Cementitious Barriers Partnership

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U.S. DOE Office of Waste Processing Technical Exchange

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Partnership Members

- **Department of Energy – Office of Environmental Management (DOE-EM)**
  - Principal supporting agency
  - Primary end-user
- **Nuclear Regulatory Commission (US NRC)**
  - Oversight & Research Divisions
  - Primary end-user
- **National Institute of Standards and Technology (NIST)**
- **Savannah River National Laboratory (SRNL)**
- **Vanderbilt University/ Consortium for Risk Evaluation with Stakeholder Participation (VU/CRESP)**
- **Energy Research Centre of the Netherlands (ECN)**
- **SIMCO**

Expert Advisory Panel organized through CRESP Independent Peer Review Board

Concrete Cancer

Courtesy of F. Sanchez, Vanderbilt U.

Project Goal

- Develop reasonable and credible set of tools to predict structural, hydraulic, and chemical performance of cement barriers used in nuclear applications over extended time frames (>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
- Reduce uncertainties in environmental assessments (e.g., risk and performance assessments) and design

Safety and Risk Issues

- Current PA approach may not adequately represent risk and uncertainty of disposal and containment systems and practices
  - Wasteform selection, contaminant loading, optimization
  - Disposal decisions
  - Remediation and D&D options evaluations
  - “Conservative” assumptions constrain future applications
- Need improved basis for understanding materials performance beyond initial design life
  - Service life extension for existing facilities
- Design improvements for future facilities may not be realized due to lack of mechanistic understanding of cementitious barrier performance

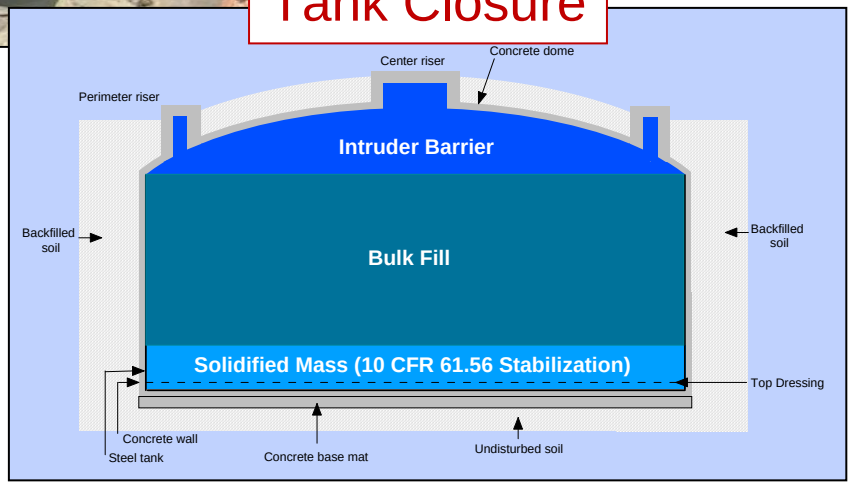
DOE Applications

Low-Activity Waste (LAW) Disposal

Components in Grout

Saltstone Vaults

Tank Closure



D & D Entombment

Environmental Management

safety ❖ performance ❖ cleanup ❖ closure

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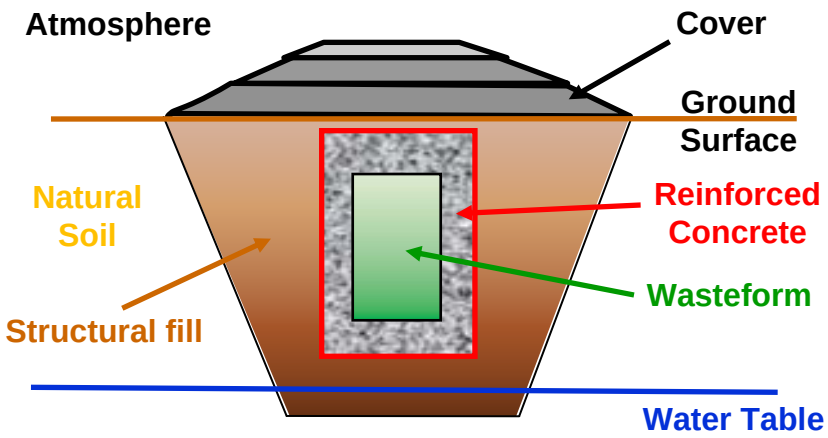
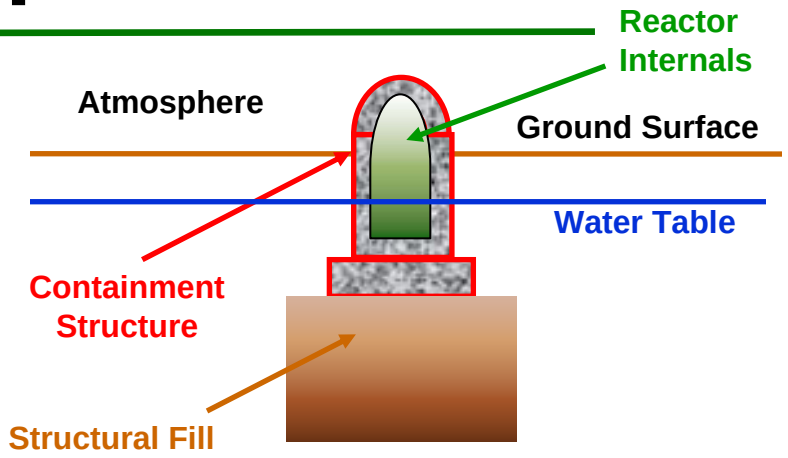
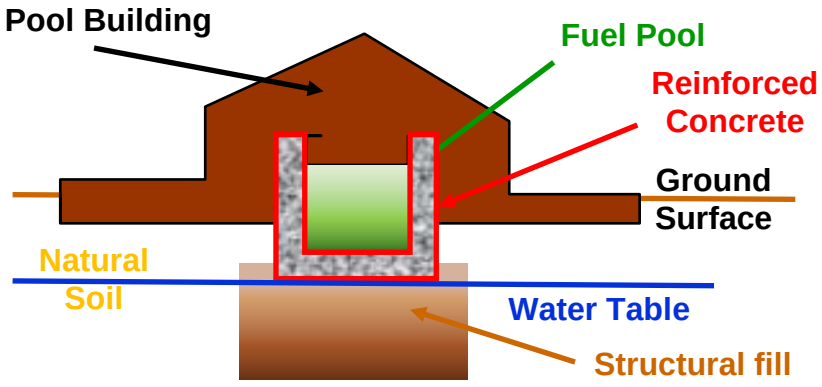
Nuclear Facility Applications



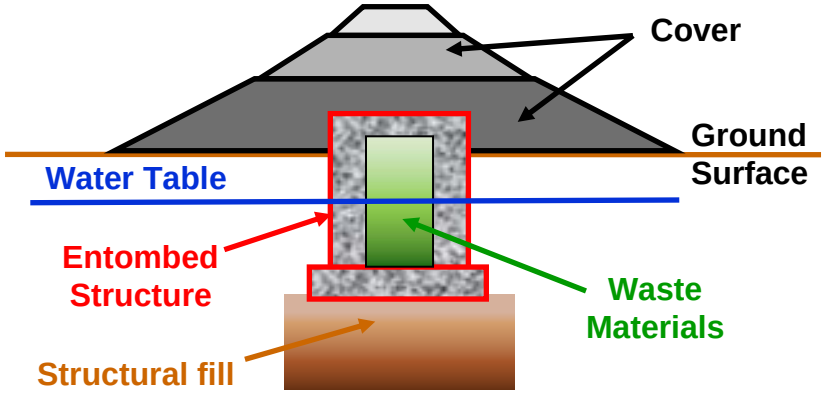
Low-Level Waste (LLW) Disposal



Nuclear Power Plant



Spent Fuel Pool

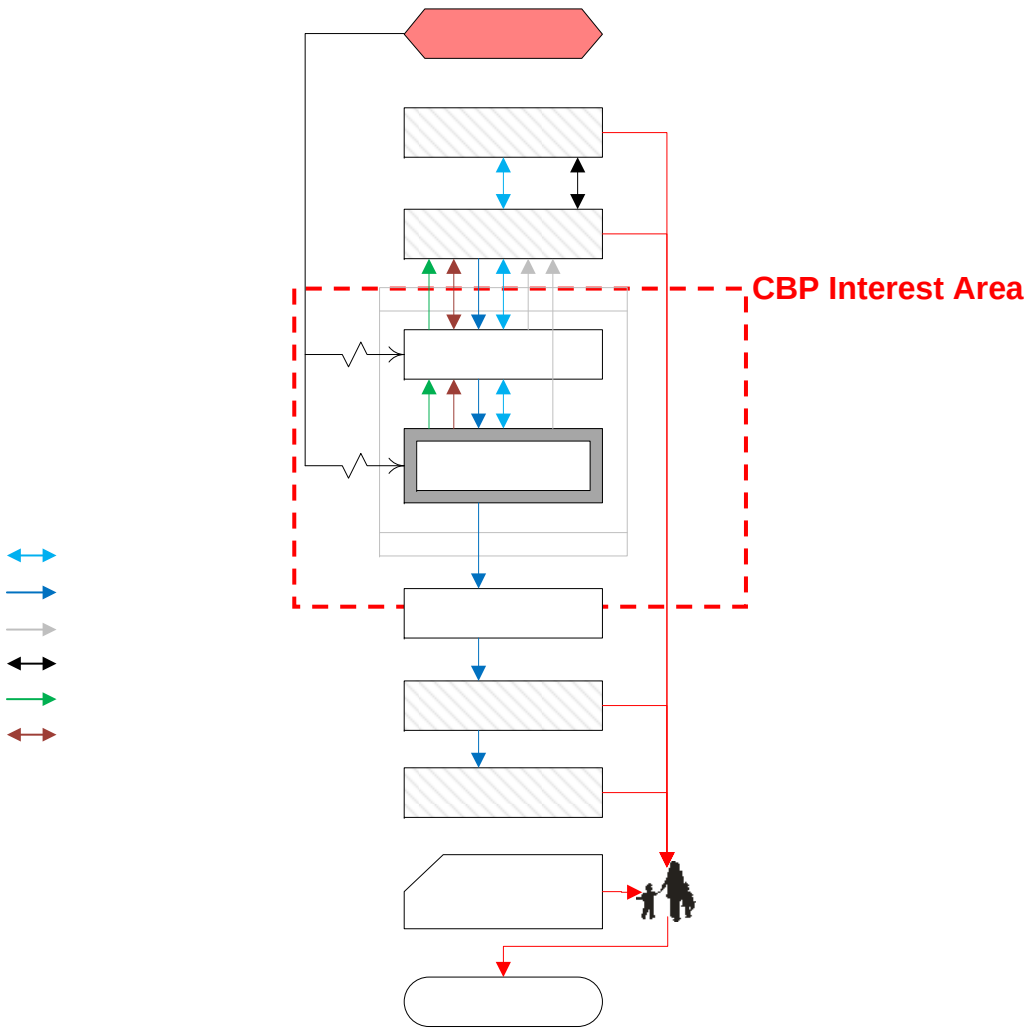


Entombment

Technical Strategy / Approach

- **Reference Cases – provide basis for comparison and demonstration of tools under development**
  - Cementitious wasteform in concrete disposal vault with cap
  - Grouted High-Level Waste (HLW) tank
  - Spent fuel pool
  - 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 and PA frameworks
- **Coordinated experimental and computational program**
  - Conceptual model improvement
  - Define test methods and parameter measurements
  - Model validation

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.

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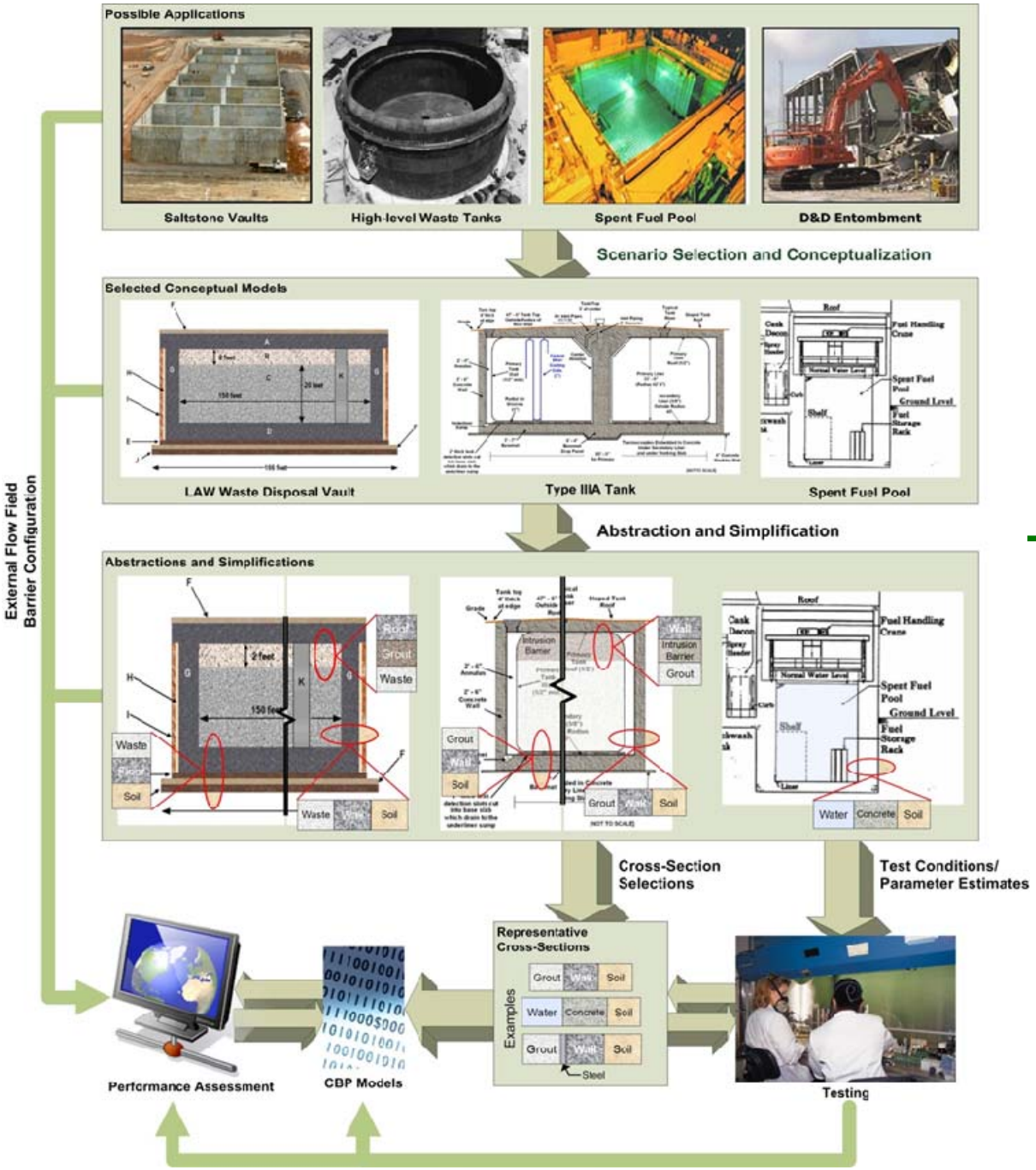
Linking Prototype Cases to Performance Models through System Abstraction



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Integrated Long-Term Degradation

Chemical degradation and physical structure evolution are coupled.

Physical stress

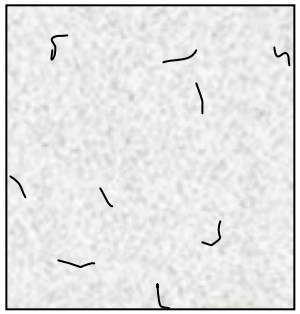
- External loading
- Drying shrinkage
- Seismic events
- Settlement

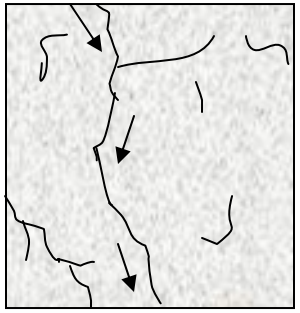
Chemical Alteration

- Oxidation and Leaching
- Pore and crack evolution
  - Dissolution and cracking
  - Precipitation and sealing
- Expansive reactions and corrosion
  - Carbonation
  - Sulfate attack
  - Rebar corrosion

Microcracks

- Increase porosity
- Increase interaction pore water/surface



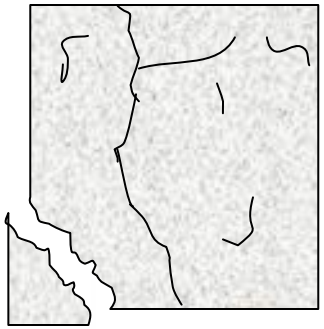


Through-cracks

- Preferential flow path
- Diffusive and convective release
- Loss of strength

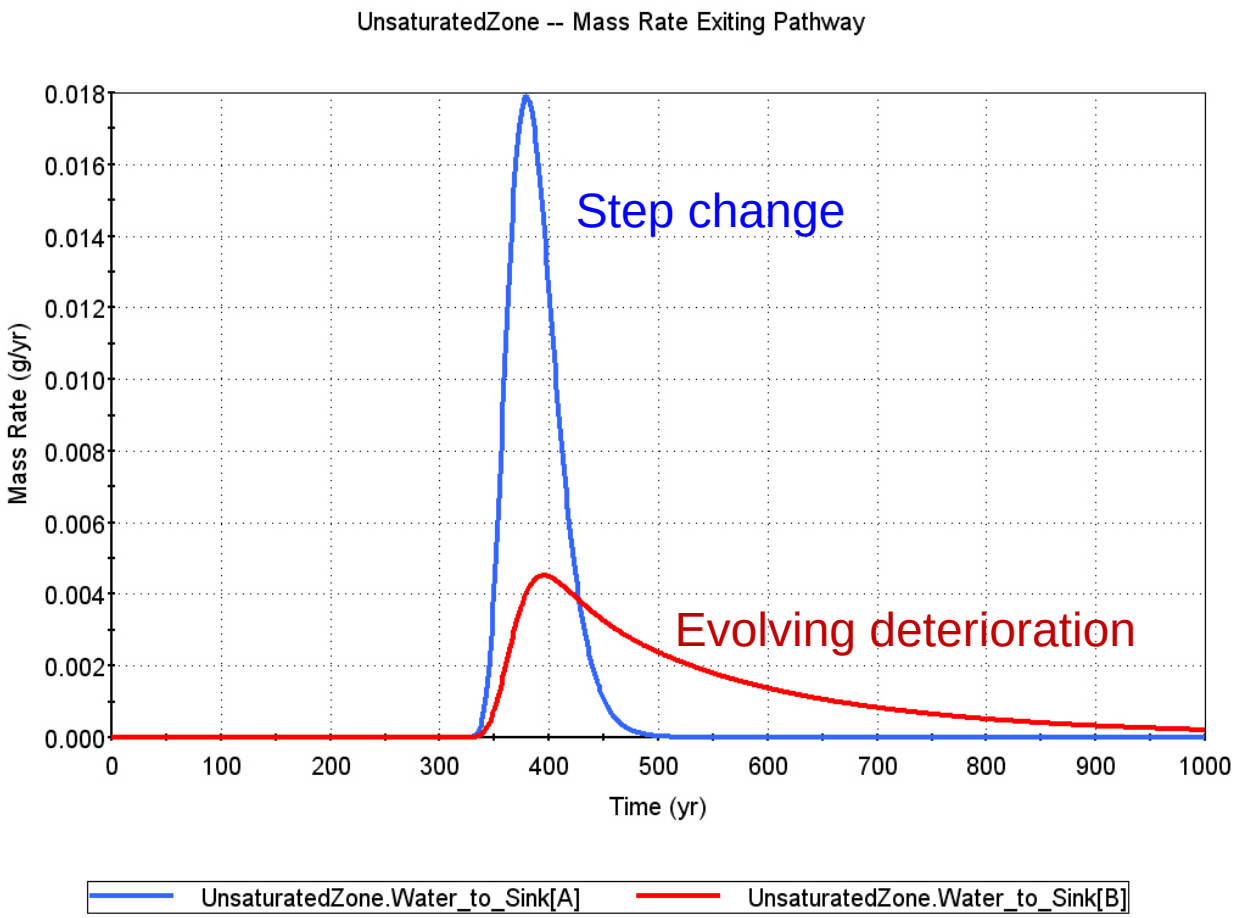
Spalling

- Loss of cohesiveness
- Two body problem
- Eventual release from "granular" material

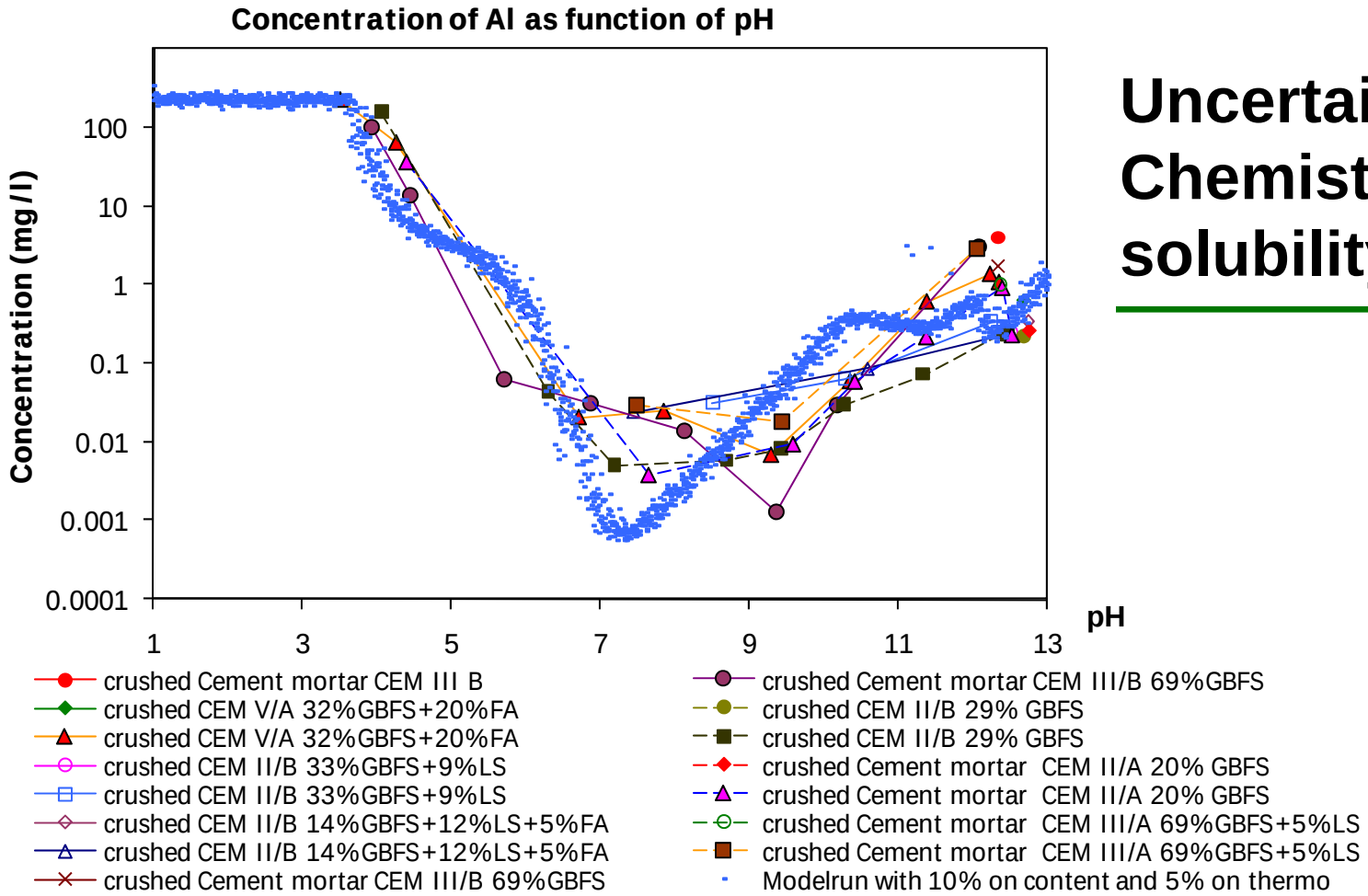


Impact of Different Degradation Pathways

(conceptual example)

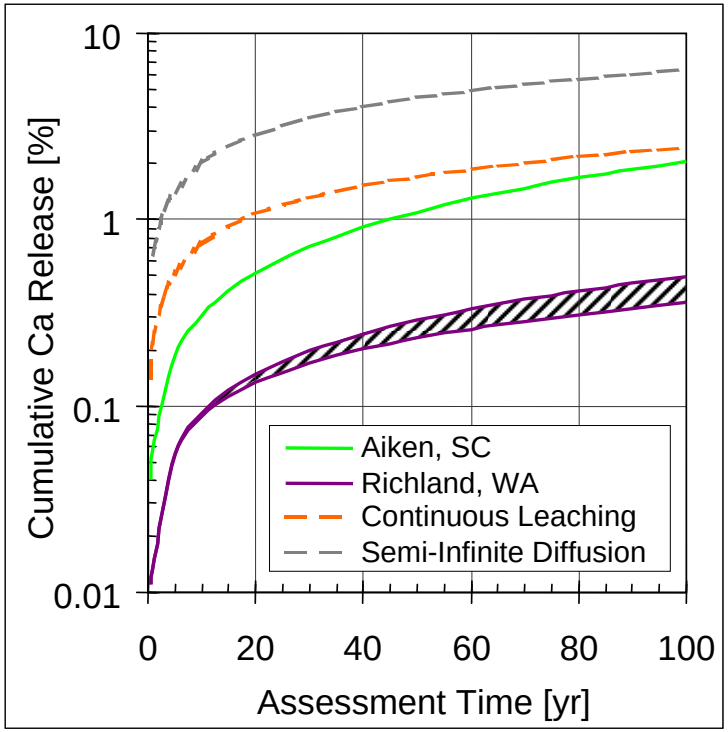


Uncertainty and Chemistry (local solubility)

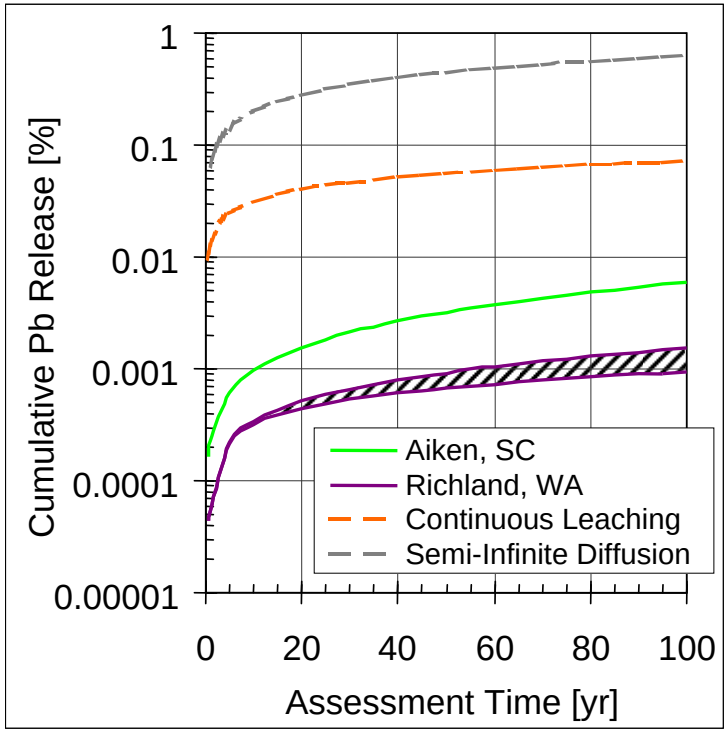


Impact of Model Assumptions – Examples

Leaching over Time: Comparison of release estimates using the (i) simple diffusion, (ii) chemistry & saturated conditions and (iii) chemistry & intermittent infiltration.

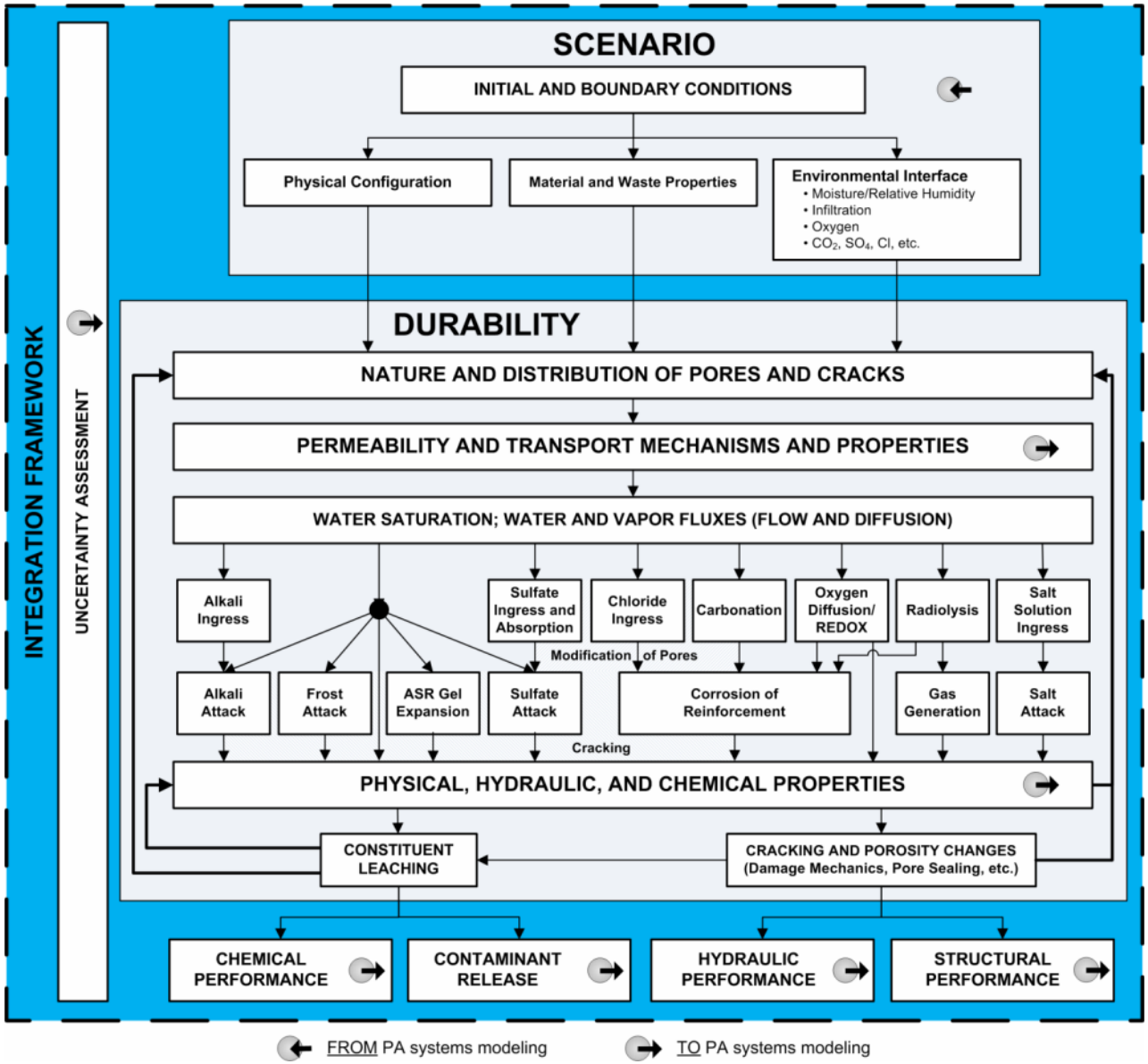


Calcium

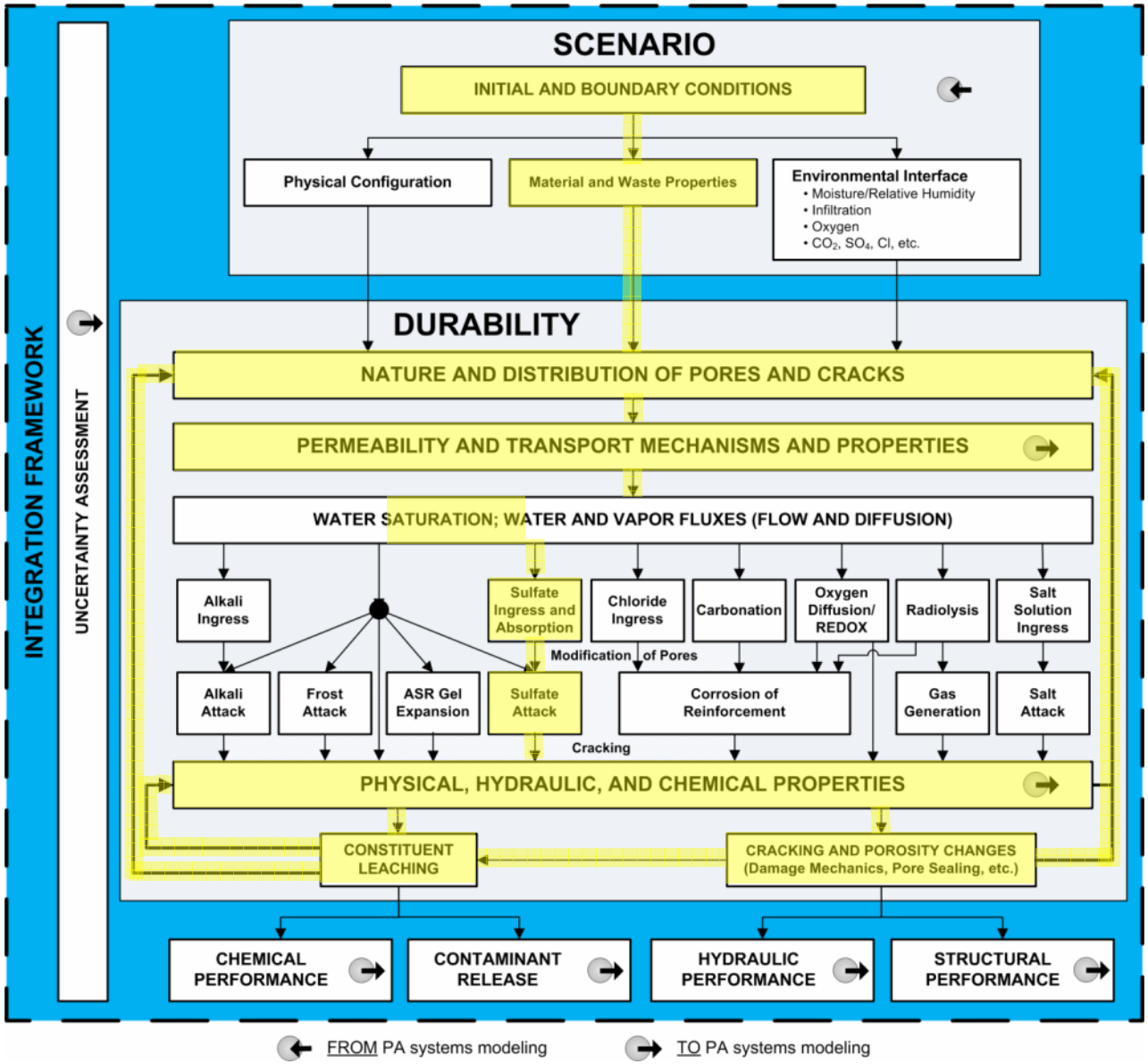


Lead

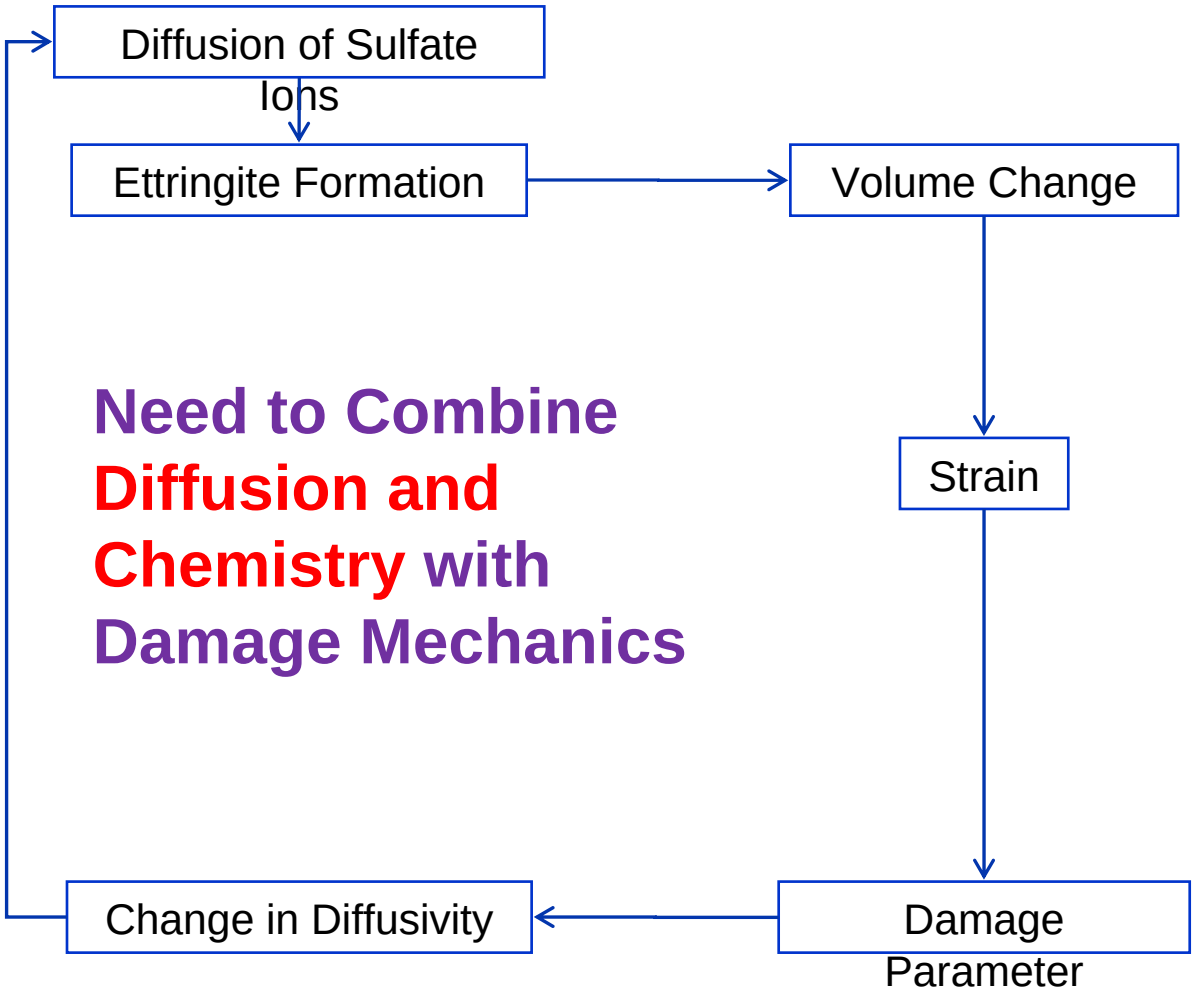
Specifications, Properties, and Phenomena for the Evaluation of Performance of Cementitious Barriers



Sulfate Attack as a "proof of principle" for coupling of phenomena

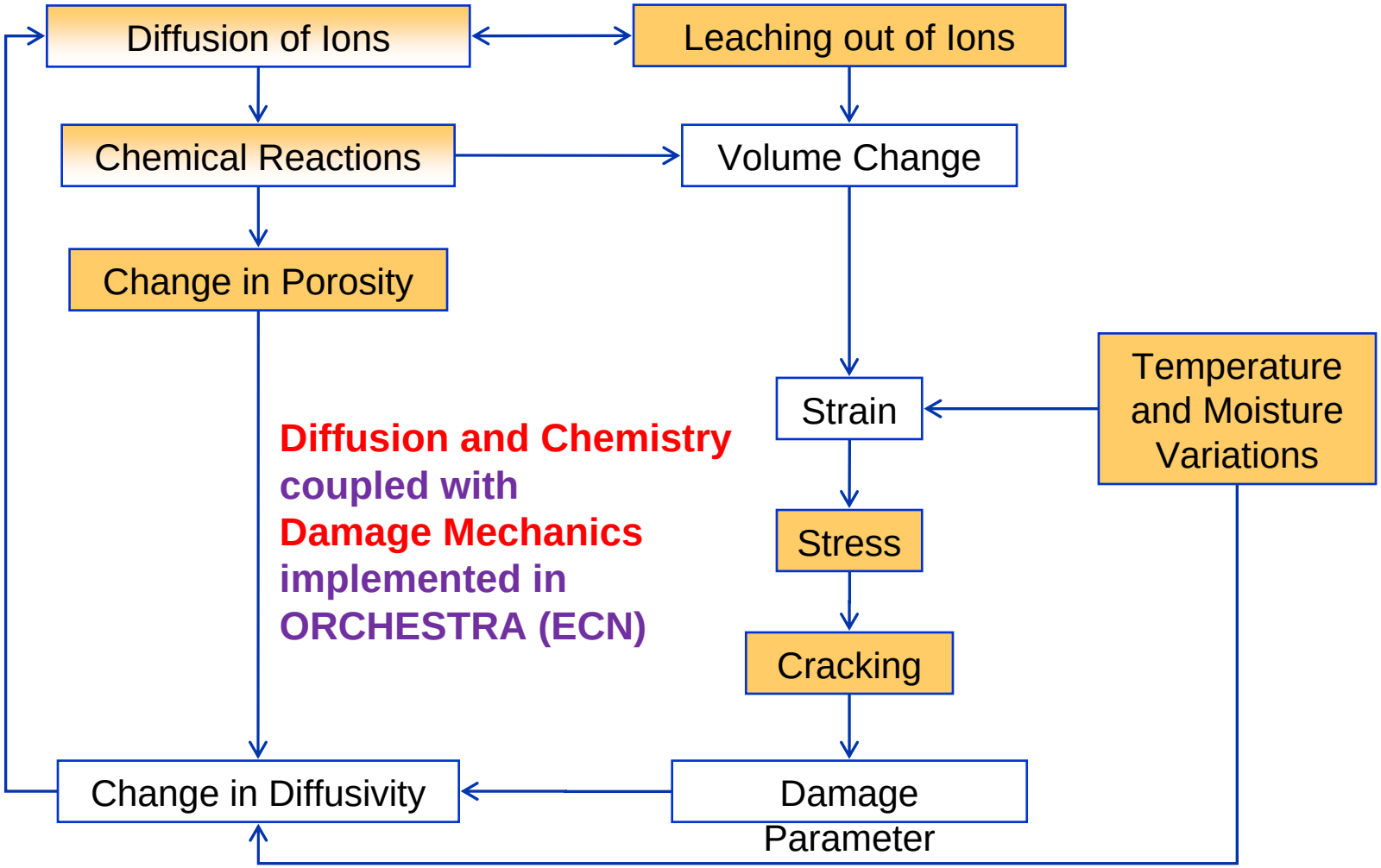


Modeling Sulfate Attack – Historical

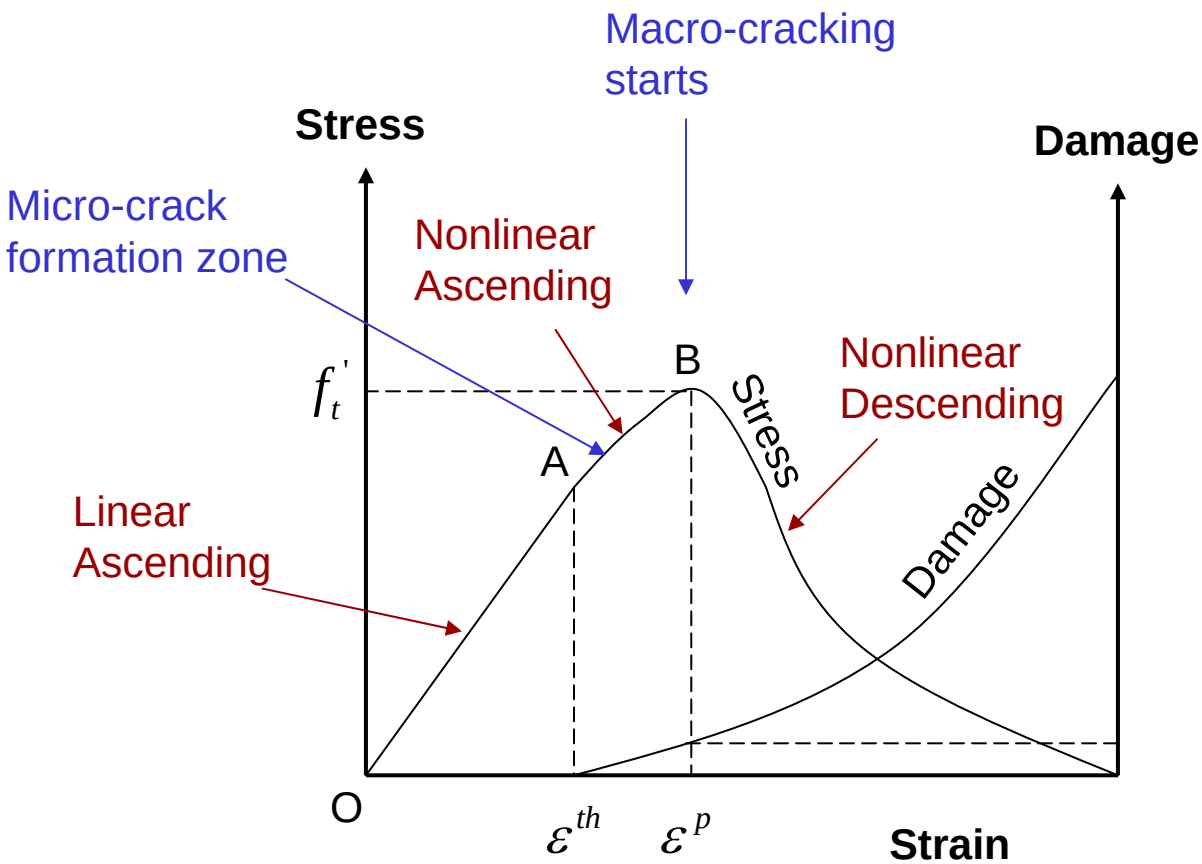


Need to Combine Diffusion and Chemistry with Damage Mechanics

Modeling Framework – Sulfate Attack



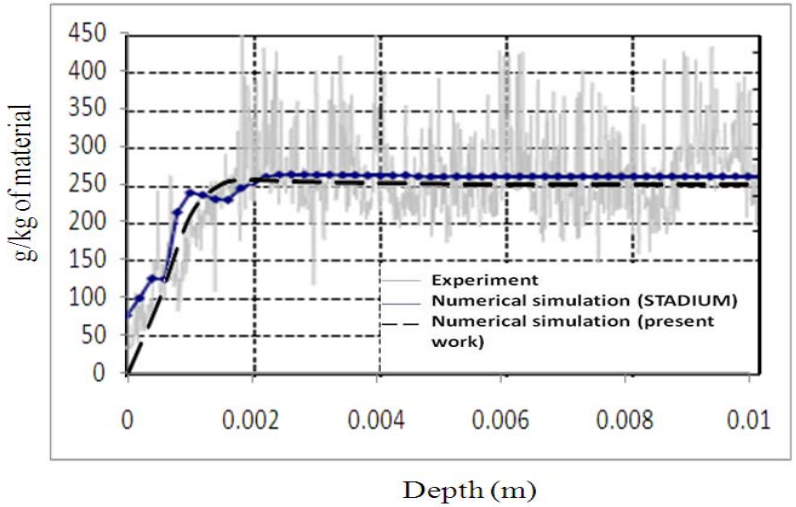
Damage Accumulation



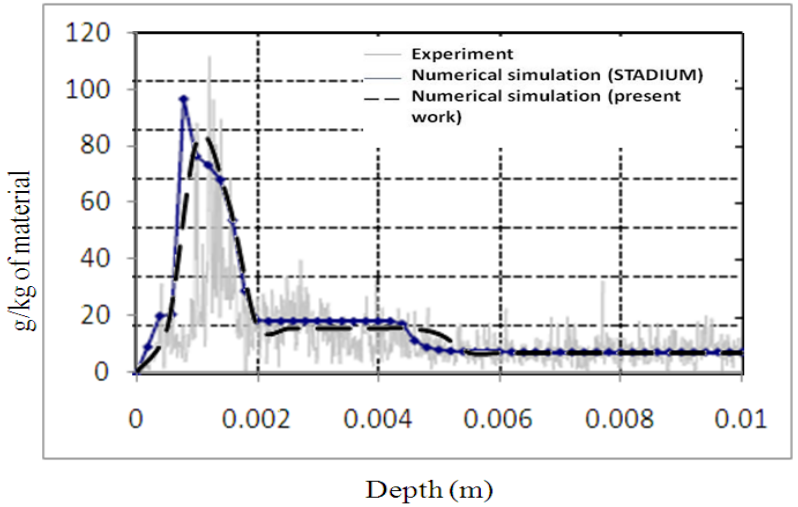
Qualitative Comparison

Calibration: 3 mo

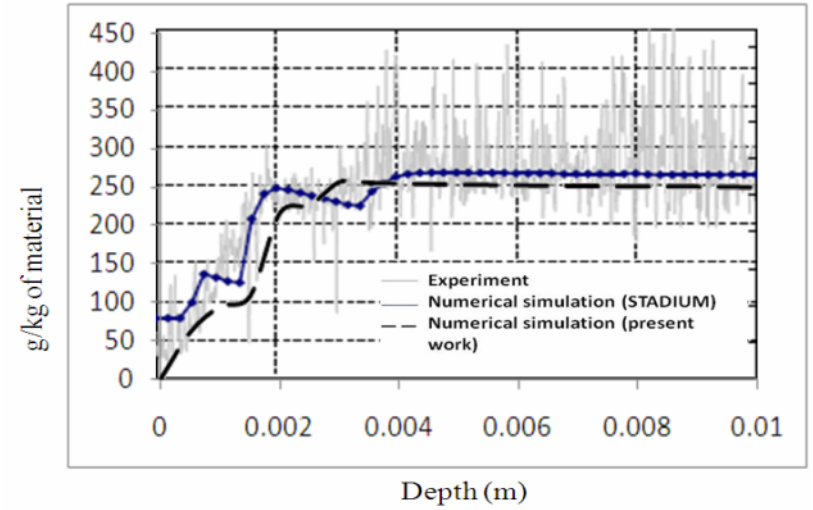
Calcium Profile (Samson *et al.*, 2007)

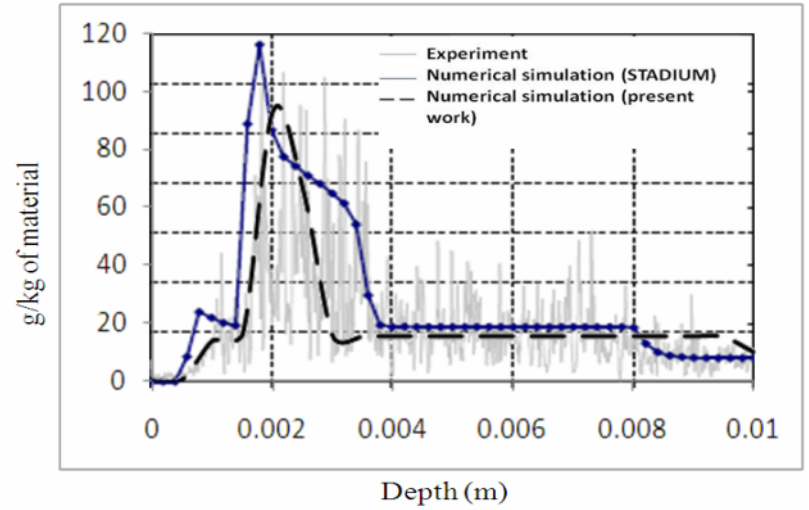


Sulfur Profile (Samson *et al.*, 2007)

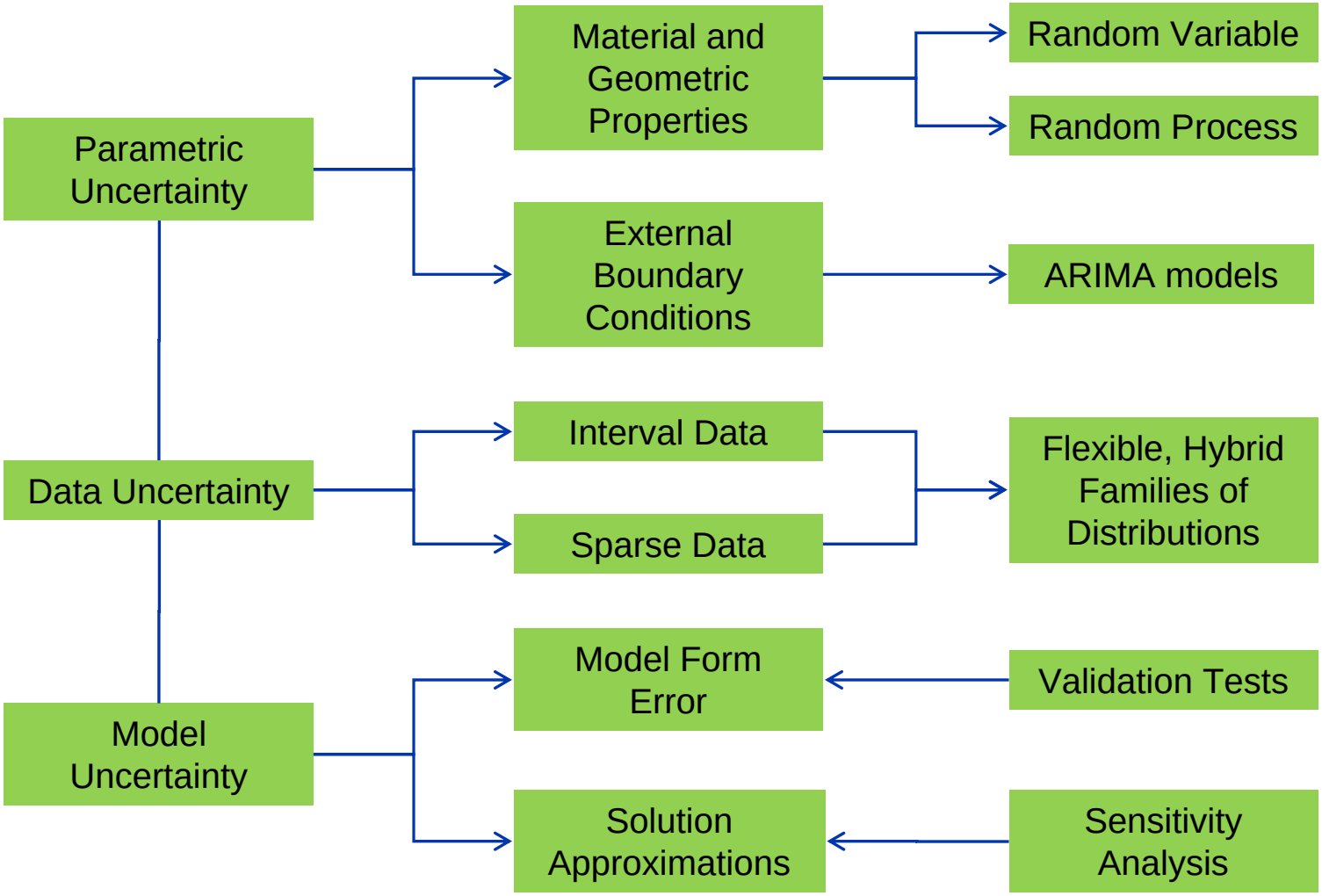


Validation: 1 yr





Sources of Uncertainty



Uncertainty Quantification

1. Parametric and Data Uncertainty

Monte Carlo Simulation

Samples of Variables and Their Distribution Parameters → Model → CDF of Model Response and Confidence Bounds

2. Model Uncertainty

Prediction vs. Observation

↓

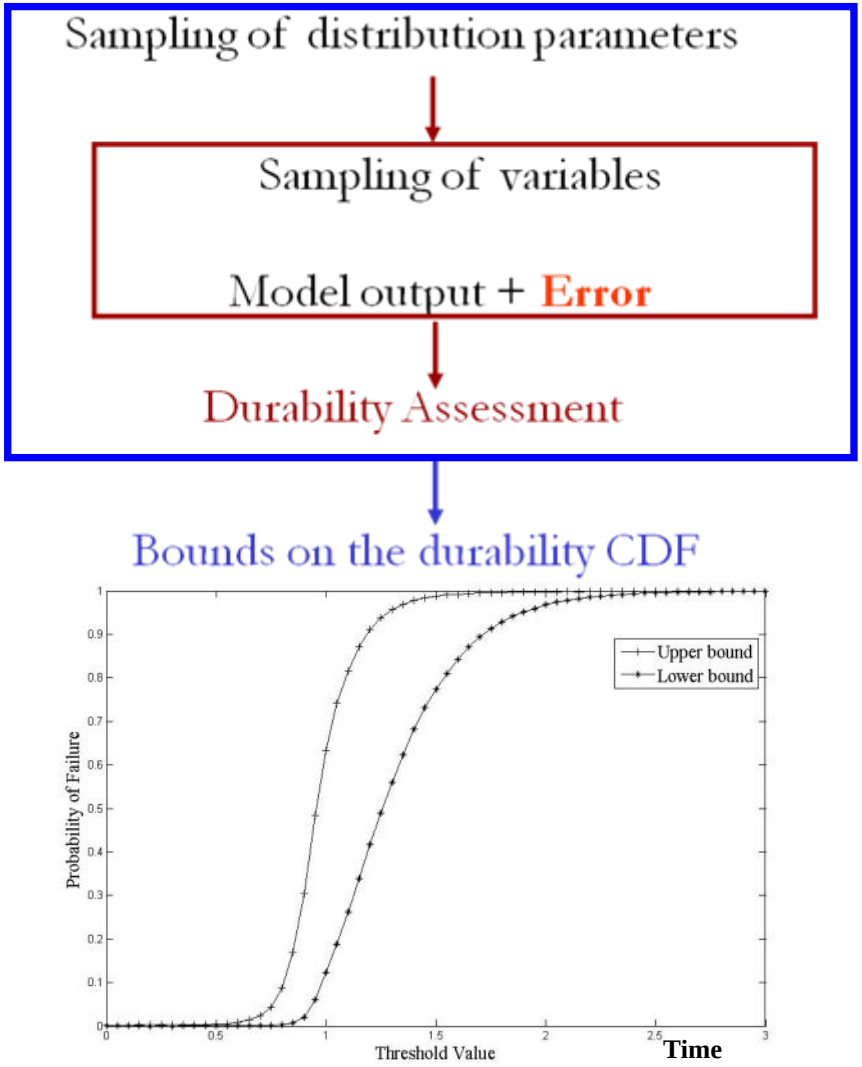
Bayesian Hypothesis Testing → $B = \frac{P(y_{\exp} | M_0)}{P(y_{\exp} | M_1)}$

↓

Confidence in Model Prediction → $C_f = \frac{B}{B+1}$

Model Error and Uncertainty Quantification

- Model error quantification
  - Solution approximation
  - Model form error
- Bayesian approach
  - Model validation
  - Calibration
  - Extrapolation
  - Confidence assessment



Expected Project Impact

- Reduced uncertainty and improved consistency for PAs
- Improved system designs (waste management and new facilities)
- Monitoring and maintenance approaches for extended (100s, 1000s yr) service life
- Updated guidance documents (assessment tools, test methods, data)
- Industry-wide technical basis for evaluation amongst stakeholders (DOE, NRC, state regulators, others)
- Assessment transparency
- Template for assessment of complex systems

Partnership Products

- Near-term
  - Review of historical PA practices including uncertainty evaluations
  - State-of-the-art reports on mechanistic and process understanding and approaches to uncertainty and integrating platforms
  - Definition of reference cases with focus on useful example cases
- Next 6 months
  - Detailed technical descriptions of candidate software and selected integrating platform (e.g., GoldSim)
  - Tier 1 integrated framework in GoldSim as proof-of-concept
  - Compilation and recommendations on test methods for model parameterization
- Long-term
  - Tier 2 (fully) integrated framework including comprehensive uncertainty analysis

Q/A

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