Technical Basis for Cementitious Barriers Partnership Models

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LeachXS/ORCHESTRA

- LeachXS
  - Database expert/decision support system that includes leaching test results for 600+ materials, scenarios and regulations
  - Platform for assessing short- and long-term release of constituents of potential concern
  - Assists in source term evaluation through reactive transport and damage progression modeling

- ORCHESTRA
  - Numerical reactive transport simulation framework embedded in LeachXS
  - Models geochemical speciation and mass transport
  - Flexible and allows users to add/modify existing equations
  - Automatic usage of multiple processors/parallelization
Multiple, Flexible Base Models Available in LeachXS/ORCHESTRA

- Select general field or laboratory scenario to model
- Select from existing CBP reference materials or customize materials
- Select interface conditions (e.g., fixed volume, continuous flow or intermittent flow/exchange & solutions (e.g., “Hanford infiltration” or “saltstone pore water”)
- Resulting model transferable to GoldSIM simulations
Cementitious Barriers Modeling Scenarios

• Currently available:
  • pH dependent equilibrium
    • Test (M1313) and prediction cases
  • Monolith leaching scenario
    • Test (M1315) and prediction cases
  • Monolith leaching with carbonation and oxidation scenario
    • Prediction cases
  • Leaching with sulfate attack scenario
    • Prediction cases
  • Percolation scenario
    • Test (M1314) and prediction cases (local equilibrium & multiple mixed regime models)
Geochemical Speciation Modeling

Progressive Carbonation of Stabilized Waste

Ca as function of pH at L/S=10

Carbonate levels

3 %

12 %

14 %

Partitioning liquid-solid, Ca

3 % carbonate

14 % carbonate

Chemical Speciation Fingerprint (CSF) developed based on Method 1313 and other information sources

Allows evaluation of conditions not readily reproduced in the Lab (e.g., redox changes, aging processes)
Monolith Diffusion

- Laboratory and field simulations
- Variable water contacting sequence, chemistry
- Saturated or unsaturated
- Carbonation, oxidation ingress
- Sulfate attack with leaching
Percolation with Mobile-Immobile Zones

- Laboratory and field simulations
- Variable water flow rate, chemistry
- Effects of preferential flow (e.g., grouted materials, contaminated soils)
Percolation with Radial Diffusion

- Laboratory and field simulations
- Cracked materials or packed beds (e.g., wasteforms, tank closure)
- Effects of preferential flow
- Variable water flow rate, chemistry
### Applications of Cementitious Barriers Models

<table>
<thead>
<tr>
<th>Models</th>
<th>Applications</th>
</tr>
</thead>
<tbody>
<tr>
<td>pH dependent equilibrium</td>
<td>Assessment of waste, waste form, grout and concrete leaching chemistry</td>
</tr>
<tr>
<td>Monolith leaching</td>
<td>Waste form leaching; grout and concrete durability</td>
</tr>
<tr>
<td>Leaching with oxidation and carbonation</td>
<td>Waste form leaching; grout and concrete durability; HLW tank integrity</td>
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<tr>
<td>Leaching with sulfate attack</td>
<td>Concrete durability and interfacial processes</td>
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<tr>
<td>Column percolation</td>
<td>Leaching from contaminated soils; leaching and pH evolution from tank grouting (cracking scenarios)</td>
</tr>
<tr>
<td>Homogeneous</td>
<td></td>
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<tr>
<td>Dual porosity w/radial and orthogonal diffusion</td>
<td></td>
</tr>
</tbody>
</table>
Finite difference method

Linear approximation of
\[
\frac{\partial c_i}{\partial t} = \frac{D_i \partial^2 c_i}{\tau \partial x^2}
\]

Three commonly employed schemes
- **FTCS** – forward in time, centered in space; “fully explicit”; “forward Euler”
- **BTCS** – backward in time, centered in space; “fully implicit”; “backward Euler”
- **CN** – Crank Nicolson; “semi-implicit”; average of FTCS and BTCS solutions

**FTCS** requires least computational expense but is only stable for \( \frac{D_i \Delta t}{\tau \Delta x^2} < \frac{1}{2} \)

**BTCS** and **CN** are unconditionally stable

For \( \Delta x = 0.5 \text{ mm} \) and \( D_i/\tau = 1.5(10^{-9}) \text{ m}^2/\text{s} \):
- \( \tau = 50 \rightarrow \Delta t_{\text{max}} < 69.44 \text{ min} \)
- \( \tau = 5 \rightarrow \Delta t_{\text{max}} < 6.94 \text{ min} \)

For \( \Delta x = 0.5 \text{ mm} \) and \( D_i = 1.5(10^{-5}) \text{ m}^2/\text{s} \) (**gas diffusion**):
- \( \tau = 50 \rightarrow \Delta t_{\text{max}} < 0.4167 \text{ s} \)
- \( \tau = 5 \rightarrow \Delta t_{\text{max}} < 0.0417 \text{ s} \) (7.6(10^{11}) timesteps for a 1000 year simulation)
Case Study: Oscillating solution example

- Model parameters
  - External (Matlab) transport model utilizing FTCS method
  - 1D model, \( L_{\text{medium}} = 10\, \text{mm}, L_S = 10 \)
  - \( \Delta x = 0.5\, \text{mm}, D_i = 1.5(10^{-9})\, \text{m}^2/\text{s}, \Delta t = 70\, \text{min}, \phi = 0.2, \tau = 50 \)

- FTCS approximates the solution at early times, but ultimately diverges from the analytical solution
- Similar results obtained in Orchestra for \( \Delta t = 71\, \text{min} \)
- For porosity opening (decreasing \( \tau \)), \( \Delta t_{\text{max}} \) may become prohibitively small
- For gas diffusion case, time steps will be prohibitively small
Understanding Carbonation at Interfaces
Microconcrete Preparation

Microconcrete sample types:

- Microconcrete with no fly ash (Control)
- Microconcretes with 45% fly ash replacement using either FA02 (bituminous coal, low calcium fly ash, ~4 wt% Ca) or FA39 (sub-bituminous coal, high calcium fly ash, ~23 wt% Ca)

Sample preparation:

- 6-month cured (100% RH)
- 6-month accelerated carbonation (5% CO$_2$, 65% RH)

<table>
<thead>
<tr>
<th></th>
<th>Control</th>
<th>Blend</th>
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</thead>
<tbody>
<tr>
<td>Nominal Mix (lb/cy)</td>
<td>866</td>
<td>866</td>
</tr>
<tr>
<td>Fly ash replacement (%)</td>
<td>N/A</td>
<td>45</td>
</tr>
<tr>
<td>Composition (wt%)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Portland Cement</td>
<td>22.2</td>
<td>12.2</td>
</tr>
<tr>
<td>Fly ash</td>
<td>N/A</td>
<td>10.0</td>
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<tr>
<td>Water</td>
<td>9.9</td>
<td>10.1</td>
</tr>
<tr>
<td>Fine Aggregate</td>
<td>67.9</td>
<td>67.7</td>
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<tr>
<td>Fly ash used (Sample code)</td>
<td>N/A</td>
<td>FA02</td>
</tr>
<tr>
<td></td>
<td></td>
<td>FA39</td>
</tr>
<tr>
<td>Microconcrete Sample Code</td>
<td>M45-00</td>
<td>M45-02</td>
</tr>
<tr>
<td></td>
<td></td>
<td>M45-39</td>
</tr>
</tbody>
</table>
Results from LEAF Methods

1. Solubility of Ca is lowered in carbonated materials compared to non-carbonated materials at their respective natural pH.

2. Initial flux of Ca is lower for carbonated materials but approaches the non-carbonated flux as the leaching front surpasses the carbonated front.
Phenolphthalein Indicator Test

A. Control (M45-00)

B. High Ca FA replacement (M45-39)

C. Low Ca FA replacement (M45-02)

- Ca wt% is of the unhydrated Portland cement and fly ash (excluding fine aggregates)
- Ca wt % estimated by Method 3052B, excludes C and B

<table>
<thead>
<tr>
<th>Type</th>
<th>Mean Depth (mm)</th>
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<tbody>
<tr>
<td>Control (no FA)</td>
<td>0.4</td>
</tr>
<tr>
<td>w/ High Ca FA</td>
<td>0.7</td>
</tr>
<tr>
<td>w/ Low Ca FA</td>
<td>1.2</td>
</tr>
</tbody>
</table>
Carbonation Microstructure

*Ex: M45-02 (low Ca FA replacement)
SEM-EDS Carbonation Profile

**Carbonation Depth Comparison**

<table>
<thead>
<tr>
<th>Type</th>
<th>Mean Depth (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Control</td>
<td>0.4</td>
</tr>
<tr>
<td>w/ High Ca FA</td>
<td>0.6</td>
</tr>
<tr>
<td>w/ Low Ca FA</td>
<td>1.8</td>
</tr>
</tbody>
</table>

- Ca wt% is of the unhydrated Portland cement and fly ash (excluding fine aggregates)
- Ca wt% estimated by Method 3052B, test does not include C
Flexible Models in LeachXS™/ORCHESTRA

- Select general field or laboratory scenario
- Select from existing CBP reference materials or add materials
- Select interface conditions (e.g., fixed volume, continuous flow or intermittent flow / exchange & solutions)
- Leaching data management integrated with chemical speciation – reactive transport modeling
Mineral Set

Thermodynamic model
- LeachXS/ORCHESTRA
  • Solves system of equations:
    • Conservation of mass
    • Laws of mass action
  • Yields solid, aqueous, and gaseous speciation
- C-S-H
  • Ideal solid solution with Tobermorite- and Jennite-like end-members (Lothenbach et al., 2008)
- Adsorption models
- Additional minerals included in the model for trace species
  • As, B, Ba, Cd, Cr, Cu, Sb, Se, Sr, Th, U, V, Zn

Major Mineral Phases

<table>
<thead>
<tr>
<th></th>
<th>Mg(OH)$_2$</th>
<th>Ca(OH)$_2$</th>
<th>CAH$_{10}$*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Brucite</td>
<td></td>
<td>Portlandite</td>
<td>Unnamed meta-stable phase</td>
</tr>
<tr>
<td>CaSO$_4$•2H$_2$O</td>
<td></td>
<td>CaCO$_3$</td>
<td>C$_3$AH$_6$*</td>
</tr>
<tr>
<td>Gypsum</td>
<td></td>
<td>Calcite</td>
<td>Hydrogarnet</td>
</tr>
<tr>
<td>SiO$_2$ (am)</td>
<td></td>
<td>C$_2$ASH$_8$*</td>
<td>C$_3$FH$_6$*</td>
</tr>
<tr>
<td>Amorphous Silica</td>
<td></td>
<td>Strätlingite</td>
<td>Fe-hydrogarnet</td>
</tr>
<tr>
<td>Al(OH)$_3$ (am)</td>
<td></td>
<td>C$_2$FSH$_8$*</td>
<td>C$<em>4$AH$</em>{13}$*</td>
</tr>
<tr>
<td>Amorphous Aluminum hydroxide</td>
<td></td>
<td>Fe-Strätlingite</td>
<td>Hydroxy AFm</td>
</tr>
<tr>
<td>Al$_2$O$_3$</td>
<td></td>
<td>C$_2$AH$_8$*</td>
<td>C$<em>4$FH$</em>{13}$*</td>
</tr>
<tr>
<td>Alumina</td>
<td></td>
<td>Unnamed meta-stable phase</td>
<td>Fe-hydroxy AFm</td>
</tr>
<tr>
<td>Fe(OH)$_3$ (am)</td>
<td></td>
<td>C$_2$FH$_9$*</td>
<td>Solid Solution:</td>
</tr>
<tr>
<td>Amorphous Iron hydroxide</td>
<td></td>
<td>Unnamed meta-stable phase</td>
<td>C$<em>{1.67}$SH$</em>{2.1}$*</td>
</tr>
<tr>
<td>K$_2$Ca(SO$_4$)$_2$•H$_2$O</td>
<td></td>
<td>CaSO$_4$</td>
<td>Jennite</td>
</tr>
<tr>
<td>Syngenite</td>
<td></td>
<td>Anhydrite</td>
<td>C$<em>{0.83}$SH$</em>{1.3}$*</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Tobermorite</td>
</tr>
</tbody>
</table>

* Notation: C = CaO, A = Al$_2$O$_3$, F = Fe$_2$O$_3$, S = SiO$_2$, H = H$_2$O
Carbonation of Cement Materials

Degree of Carbonation
• Modeled by input CO$_3$ content
• 2000-yr-old Roman Cement (green diamonds) – completely carbonated
Speciation of Cement Materials

Uncarbonated (Control)

Carbonated

M45-00 (no FA)

M45-02 (low Ca FA)
Monolith Diffusion Modeling

Modeling Options

- Laboratory and field simulations
- Variable water contacting sequence, chemistry
- Saturated or unsaturated
- Carbonation, oxidation ingress
- Sulfate attack with leaching

For this study

- 180 days simulated to represent experimental results
- Saturated conditions with tortuosity and porosity at upper ends of reasonable ranges
- No fluxes at boundaries – diffusion only
- Five (5) millimeters “pre-carbonated” based on field results

local equilibrium based on CSF model

finite volume (well mixed)

new leachant refresh at scheduled times

leachate

Carbonated

Monolith

Bath

Diffusion

For this study

- 180 days simulated to represent experimental results
- Saturated conditions with tortuosity and porosity at upper ends of reasonable ranges
- No fluxes at boundaries – diffusion only
- Five (5) millimeters “pre-carbonated” based on field results
Monolith Diffusion Results

M-45-00 (no fly ash replacement)

M-45-02 (low Ca fly ash replacement)

Depth (mm)

pH

Sigma Ca^2+/Sigma Ca^2+ (∞) (mols/mols)

Diameter (mm)

M-45-00 (no fly ash replacement)

M-45-02 (low Ca fly ash replacement)
Diffusion Modeling – Phases

Time = 0.125 days

Time = 180 days

*Ex: M45-02 (low Ca FA replacement)
Modeling Carbonation and Leaching through Cracked Concrete for HLW Tank Integrity and Closure

K.G. Brown¹, S. Sarkar¹, J. Arnold¹, D.S. Kosson¹
J.C.L. Meeussen², H. van der Sloot³, G. Flach⁴

Consortium for Risk Evaluation with Stakeholder Participation (CRESP)
¹Vanderbilt University and CRESPP
²NRG, Energy Research Centre of The Netherlands
³Hans van der Sloot Consultancy
⁴Savannah River National Laboratory
Motivation: Stabilize Residual High-Level Waste

200+ High-level waste (HLW) tanks require waste removal and closure:

- Tanks in service:
  - Capacity of ca. 4 million liters
  - Carbon steel liner within a reinforced concrete shell

- Tank closure
  - HLW retrieved to extent practical and filled with grout
  - Grout – cement mixed with supplementary materials
  - Grout intended to provide structural stability and to retain residual radionuclides

**Challenge** – predict timeframe and radionuclide rate of release

Source: SRNL-STI-2012-00372
Primary Degradation Mechanisms

Important degradation phenomena that can lead to radionuclide release:

- **Dome:**
  - CO₂ ingress (carbonation) and major constituent leaching
  - Depassivation of embedded steel (pH<9) and cracking leading to water infiltration

- **Grout:**
  - Cracking allowing water percolation, constituent leaching, and release to environment
  - Grout: CO₂/O₂ ingress resulting in pH change and respeciation of grout and waste constituents (future)

- LeachXS/ORCHESTRA used to model phenomena
Decouple carbonation of the dome from transport in the grout (dual regime reactive transport) model

- Carbonation of dome is a very slow process (e.g., << 1mm/yr)
- Transport in the grout assumed negligible until dome is carbonated and cracked (allowing infiltration)
- Thus, stochastically model dome carbonation to generate distribution of times until cracked
- Time distribution then used to delay impact on cracked grout pH using dual regime model
Assume that transport through the grout is negligible until the dome is carbonated and cracked (allowing infiltration)

Arnold, Joshua Robert, 5/3/2013
Multiple, flexible base models are available in LeachXS/ORCHESTRA

- Select general field or laboratory scenario to model
- Select from existing CBP reference materials or customize materials
- Select interface conditions (e.g., fixed volume, continuous flow or intermittent flow / exchange & solutions
- Resulting model transferable to GoldSim probabilistic framework (CBP Software ToolBox)
Representative HLW Tank

- Roof constructed of reinforced concrete assuming minimum 0.040 m concrete cover (to rebar) – no steel liner under roof
- Selected thinnest dome concrete (0.18 m) where SRS tank domes range up to 1.22 m
- Selected vertical (grouted) span of 9 m that is the shortest path for SRS HLW tanks
- Material of construction assumed to be Ordinary Portland Cement (where tanks built in late 1950s)
- Closed HLW tank will be buried in at least 3 m of backfill material (properties assumed similar to SRS clayey vadose zone soil)

Source: SRS-REG-2007-00002, Rev. 1
Conical as opposed to hemispherical?
Arnold, Joshua Robert, 5/3/2013
**Thermodynamic model**

- **LeachXS/ORCHESTRA:**
  - Solves system of equations:
    - Conservation of mass
    - Laws of mass action
  - Yields solid, aqueous, and gaseous speciation

- **C-S-H:**
  - Ideal solid solution with Tobermorite- and Jennite-like end-members (from Lothenbach et al., 2008)
  - No adsorption and (some) additional minerals in the model
  - Dome construction material assumed to be Ordinary Portland Cement

**Mineral phases**

<table>
<thead>
<tr>
<th>Mineral</th>
<th>Formula</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Brucite</td>
<td>Mg(OH)₂</td>
<td>Mg(OH)₂</td>
</tr>
<tr>
<td>Portlandite</td>
<td>Ca(OH)₂</td>
<td>Ca(OH)₂</td>
</tr>
<tr>
<td>Hydrogarnet</td>
<td>C₃AH₆</td>
<td>C₃AH₆</td>
</tr>
<tr>
<td>Hemi-carbonate</td>
<td>C₄Ac₀.₅H₁₂</td>
<td>C₄Ac₀.₅H₁₂</td>
</tr>
<tr>
<td>Ettringite</td>
<td>C₆As₃H₃₂</td>
<td>C₆As₃H₃₂</td>
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<td>Gypsum</td>
<td>CaSO₄·2H₂O</td>
<td>CaSO₄·2H₂O</td>
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<td>Calcite</td>
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<td>Fe-hemi-carbonate</td>
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<td>C₄Fc₀.₅H₁₂</td>
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<td>Fe-ettringite</td>
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<td>C₆Fs₃H₃₂</td>
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<td>M₄AcH₉</td>
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<td>SiO₂ (am)</td>
<td>SiO₂ (am)</td>
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<td>Solid Solution</td>
<td>C₃₁₆₇SH₂₁₂₁</td>
<td>C₃₁₆₇SH₂₁₂₁</td>
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<td>C₁₆₇SH₂₁₂₁</td>
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<td>C₅₇₈SH₁₃</td>
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<td>CaSO₄</td>
<td>CaSO₄</td>
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<tr>
<td>Hydrotalcite</td>
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<td>Microcrystalline Iron Hydroxide</td>
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<td>C₀₈₃SH₁₃</td>
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<tr>
<td>CO₃⁻</td>
<td>C₀₈₃SH₁₃</td>
<td>C₀₈₃SH₁₃</td>
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</tbody>
</table>
Comparison of Data [USEPA 1313] and Thermodynamic Model Predictions [LXS]

Experimental data from USEPA Method 1313 (SW-846)
Probabilistic Dome Analysis

Non-Stochastic Parameters

- Dome thickness 0.18 m (7 in)
  - Varies between 0.18 and 1.22 m (SRS-REG-2007-00002)
- Burial depth 3 m (10 ft) (SRR-CWDA-2010-00128)
- Temperature 20°C at 3 m (WSRC-STI-2007-00184, Rev. 2)

Stochastic Parameters

- CO₂ and O₂ Diffusivities – $U(D_m \text{ at } 20°C, \pm 5\%) \text{ m}^2/\text{s}$
  - Based on data from Marrero and Mason (1972)
- Infiltration Rate – $N(0.18, 0.051) \text{ m/yr}$
  - Distribution of 1,000-yr rates (WSRC-STI-2007-00184)
- Soil: $\phi$ – $N(0.37, 0.011)$, $\tau$ – $\Delta(0.202, 0.331, 0.557)$, and $S$ – $\Delta(0.843, 0.858, 0.873)$
  - Concrete: $\phi$ – $N(0.221, 0.013)$, $\tau$ – $\Delta(0.011, 0.05, 0.217)$
  - Information from WSRC-STI-2006-00198
- Concrete Saturation $S$ – $U(0.74, 0.90)$
  - Rubble min (WSRC-TR-2005-00054); max to allow CO₂ ingress
- Soil-Gas CO₂ – $\Delta(0.01, 0.015, 0.032)$
  - Distribution of well data (SRNL-L3200-2012-00017)
• Simulation times to estimate when pH<9 were prohibitive
• Simulated when carbonation front reached 0.04 m (cover to rebar) and 0.18 m (dome)
• Used previous results to estimate time after front reaches 0.04 m that pH < 9
  — Time to pH < 9 -- N(570, 20) years
• Assumed that concrete (0.14 m with rebar) cracking would proceed at 0.001 m/yr
• Assumptions result in much shorter estimates than times to carbonate through dome

Note log scale ordinate
Equilibrium approach

Mobile-immobile zone

Inflow

Advection and diffusion

Homogenized structure

Outflow

Mobile

Inflow

Advection

Exchange

Immobile

Outflow

Relative concentration ($C/C_0$)

Time (days)

0 2 4 6 8 10

0.2 0.4 0.6 0.8 1

Mobile zone controlled

0 2 4 6 8 10

0.2 0.4 0.6 0.8 1

Relative concentration ($C/C_0$)
Flow through Heterogeneous Media

- Refined mobile-immobile approach
- Can capture micro-macro pore and particle size distributions
Conceptual Simulation Scenario

- Inflow
- Advection through mobile zone
- Diffusion in/out of stagnant zone
- Chemical Reactions

- Solids with cracks and macropores: Mobile zone
- Solid matrix with micropores: Immobile zone

Source: van Beinum et al., 2000
Mineral set selected to achieve best agreement with pH dependence test data (USEPA method 1313) for major species

Databases used: MINTEQA2 (Allison et al., 1992) and CEMDATA07 (Lothenbach et al., 2006 and 2008)
Non-Stochastic Parameters

• Grout thickness 10.5 m (SRS Type IV Tank)
  – Varies between 9 and 16 m (Sites, et al. 2006)

Stochastic Parameters

• Crack spacing – U(1,2) m
  – Sarkar, et al. (2013)
• Infiltration Rate – N(0.18, 0.051) m/yr
  – Distribution of 1,000-yr rates (WSRC-STI-2007-00184)
• Total porosity: $\phi_t$ – U(0.20, 0.30)
  – Sarkar, et al. (2013)
• Immobile zone porosity: $\phi_{im}$ – N(0.221, 0.013)
  – Information from WSRC-STI-2006-00198
• Mobile volume fraction: U(0.10,0.20)
  – Sarkar, et al. (2013)
• Solid composition: N(mean, ±10%)
  – Sensitivity evaluation
Coupled Analysis Results

- Simulated pH response at grout – waste layer interface
- Upper graph indicates fairly insensitive pH response to infiltration rate *for nominal grout parameters*
  - Especially at longer times where responses converge
- Lower graph (red) indicates some initial variability in pH response *at maximum infiltration rate* but pH responses tend to approach nominal values at long times
• Simulated pH response at grout – waste layer interface
• Upper graph (blue) indicates sensitive pH response at minimum infiltration rate
• Lower graph indicates sensitive pH response depending on infiltration rate
  – Similar sensitive response found at median (green) infiltration rate
  – Waste layer not impacted until after 700 years (and likely much longer)
• Significant pH effects over the first two millenia tend to be observed as the infiltration rate is lower
  – Longer simulations required to better evaluate
Summary

- Implemented both a 1) concrete carbonation model and 2) dual regime reactive transport model for simulating percolation through cracked grout
  - Carbonation model results previously compared to Hanford HLW tank dome core measurement
  - Dual regime model calibrated and validated using up-flow column percolation test data

- Probabilistic analyses were carried out for both models
  - Carbonation to pH 9 (depassivation of embedded steel) requires at least on the order of 700 years (and likely 10X this estimate)
  - Significant pH effects at the grout – waste layer interface over the first two millenia tend to be observed as the infiltration rate is lower

- An efficient method for assessing effectiveness of current closure grouts and designing of future grouts
  - Longer simulation times and coupling of nominal cases would provide useful additional information
  - Consider gas phase exchange reactions (e.g., CO$_2$ and O$_2$) for future models
Significance of CBP Modeling Scenarios

• Applicability:
  • Evaluation of waste forms and treatment process effectiveness
  • Concrete vault durability and radionuclide release
  • Source term for contaminated soils/vadose zone and waste disposal scenarios
  • HLW tank integrity analysis and closure

• Flexible framework that can be easily modified to reflect various testing and field conditions

• Can be compared with available test results from the database of a large selection of materials

• Useful framework for designing future structures and maintenance scheduling for existing structures