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Subsurface Engineering Challenges - Towards Tools and Methods for Improved Understanding of Chemo-Mechanics in Cementitious Materials

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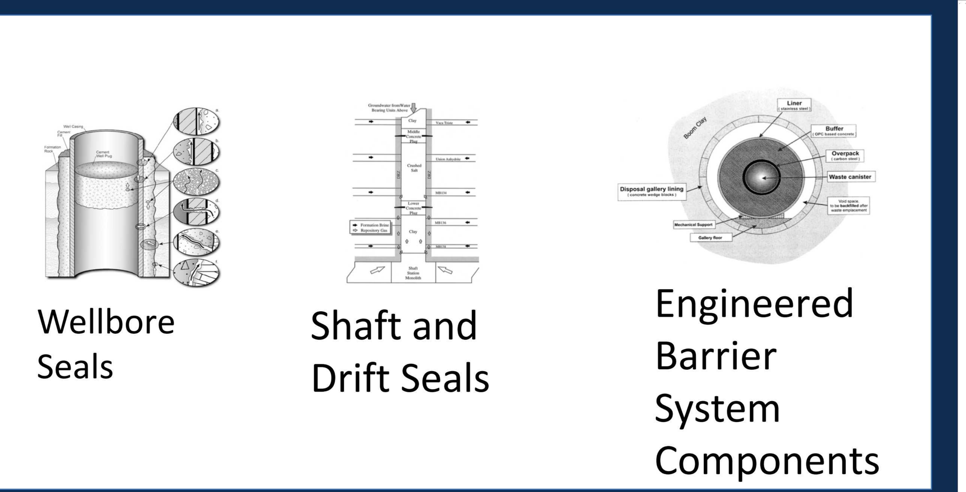
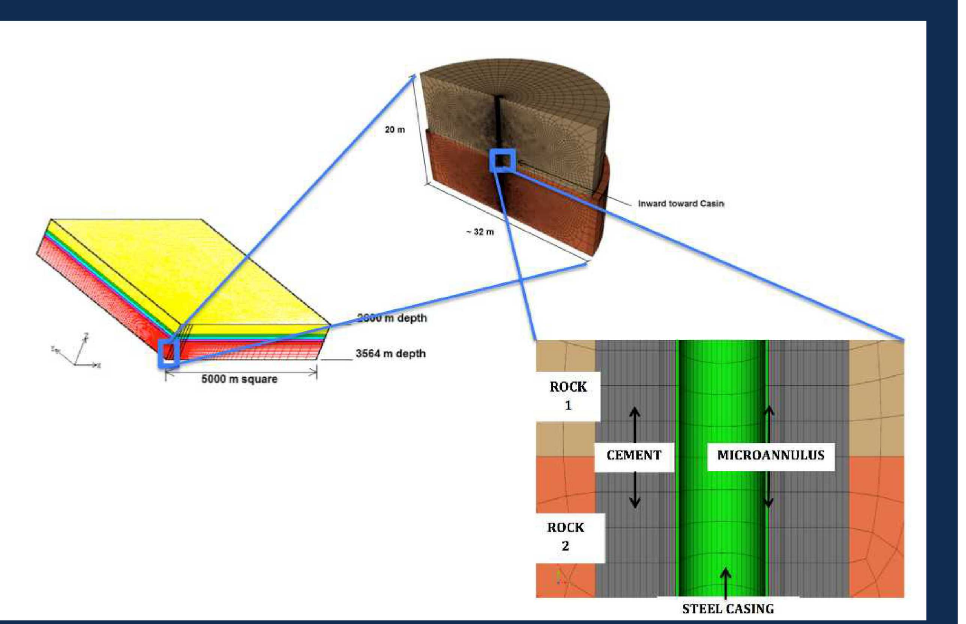
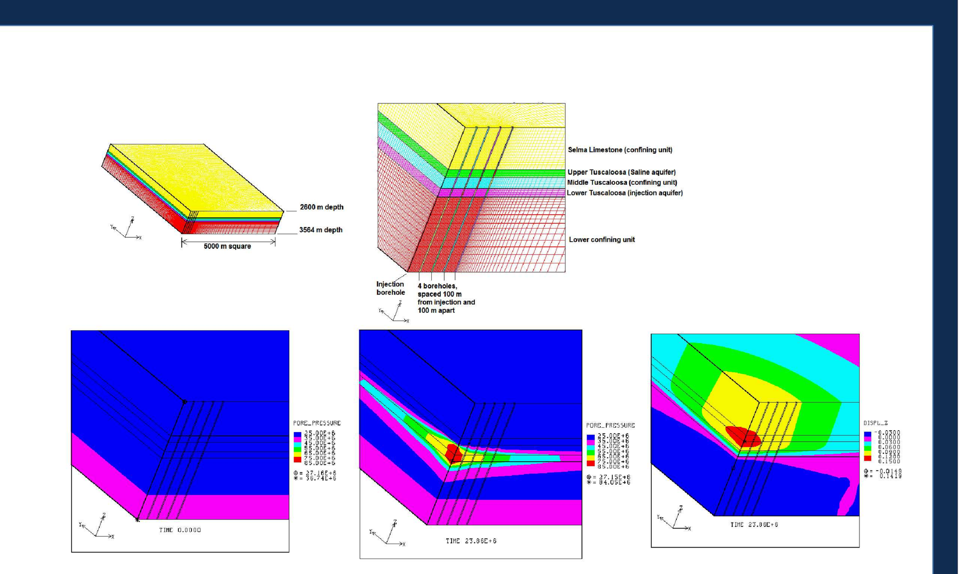
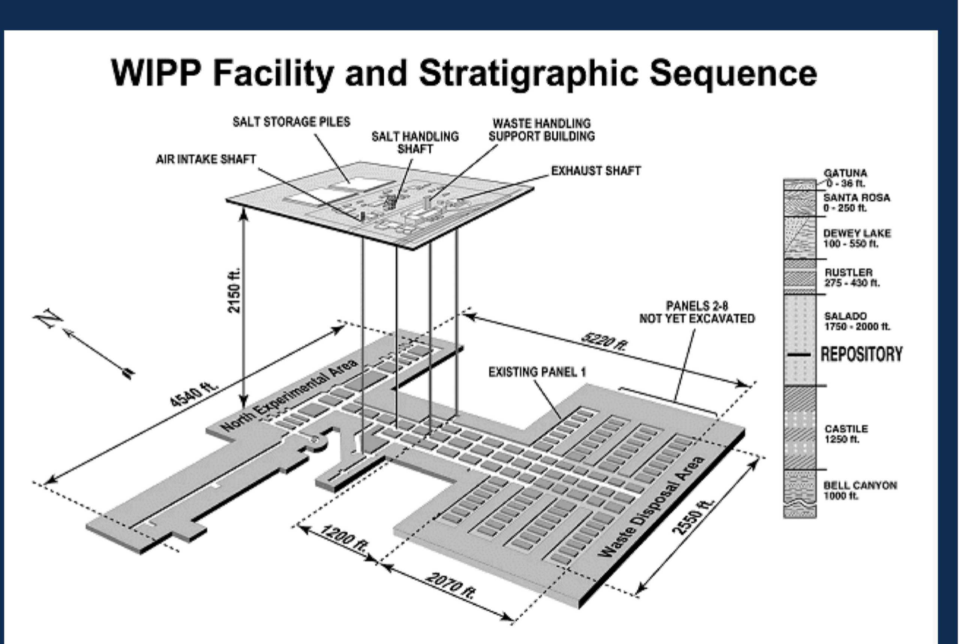
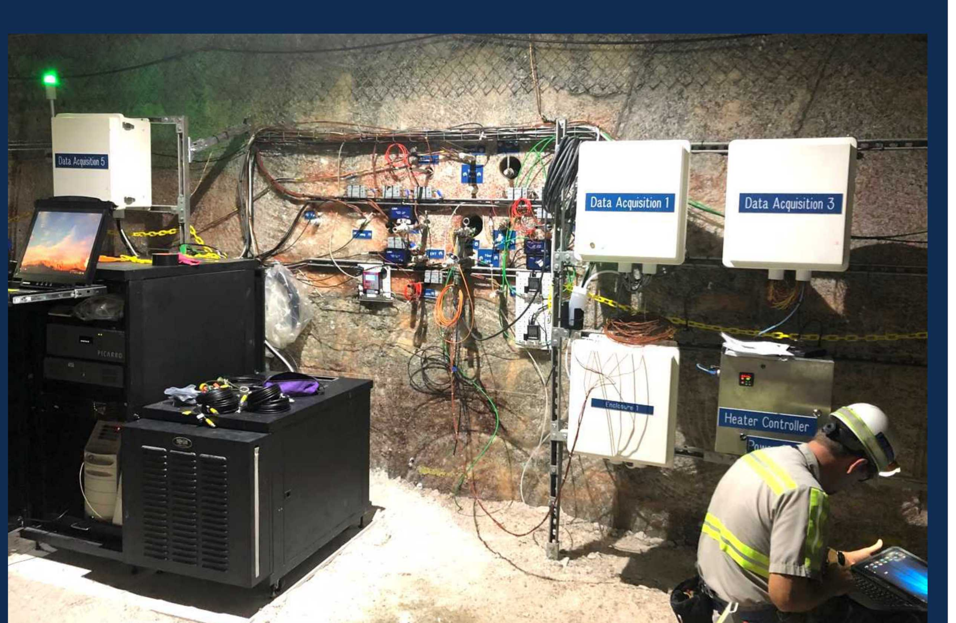










Overview

Cementitious materials play important roles in subsurface engineering applications as structural support for excavations, engineered barriers, and subsurface seal materials.

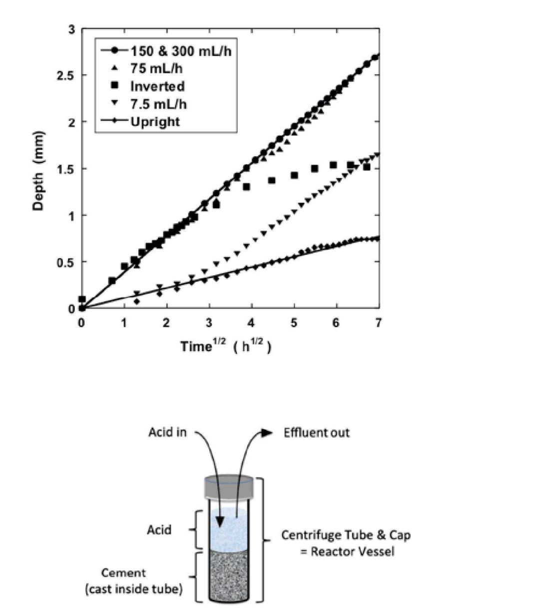
Challenges

1) Complex and dynamic subsurface geochemistry and geomechanics

2) Multi-scale and coupled processes (i.e., combinations of thermal, chemical, mechanical, hydrologic processes)

Background, Part I- Effect of Boundary Conditions on Leaching Rate

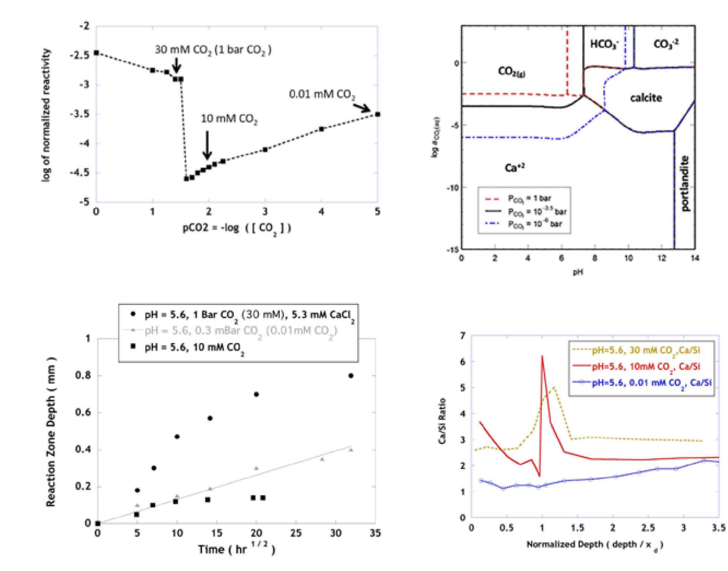
- Batch and flow-through tests to determine effect of leachant accumulation of leaching rate
- High flowrate
  - Fastest leaching rate, diffusion dominated
- Inverted batch (where leachant gravity-settled away from acid-cement surface)
  - Initially, fast rate of attack, but deviated from diffusion dominated rate after ~3 hrs.
- Upright batch (where leachant gravity-settled onto cement-acid interface) had the slowest rate, presumably because the leachant accumulation decreasing the concentration driving -> Leaching rate.
- Definition of the degradation zone and leaching front…



From Matteo and Scherer, IJGGC 2012

Background, Part 2 - Investigating the Controls/Mechanisms of Pore Clogging

- Reactive transport modelling showed dramatic decrease in cement reactivity ~ 10 mM CO2
- Hypothesis : pore-clogging
- Design experiments to verify
- By pushing solution conditions into calcite region on activity phase diagram, pore clogging was experimentally achieved
- These tests showed:
  - Activity phase diagram can help understand pore-clogging regime
  - Pore-clogging can be seen in deviations from diffusion-controlled degradation rates (linear w.r.t. to square root of time)
  - Transport across the degradation zone (heavily leached



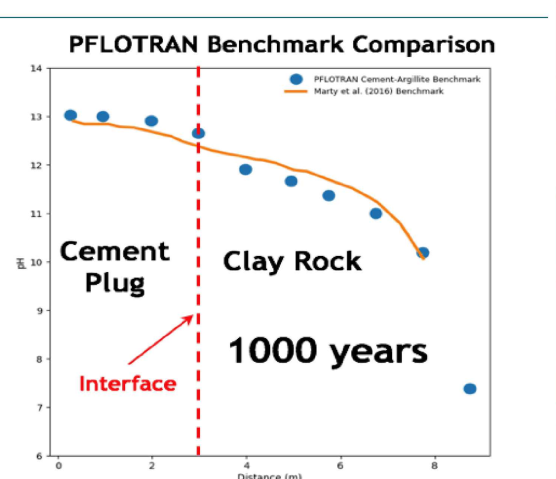
From Matteo et al., CCR 2018

PFLOTRAN Benchmark for Reactive Transport Modeling of Cement-Geomaterial Interfaces

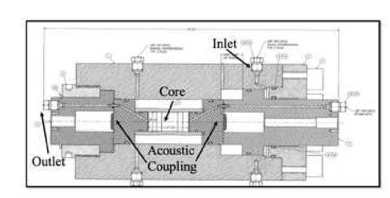
PFLOTRAN reactive transport simulations:
- Full saturation
- Diffusion only
- Isothermal
- Kinetic rate & equilibrium scenarios

Comparison with parameters & results from multicomponent reactive transport between cement - clay rock (Marty et al. 2015)
- Comparison of species concentration with distance profiles across 1-D domain
- Effective diffusivities defined for each medium
- Effects of cement/mineral phase kinetic rate law parameters
- Phase volume fraction & transport parameter sensitivities

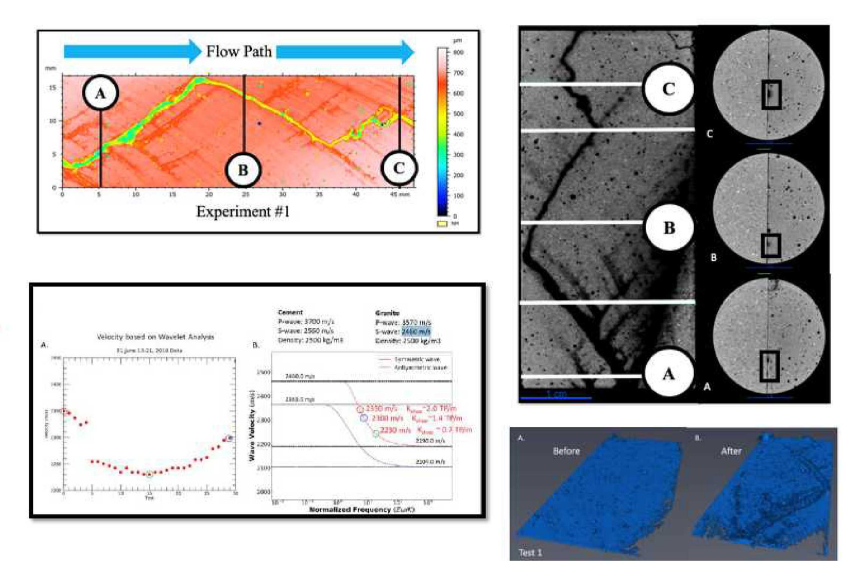
Preliminary Results
- Good agreement on pH predictions at 1000 years
- Still working on comparisons with other chemical components



Triaxial deformation with reactive flow though cement-host aperture

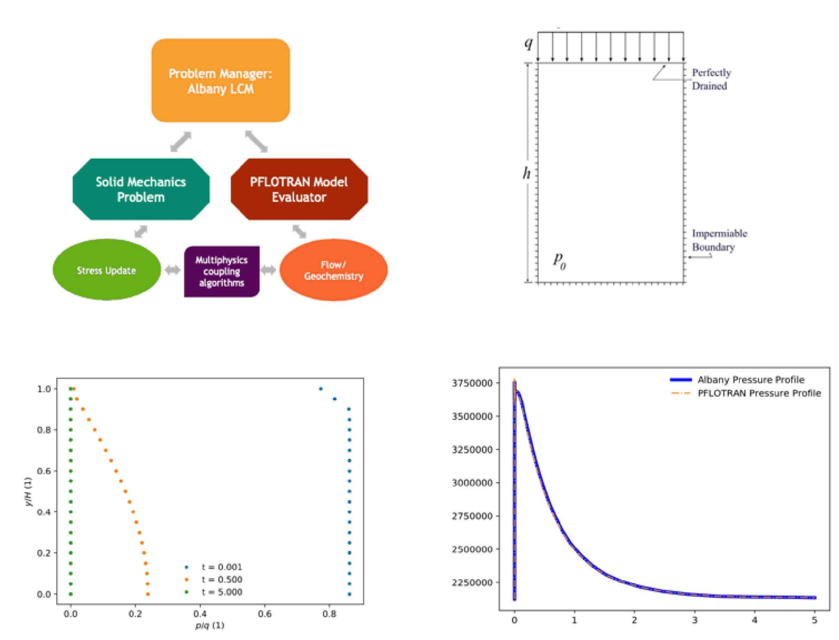


- Leaching of cement-granite interface under triaxial stress conditions
  - Confining pressure ~13. Mpa
  - Axial load ~16.8 Mpa
  - pH 3 HCl leachate flowed through cement-granite aperture
  - Ultrasonics and microCT used to characterize the interface



Albotran - A Code to Couple Solid Mechanics and Reactive Transport/Flow

- Coupling of two open-source codes
  - PFLOTRAN
    - Reactive flow
  - Albany
    - Solid Mechanics
- Rigorous testing of coupling algorithm
  - Terzhagi consolidation problem as a test case
- Expanding into more relevant cement leaching problems



Field Test of Cementitious Seals: Recipes for Emplaced Plugs

Sorel Cement D4 (5-1-8 phase)

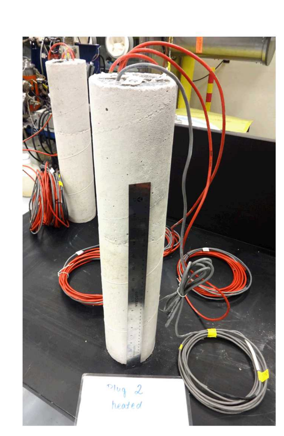
- Proportions similar to Popp et al. 2018
  - Density = 2240 kg/m^3
- Desired fast setting
- Used MgO currently emplaced with waste at WIPP
  - Crushed and sieved <75 um
  - reactivity = 272 s
- Aggregate: Run of mine WIPP salt <4 mm grain size

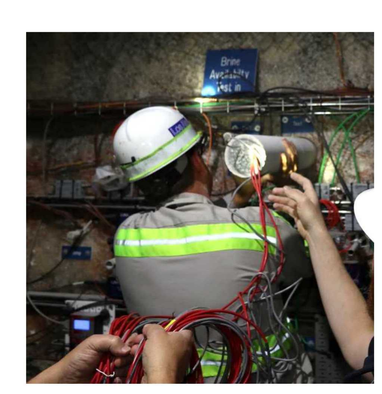
Sorel D4	Composition (mass-%)
5 M $MgCl_2$	18.3
< 75 um MgO	18.3
Salt Aggregate	63.4

Salt Concrete

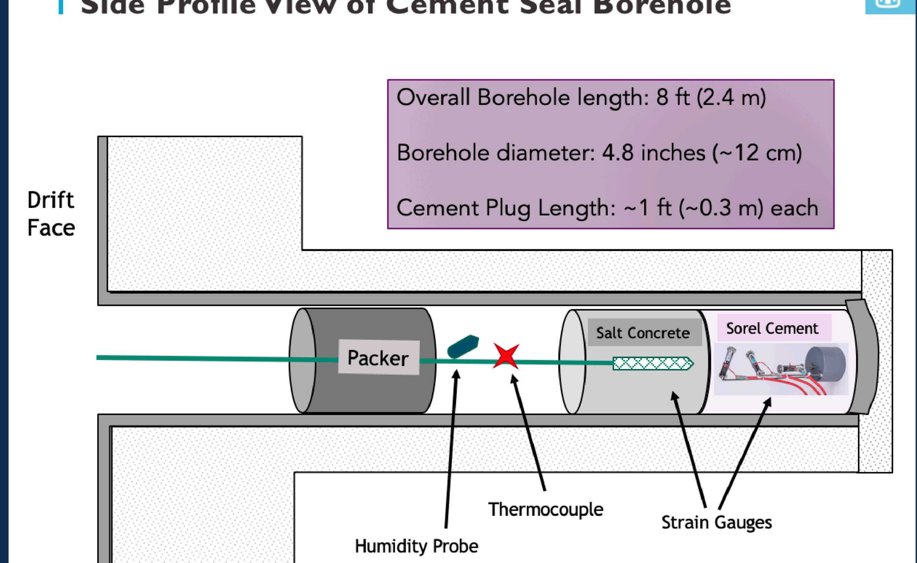
- Followed recipe from Muller-Hoppe et al. 2010 (LAVA2)
- Ground Blast Furnace Slag
- Aggregate: Run of mine WIPP salt <4 mm grain size
  - Impurities affected mixture
- Required to be mixed in glove box

Salt Concrete	Composition (mass-%)
Saturated NaCl	14.7
Blast Furnace Slag	28.4
Salt Aggregate	56.9





Side Profile View of Cement Seal Borehole



Summary:

- Subsurface engineering demands computational tools that can represent multi-scale and coupled phenomena, with accuracy and efficiency
- These tools need to be integrated with and validated against bench-top and field-scale experimental tests

References:

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