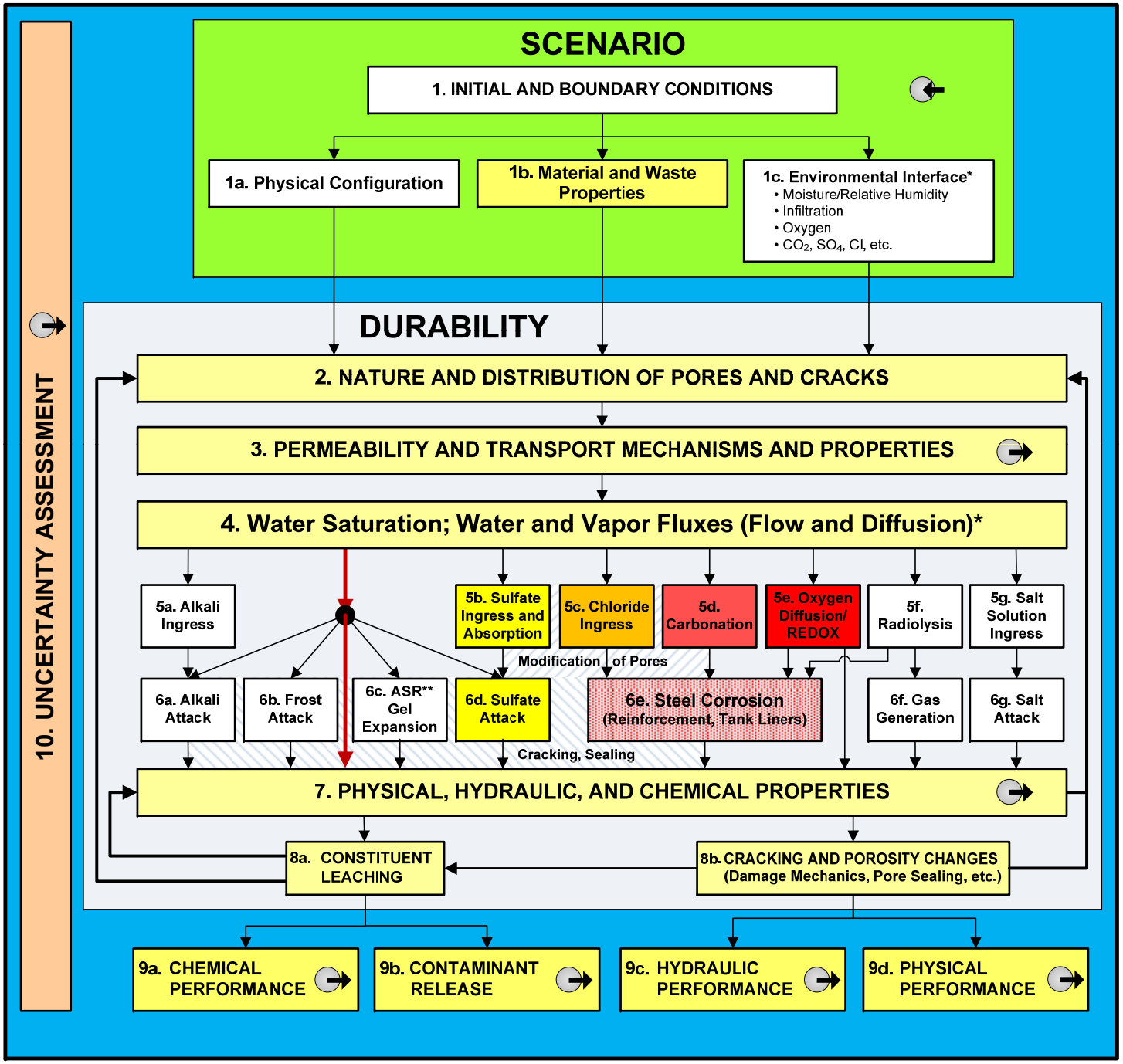
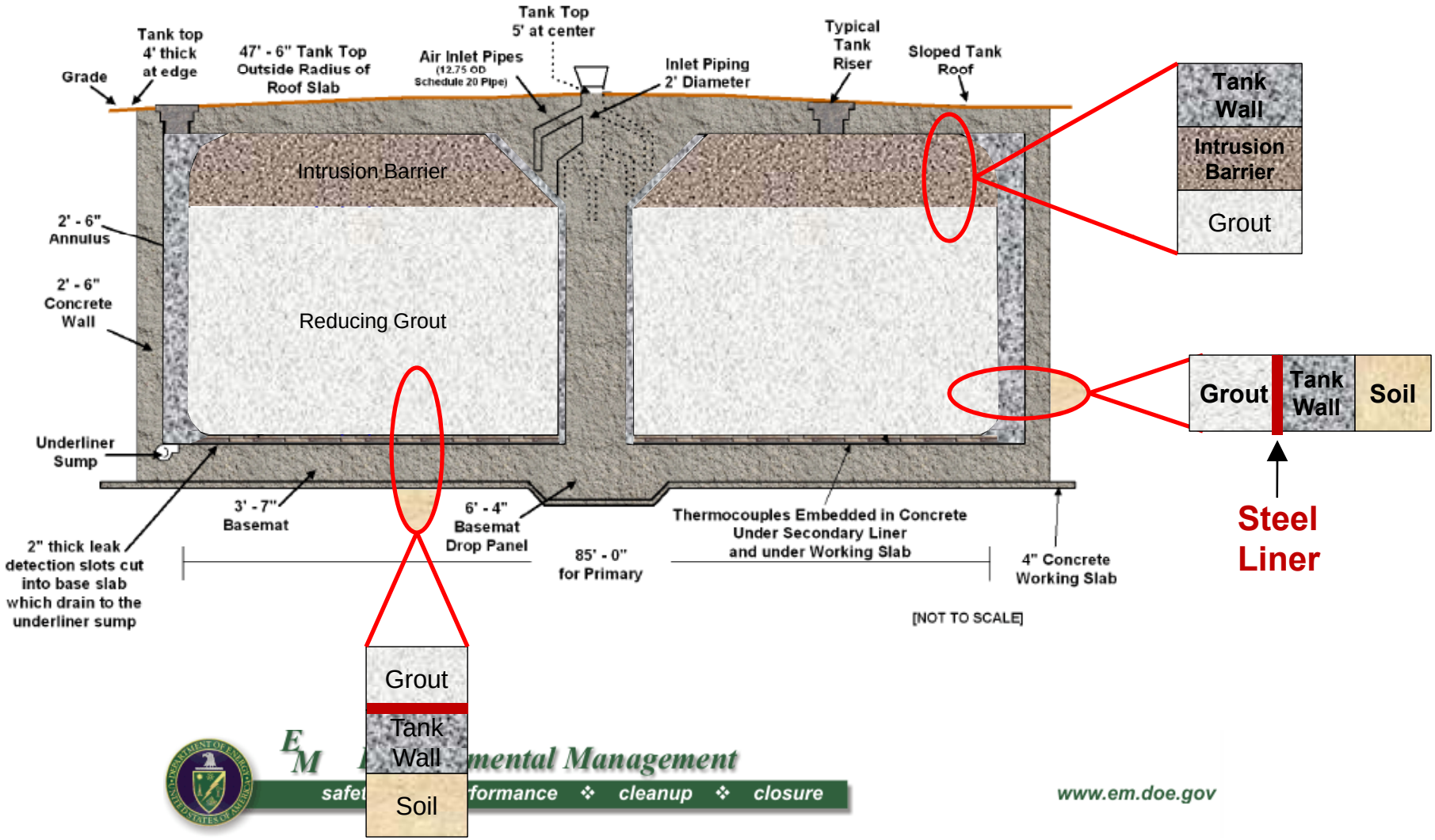
Specifications, Properties, and Phenomena for the Evaluation of Performance of Cementitious Barriers



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
  - LeachXS/ORCHESTRA – Chemical Performance & Constituent Release
- Vanderbilt University/CRESP
  - Chemical Performance & Constituent Release (experimental)
  - Uncertainty Analysis Framework
  - Model Integration

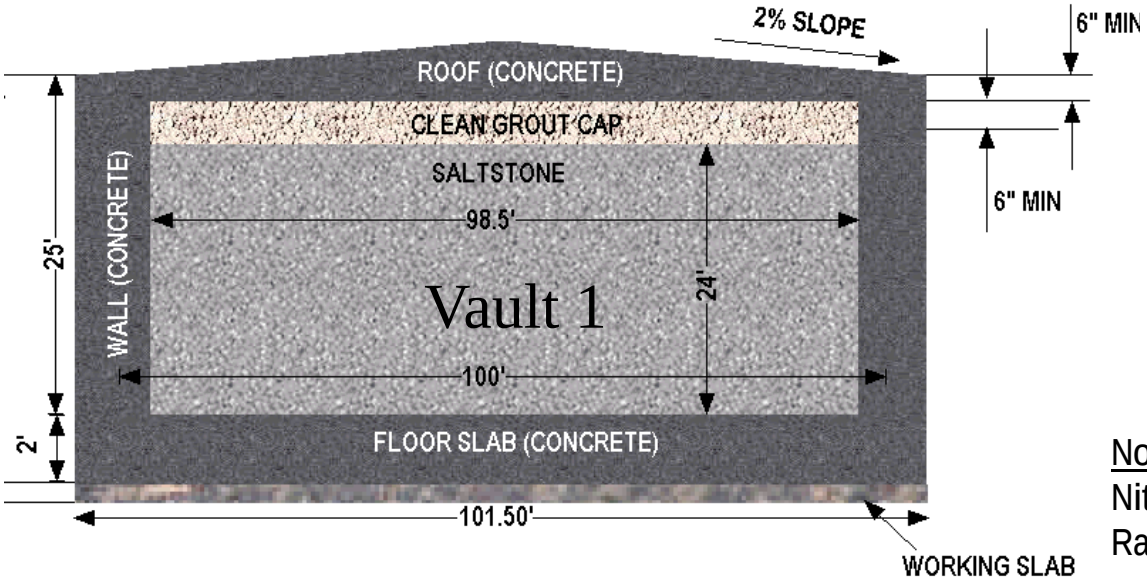
Type IIIA Tank – Conceptual Closure Model

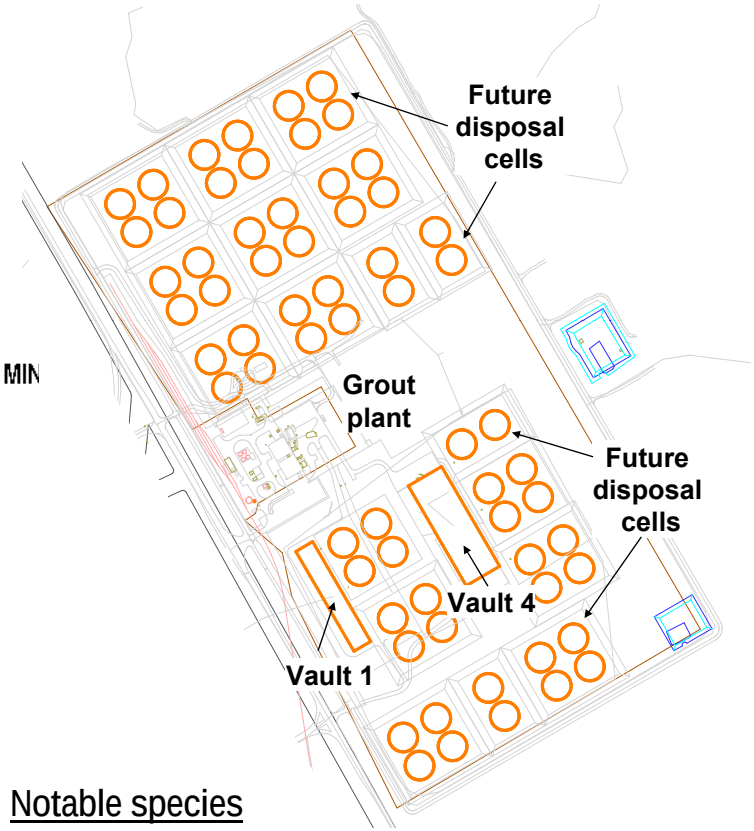


Contaminant Release from Cementitious Materials: Savannah River

►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

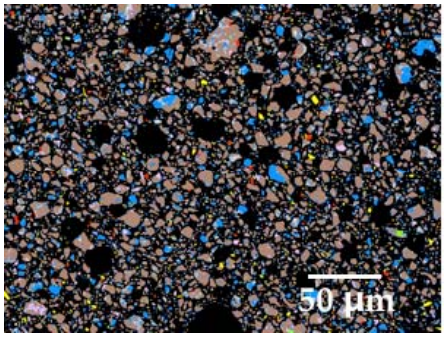




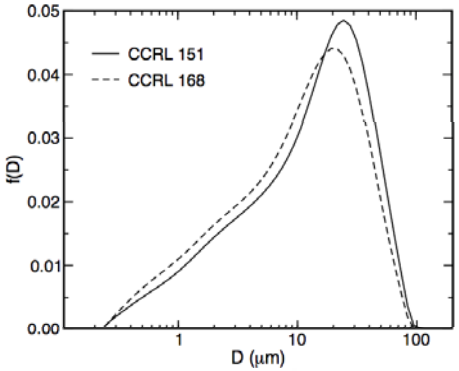
Notable species
Nitrate, Tc-99, I-129 and Ra-226 ingrowth from Th-230

THAMES

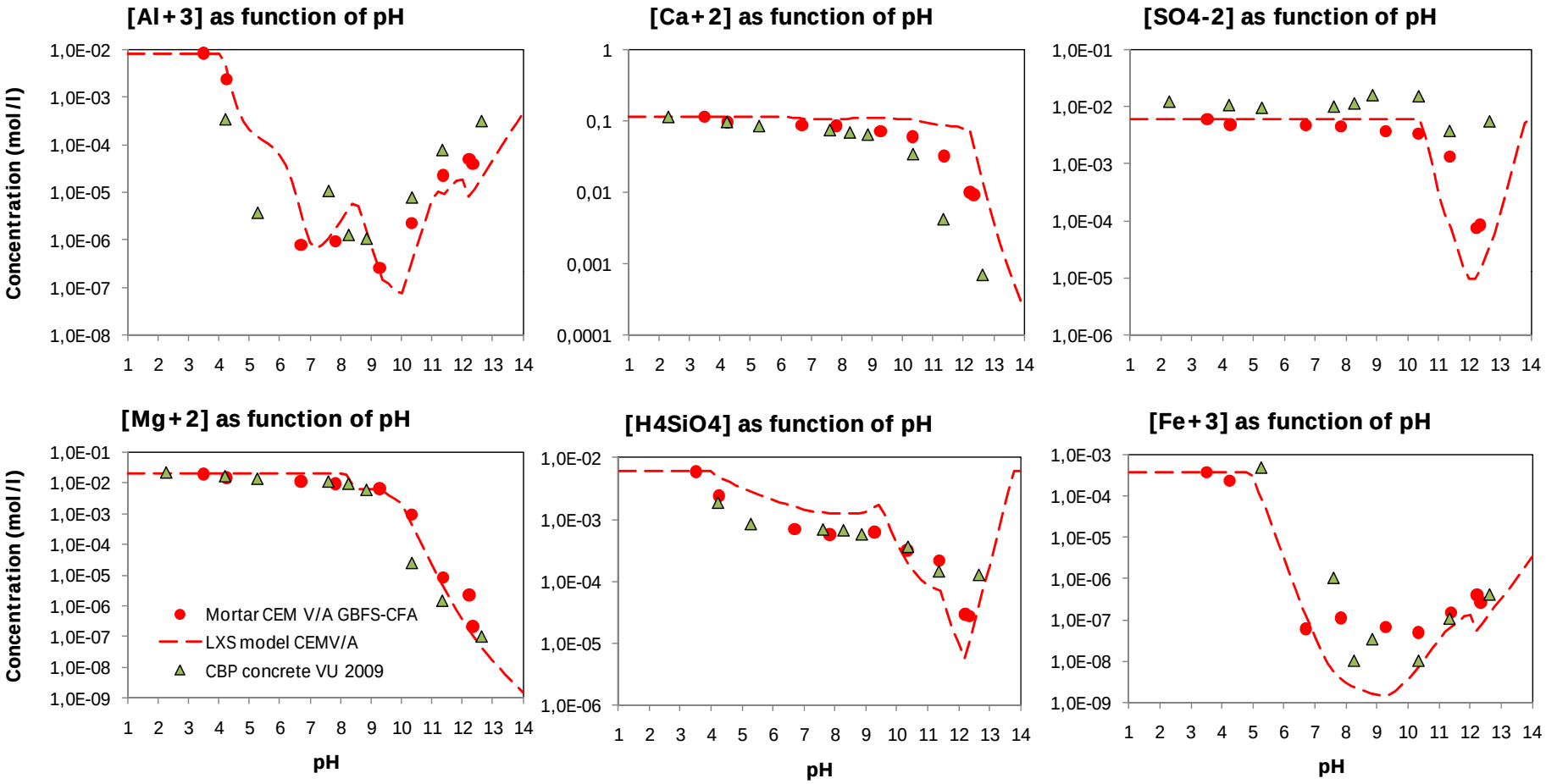
- Chemical and physical properties for a (100 μm)^3 microstructure.
  - ➢ Phase mass fractions & pore solution vs. time
  - ➢ Quantitative microstructure in 3-D vs. time
    - Simulated micrographs of microstructure at various ages
    - Porosity, pore connectivity (percolation), correlation functions
- Parallelization of THAMES in order to be able to generate 1000^3 size models (e.g. for fluid permeability and for computational speed), cracking



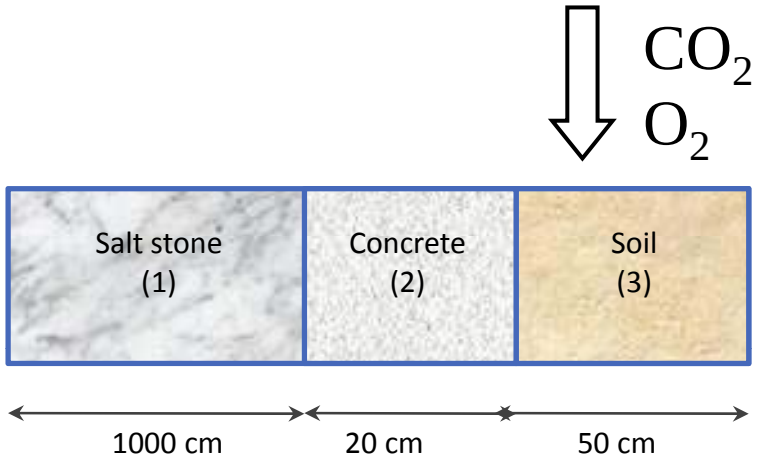
C_3S (brown)
C_2S (blue)
C_3A (gray)
C_4AF (white)
gypsum (yellow)
calcite (green)
periclase (pink)



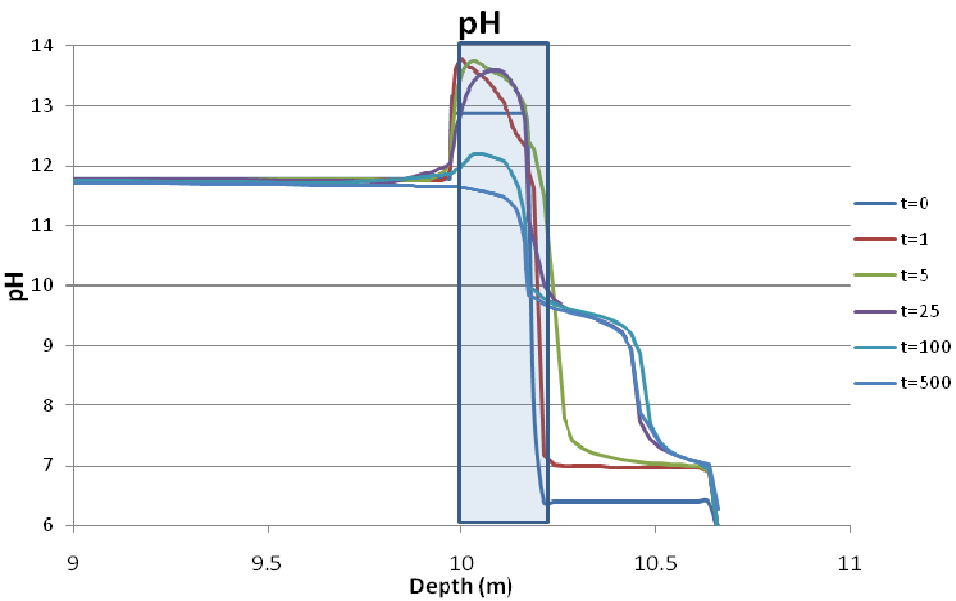
Comparison of Cement Mortar Data and Thermodynamic Model

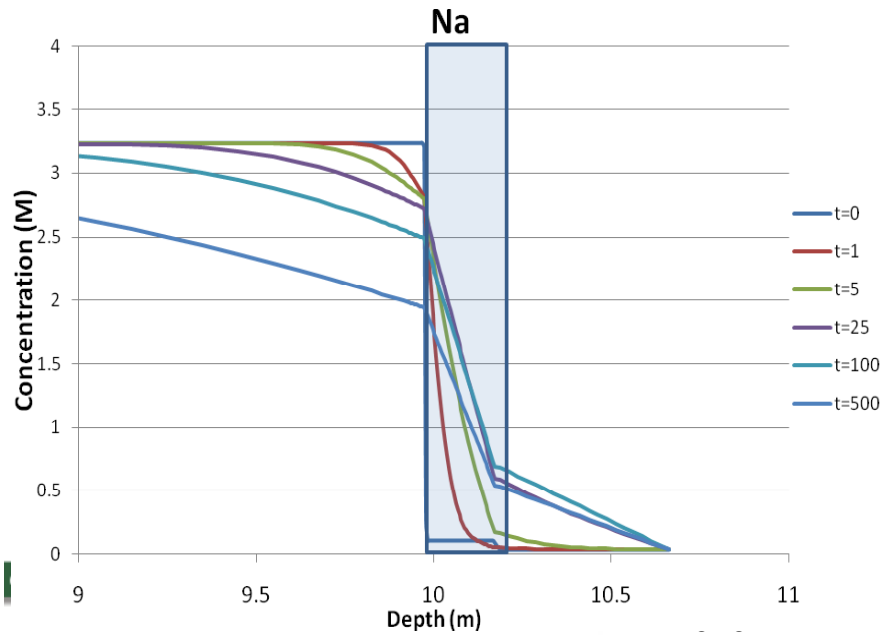


3-Layer Reference Scenario

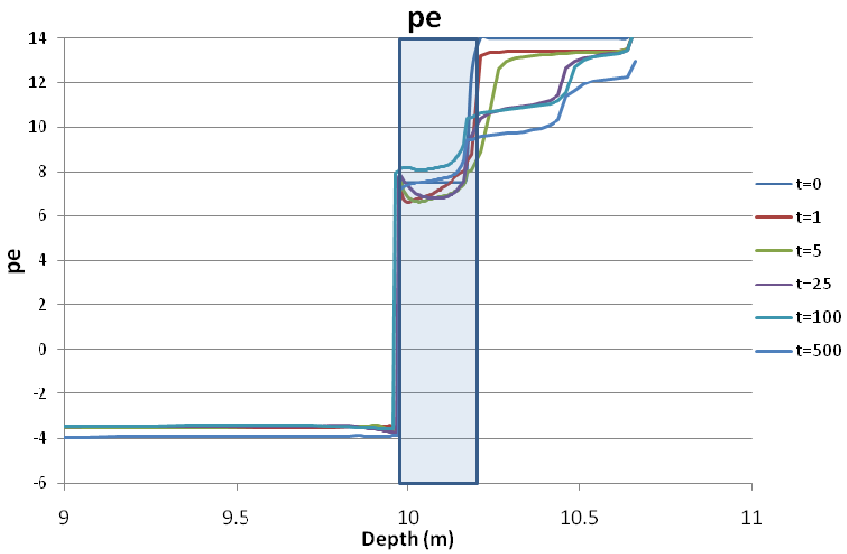


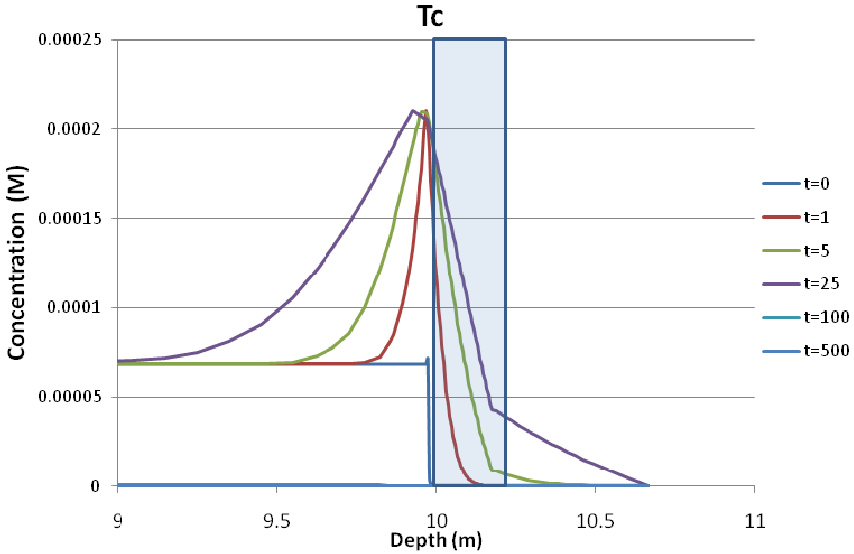
- 3-Layer, 1-D diffusion model for reactive substances
- CO_2 and O_2 influx in soil layer proportional to partial pressure difference air-soil.



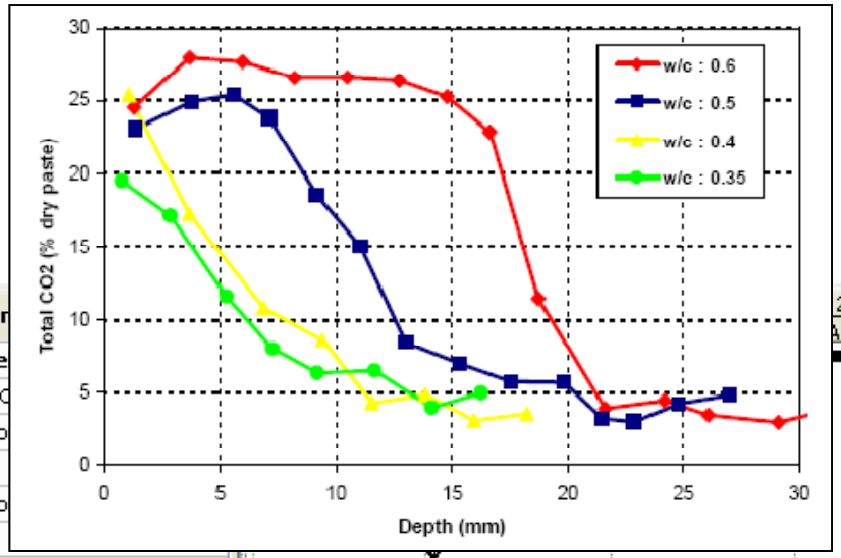


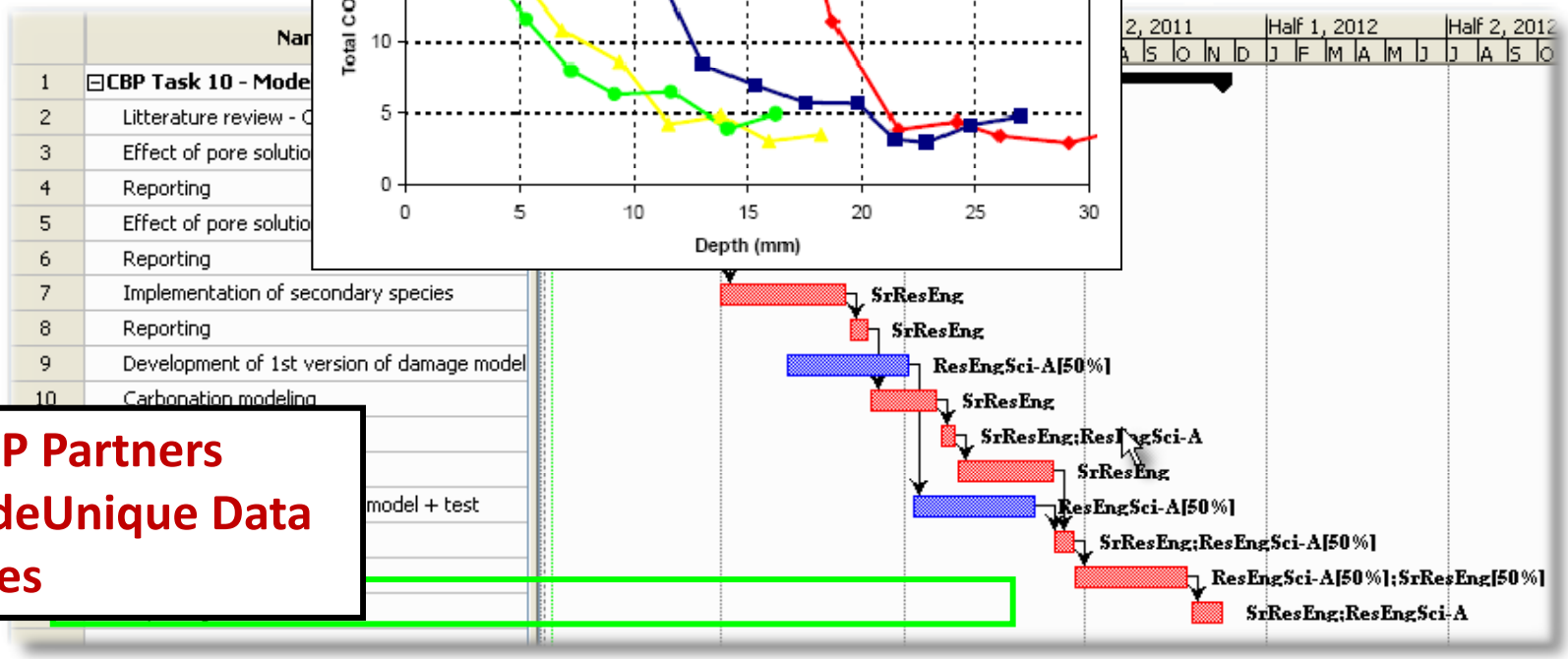
Effect of Redox Gradient Evolution on Tc Release





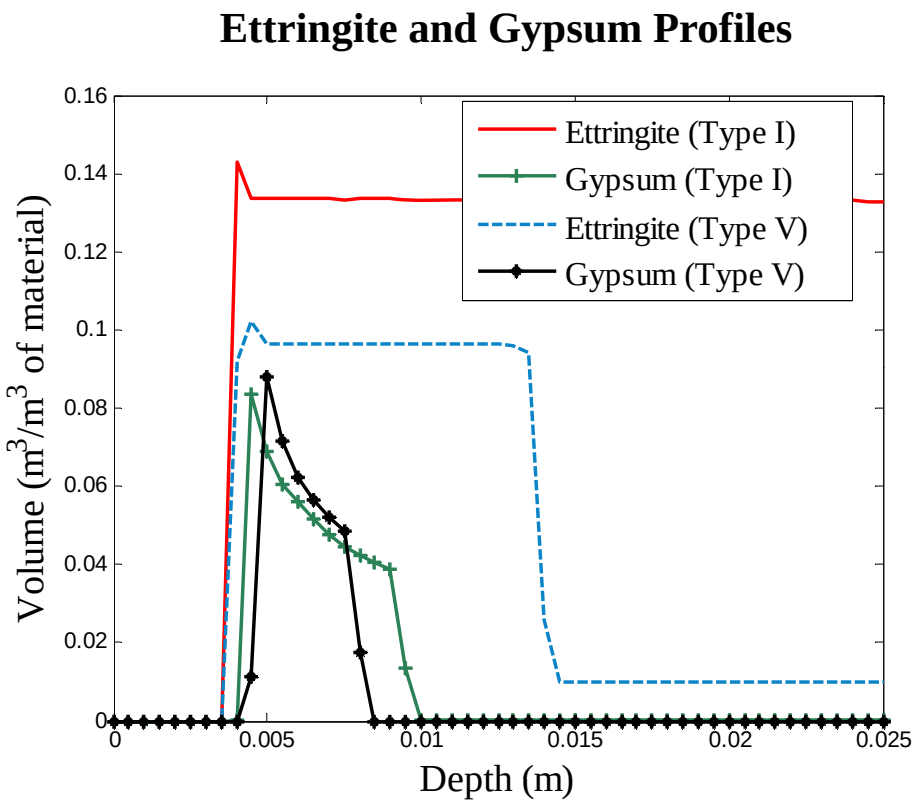
Carbonation modeling –
SIMCO Experimental results for validation.

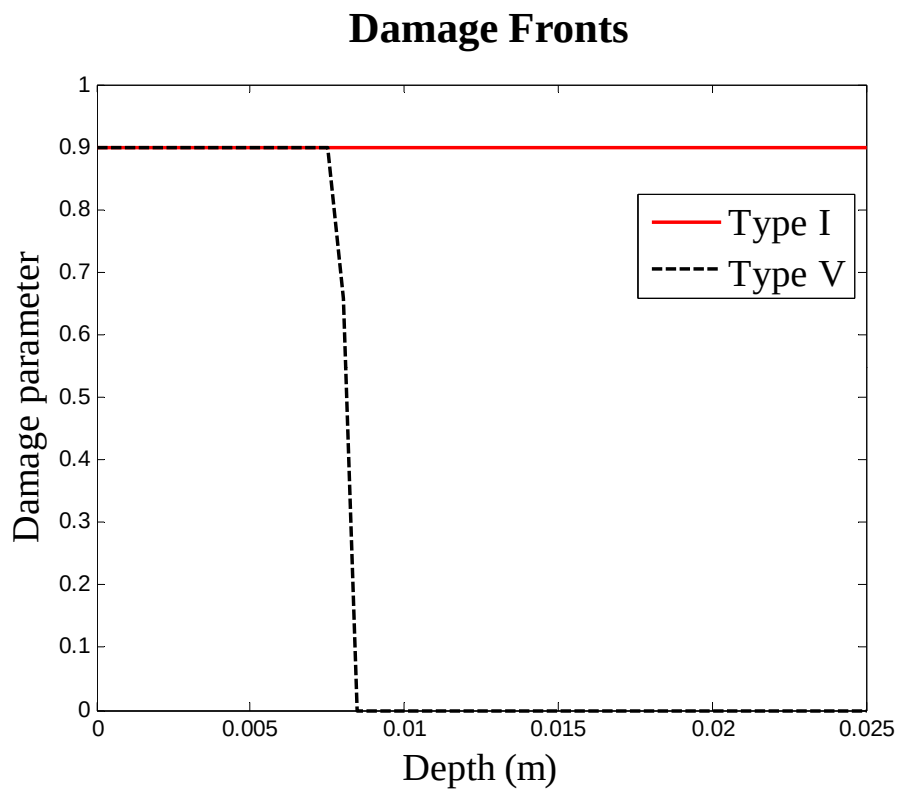




All CBP Partners ProvideUnique Data Sources

Cement Type





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

Uncertainty Quantification

Method 1

Repeat N_2 times

Generate samples for parameters having Data Uncertainty

Repeat N_1 times

Generate samples for parameters having Physical Variability

Perform simulation

Generate sample for Model Error

Durability Assessment

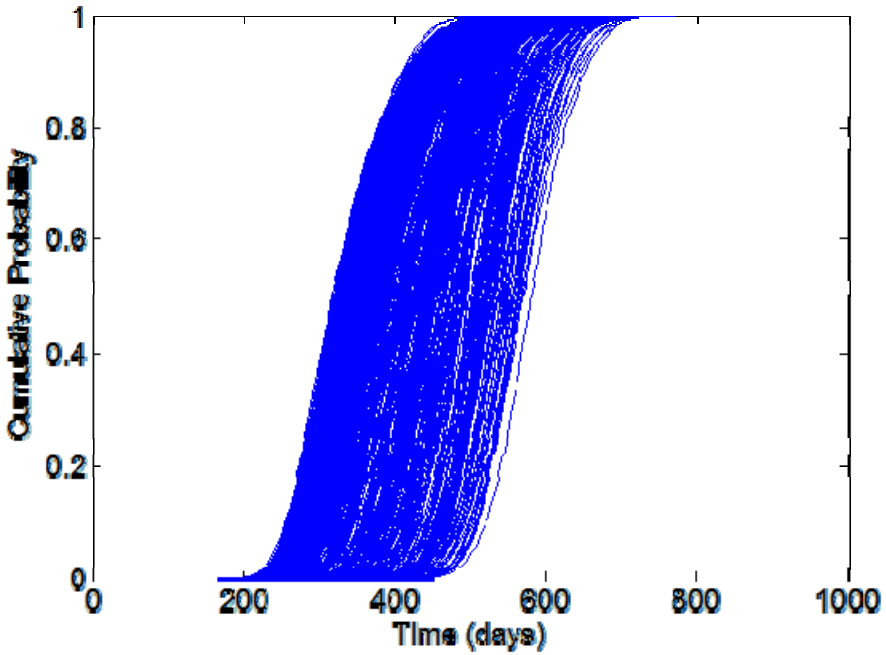
Distribution of Durability **Method 2**

Confidence Bounds on Durability Curve

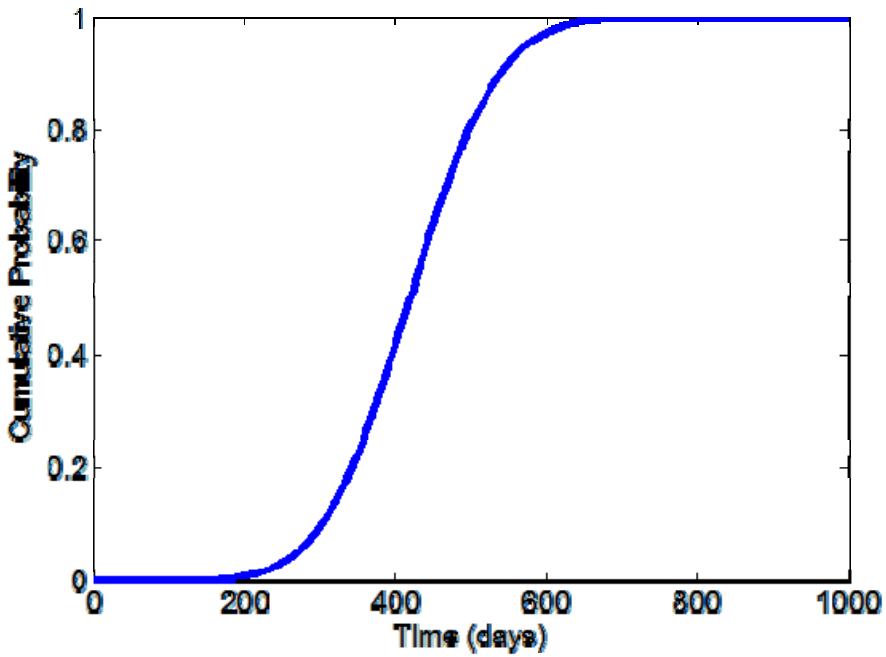
Assessment of Time to Failure

(accelerated case for demonstration of approach)

Method 1



Method 2



- **Failure Criterion : 50% of the structure reaches maximum damage level (damage parameter = 0.9)**