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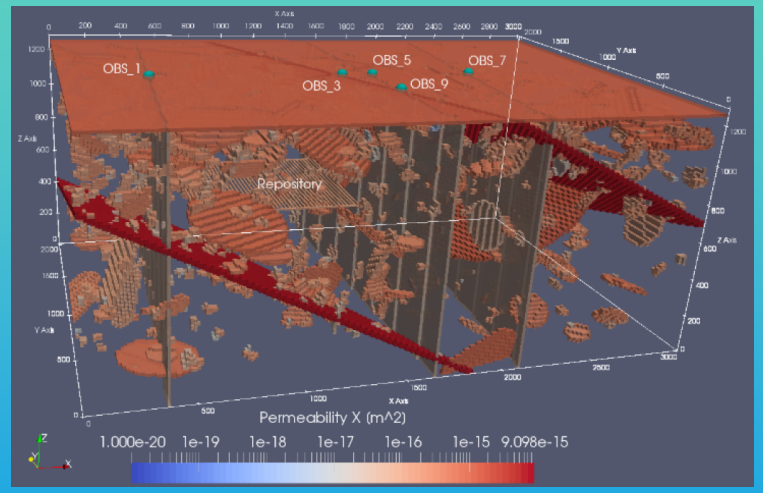

Engineered Barrier Systems Research Overview

2021 SFWD Annual Working Group Meeting
May 17- 20, 2021

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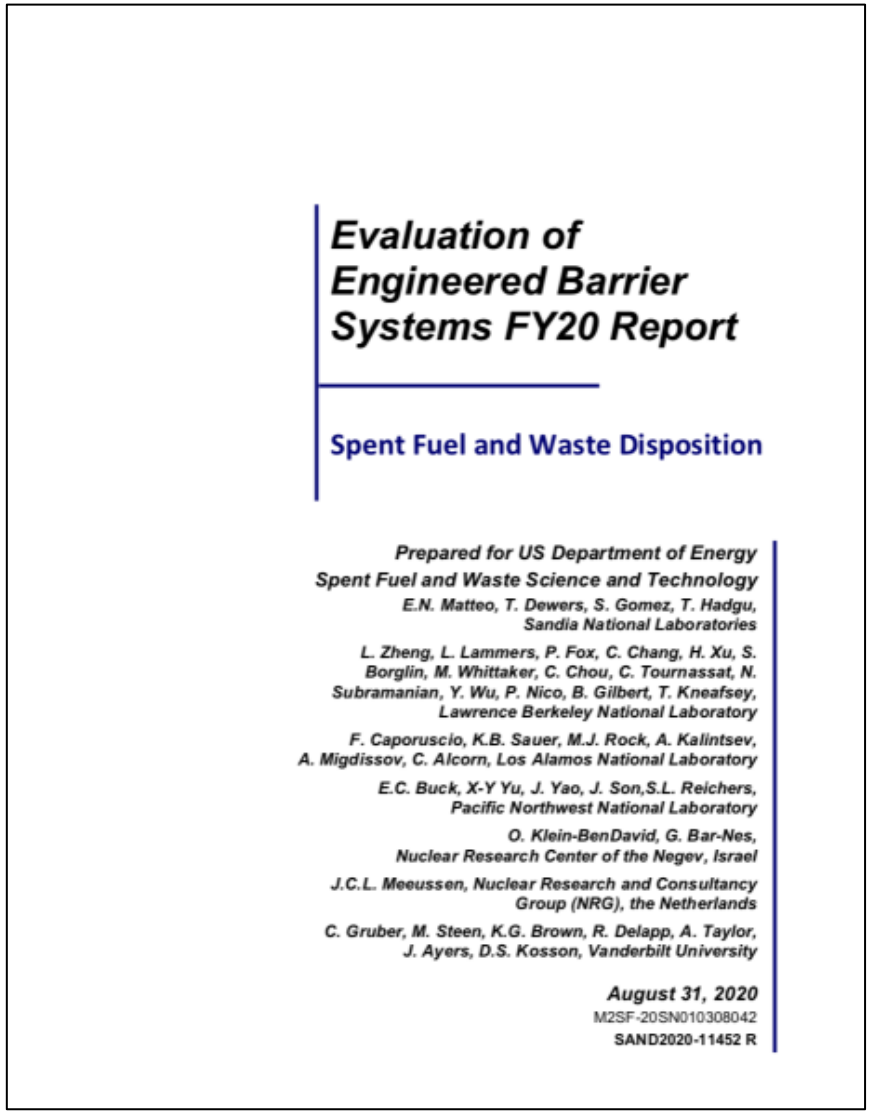
Ed Matteo
Sandia National Laboratories
Dept. of Nuclear Waste Disposal Research and Analysis

Session Layout

- EBS Overview
- *Developing Process Models and Refining Code Capabilities: Comparing COMSOL and PFLOTRAN*
- *Estimating Long-term Performance of Cement-Rock Interfaces*
- *EBS and Hot Bent (Int'l) hydrothermal experiments - Summary for FY20-FY21*
- *Radionuclide Complexation at Clay Mineral Interfaces*
- *Experimental Investigations in Compacted Clay: Radionuclide Diffusion and Microbial Incubations*
- *Models and experiments to study the THMC processes of bentonite barrier*
- Questions and Discussion

EBS Activities and Scope



Evaluation of Engineered Barrier Systems FY20 Report

Spent Fuel and Waste Disposition

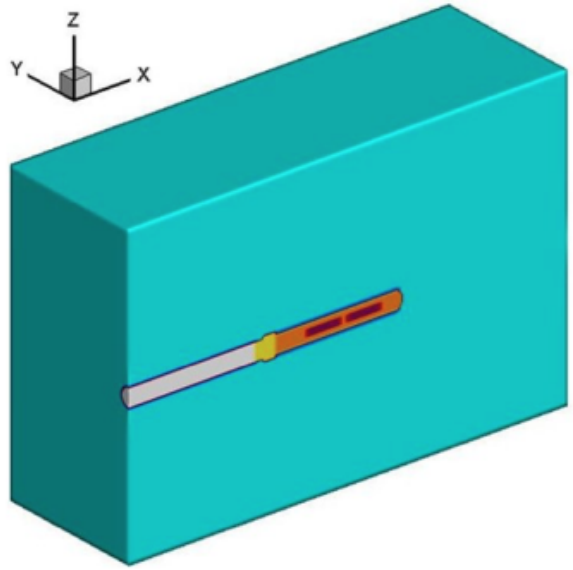
Prepared for US Department of Energy
Spent Fuel and Waste Science and Technology
E.N. Matteo, T. Dewers, S. Gomez, T. Hadgu, Sandia National Laboratories
L. Zheng, L. Lammers, P. Fox, C. Chang, H. Xu, S. Borglin, M. Whittaker, C. Chou, C. Tournassat, N. Subramanian, Y. Wu, P. Nico, B. Gilbert, T. Kneafsey, Lawrence Berkeley National Laboratory
F. Caporuscio, K.B. Sauer, M.J. Rock, A. Kalintsev, A. Migdissov, C. Alcorn, Los Alamos National Laboratory
E.C. Buck, X-Y Yu, J. Yao, J. Son,S.L. Reichers, Pacific Northwest National Laboratory
O. Klein-BenDavid, G. Bar-Nes, Nuclear Research Center of the Negev, Israel
J.C.L. Meeussen, Nuclear Research and Consultancy Group (NRG), the Netherlands
C. Gruber, M. Steen, K.G. Brown, R. Delapp, A. Taylor, J. Ayers, D.S. Kosson, Vanderbilt University

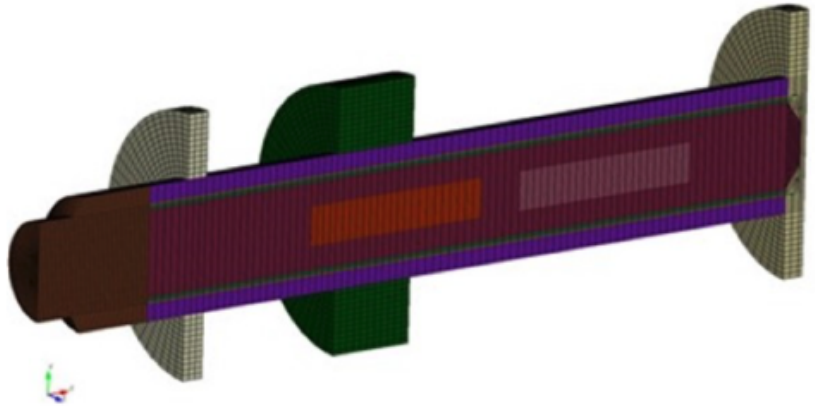
August 31, 2020
M2SF-20SN010308042
SAND2020-11452 R

- Working to understand of fundamental processes
  - Integrity of Repository Seals
    - Drift and shaft seals
    - Degradation evolution, esp. permeability evolution
  - Processes at material interfaces
    - Engineered materials and Disturbed Rock Zone (DRZ)
    - Waste Package materials and backfill/buffer
  - Representing and understanding complex processes
    - Coupled processes
      - Chemo-mechanics
      - Thermal-Hydrologic-Mechanical-Chemical
    - Multi-phase flow
    - Multi-scale phenomenon
      - Linking microstructural scale to continuum scale

TH Models for Engineered Barrier Systems Task Force Task 9

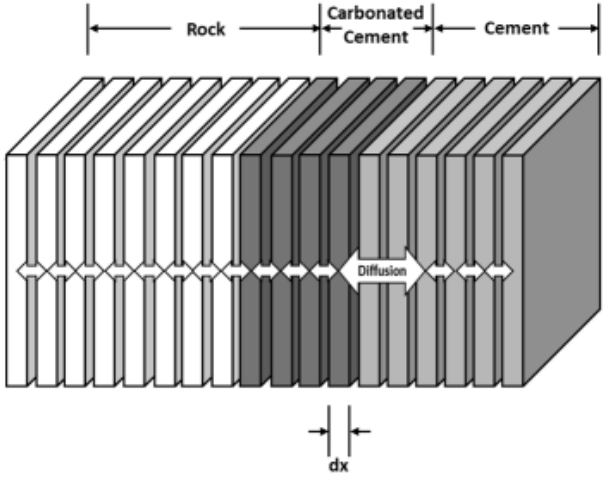
- Modelling teams simulate the FEBEX Test at the Grimsel Test Site in Switzerland
- 3-dimensional Thermal-Hydrologic Model using PFLOTRAN
- Good agreement with experimentally measured temperatures and liquid saturations
- Sensitivity study using DAKOTA-PFLOTRAN to examine model sensitivities, including heater power, buffer and host thermal conductivity, relative humidity, air entry pressure, and van Genuchten parameter

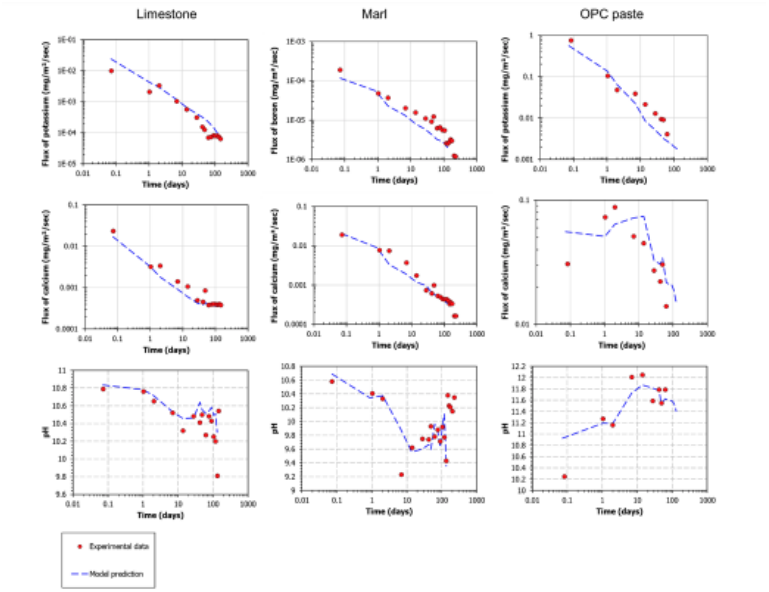


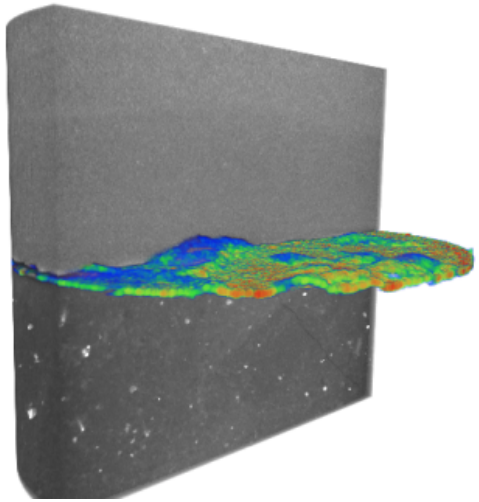


Cement-degradation and Cement-Geomaterial Interactions

- Cement-geomaterial interaction (chemical alteration, mechanical effects)
- Leaching tests using EPA 1315, 1315 leaching methods coupled with state-of -the-art characterization: X-ray micro-CT, nano-indentation, mineralogy/elemental analysis via electron microscopy
- LeachXS software is the 1-dimensional analysis method
- Compare and extend capabilities with 3-dimensional PFLOTRAN simulations

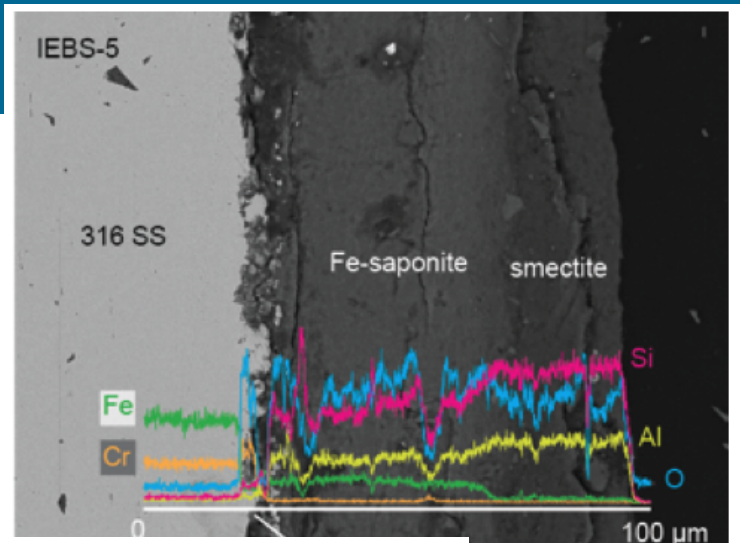


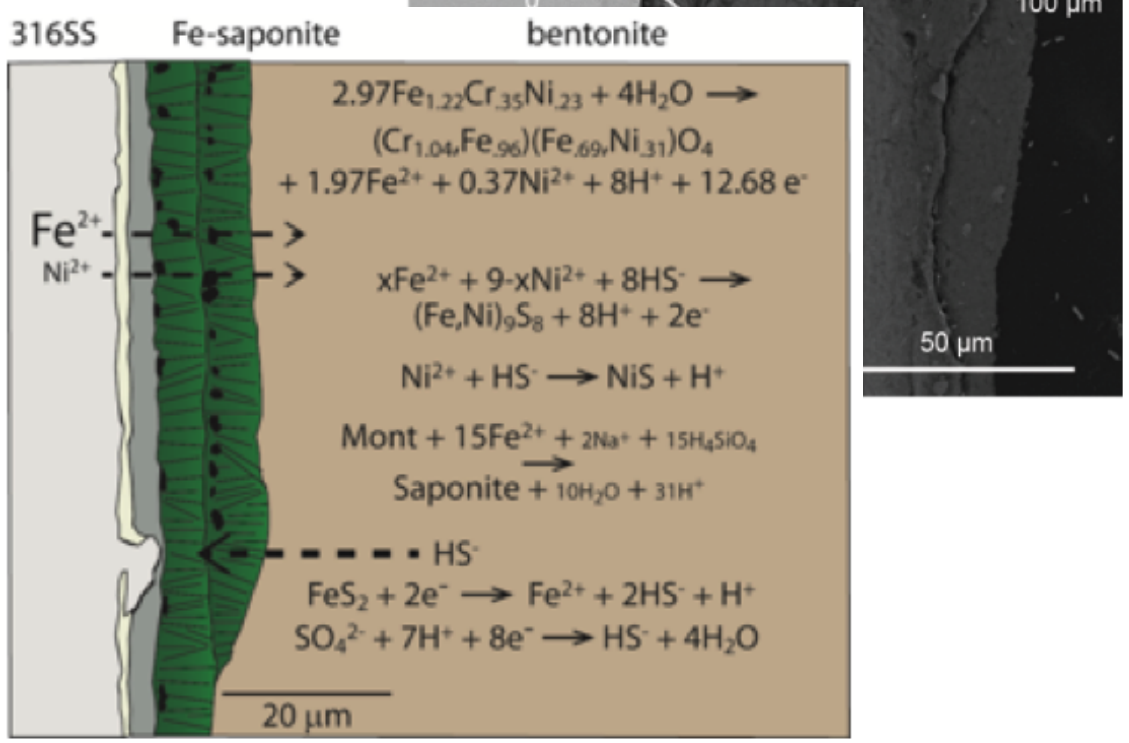




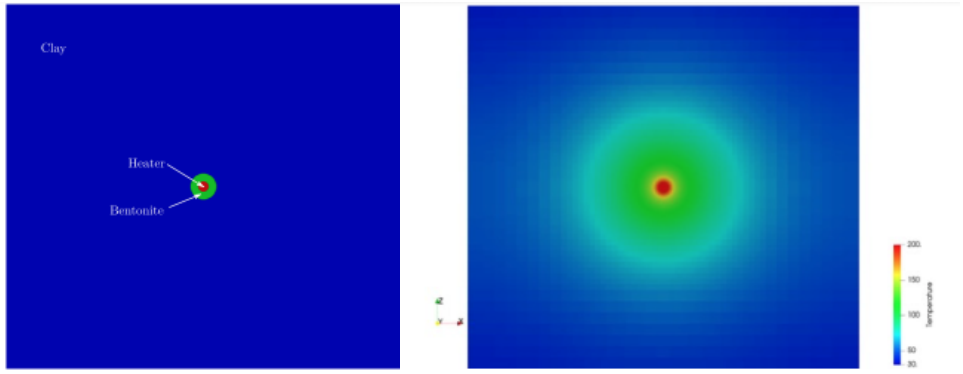
Hydrothermal Alterations at Material Interfaces

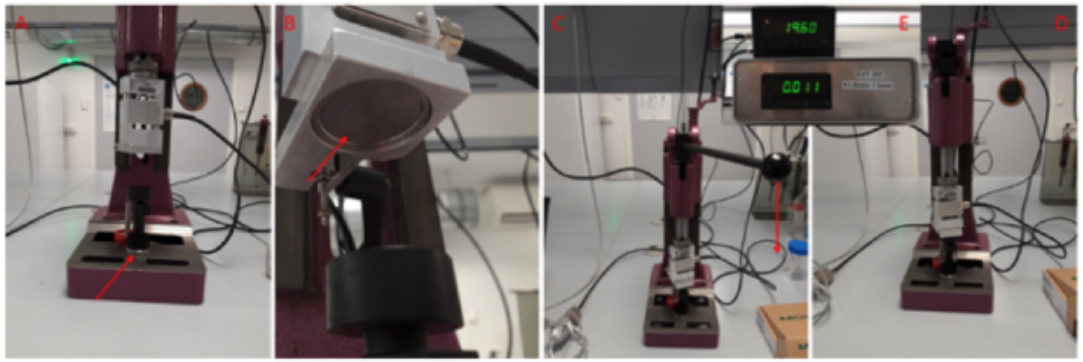
- Waste canister-buffer-host interactions investigated at hydrothermal conditions (e.g. steel-bentonite-granite in representative host pore solution)
- Recent tests have been also adding cementitious materials to the hydrothermal tests
- Post-test elemental fluid analysis and X-ray diffraction and electron microprobe analysis for mineralogic and elemental analysis of interfaces and surfaces alteration
- Testing to support high temperature studies, e.g. HotBENT

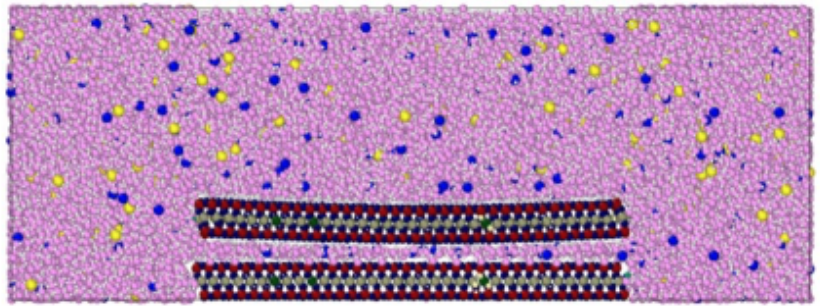




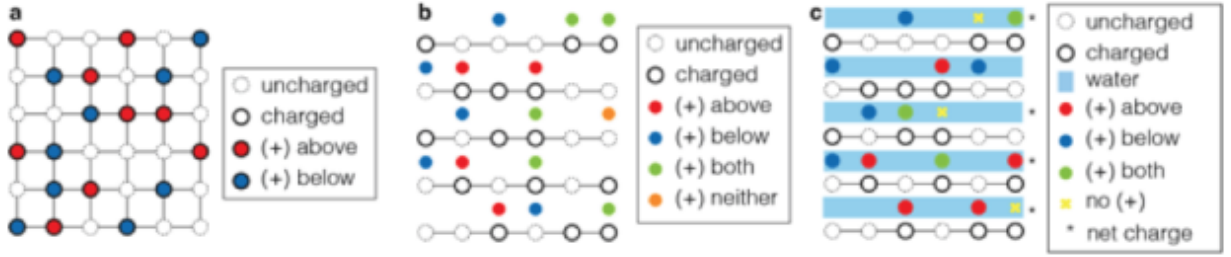
Bentonite Buffer Studies across Processes and Length Scales





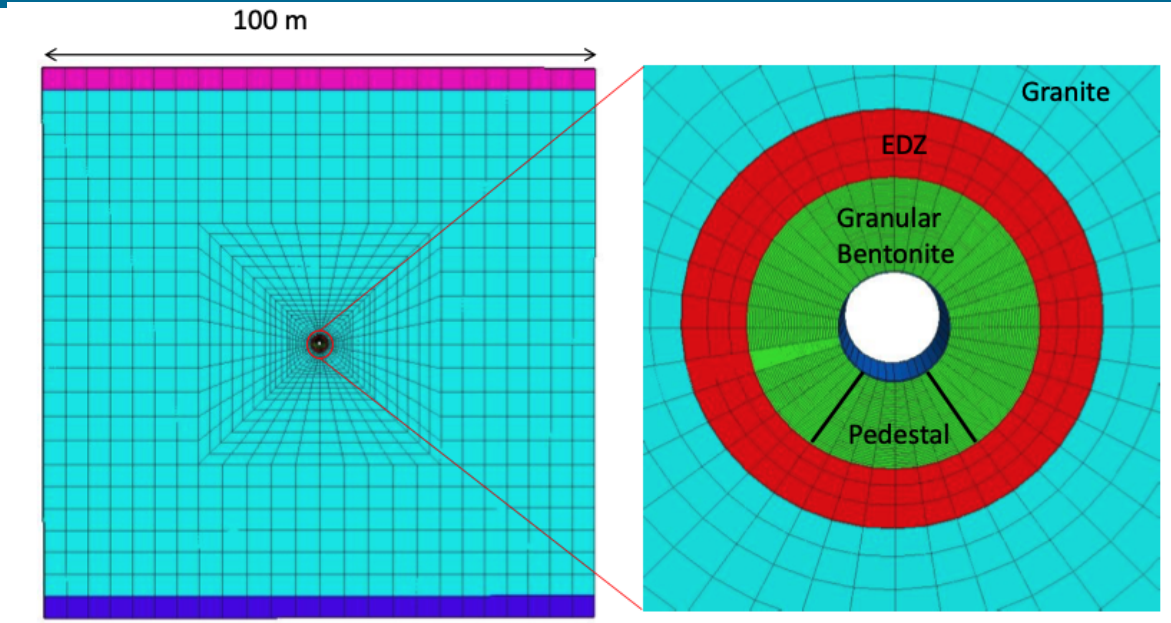


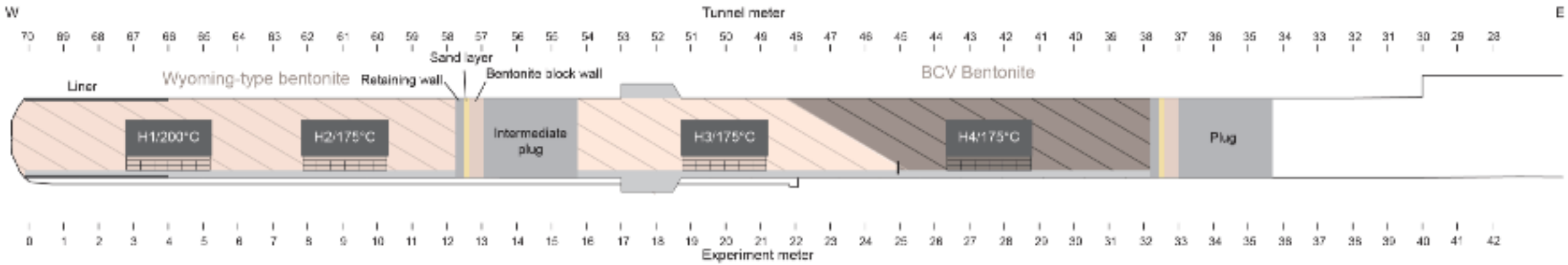
- Thermal-Hydrologic-Mechanical-Chemical modeling of buffer evolution using specialized constitutive models for clay swelling, esp. at high temperatures
- Uranium Sorption to bentonite to determine/improve distribution coefficients, so-called Kd values.
- Oedmetric swelling tests coupled with molecular dynamics simulations
- Microscopic origins of coupled transport in bentonite



LBNL Benchtop Column Test to Support Hot BENT

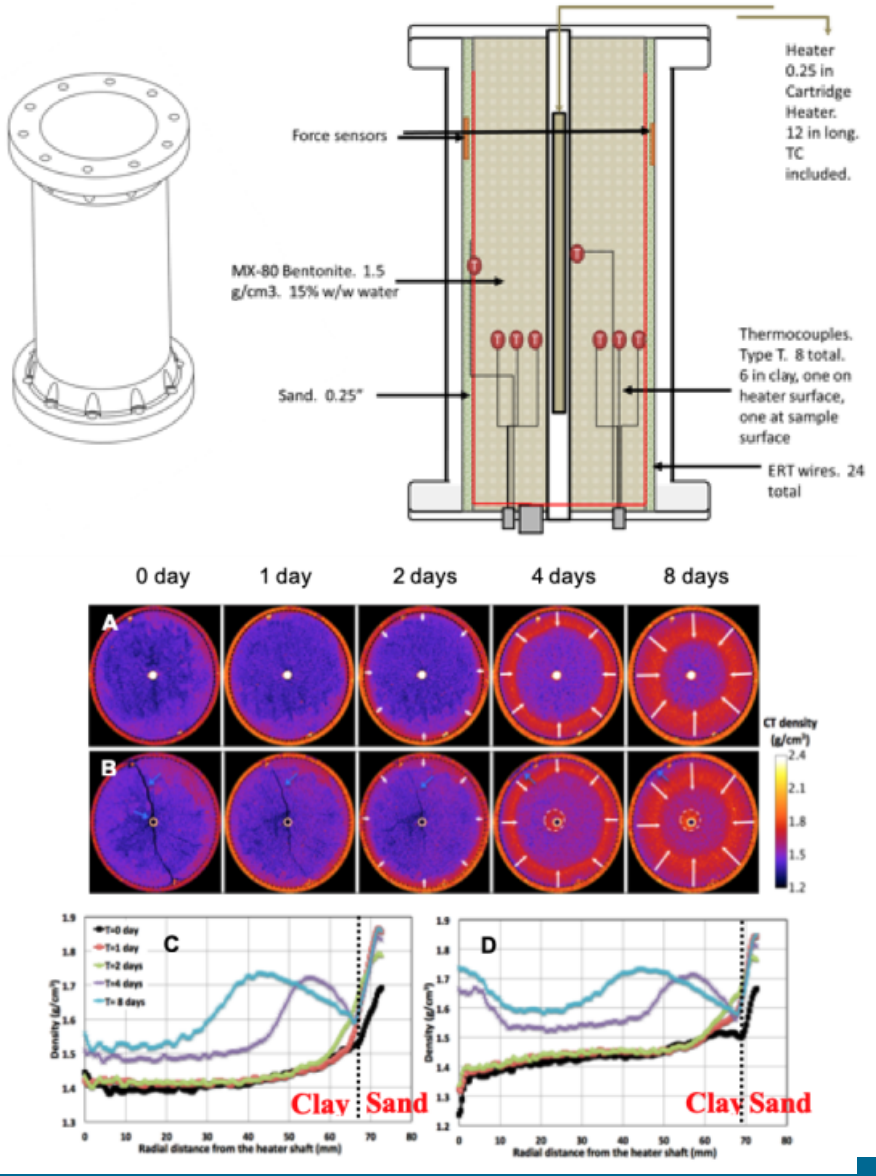
- THC model to predict the evolution of Wyoming bentonite (MX-80) to be used in the HotBENT field test
- ~ 3 years, most of bentonite would become fully saturated, but a narrow zone about 3 cm thick in the close vicinity of heater would remain unsaturated with a water saturation degree from 95% to 98% until 20 years.





Hot BENT and the LBNL Hot BENT Column Test

- In June 2019, hydration was started in both columns, and heating was applied to one colun
- In FY19–20, columns were monitored continuously for hydration, temperature distribution, effluent chemistry, and density changes
- Effluent chemistry showed differences betweer. the heated and non-heated columns, specifically, sulfate, calcium, potassium and magnesium reduction and silicon and potassium production occurred in the heated column.
- Feature Test for EBS Task Force Modelling Exercise



EBS Involvement with International Activities

- DECOVALEX 2023 Task B and Task C
- Engineered Barrier System Task Force New Tasks
  - Cement-Bentonite Interactions
  - HotBENT Column Test at LBNL
- RANGERS - shaft and drift performance study in collaboration with Germany
- HotBENT Field Test
  - High temperature bentonite field test
  - HotBENT Column Test at LBNL

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