

## EBS Research and Development

SNL-NUMO NDA Kick-off Meeting  
October 28, 2020

National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525. SAND2020-xxxx

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

# SFWST EBS Research Teams

## **Sandia National Laboratories**

***E.N. Matteo, T. Dewers, S. Gomez, T. Hadgu,***

## **Lawrence Berkeley National Laboratory**

***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,***

## **Los Alamos National Laboratory**

***F. Caporuscio, K.B. Sauer, M.J. Rock,,***

## **Vanderbilt University**

***C. Gruber, M. Steen, K.G. Brown, R. Delapp, A. Taylor, J. Ayers, D.S. Kosson,***

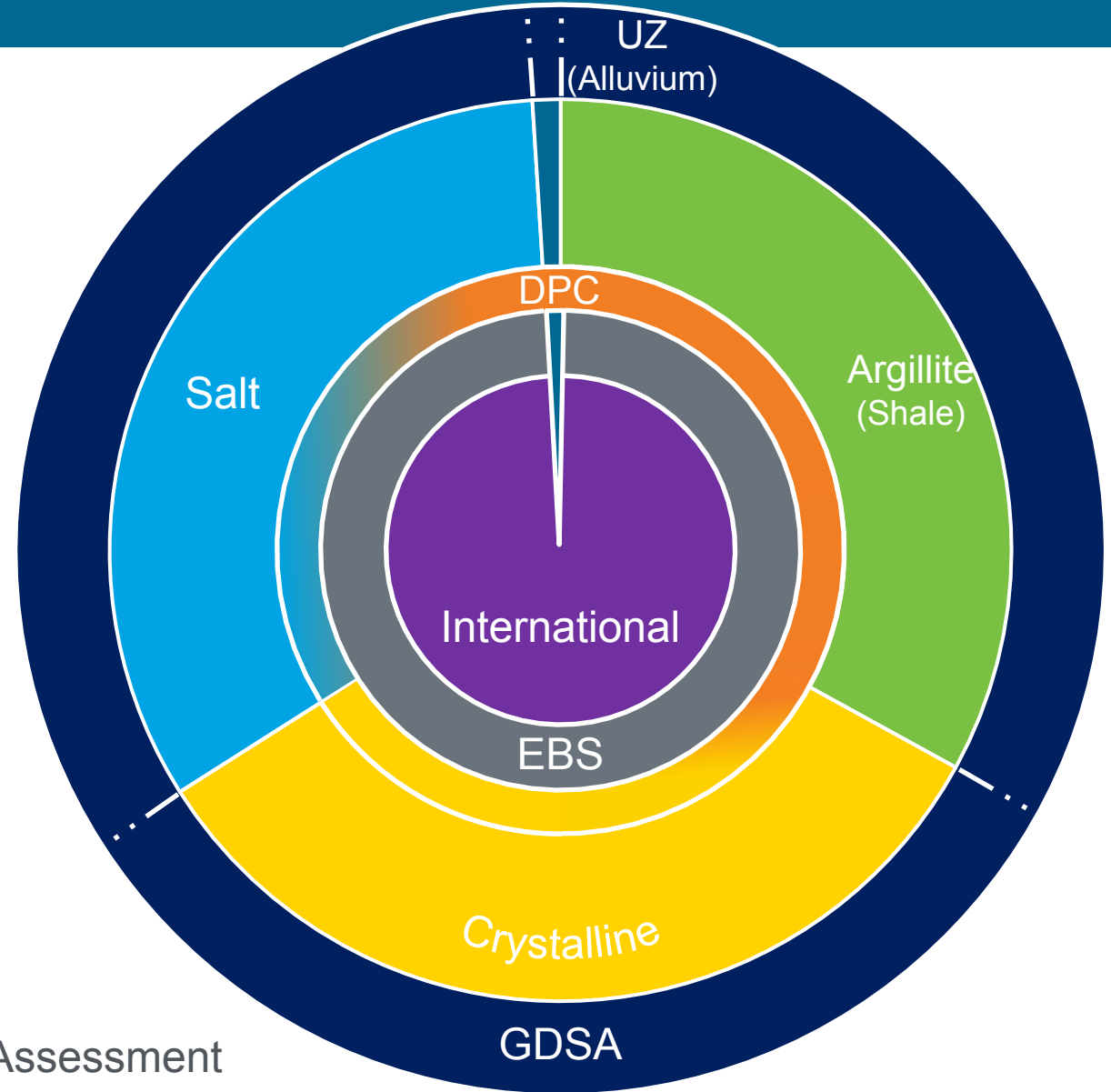
# Overview

- Engineered Barrier Systems(EBS) Research relative to other SFWST research areas
- Knowledge and Capability Gaps
- Research Priorities
- Summary of current EBS Research in the the EBS

# R&D Priorities

- Gaps in understanding 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, buffer, and host rock

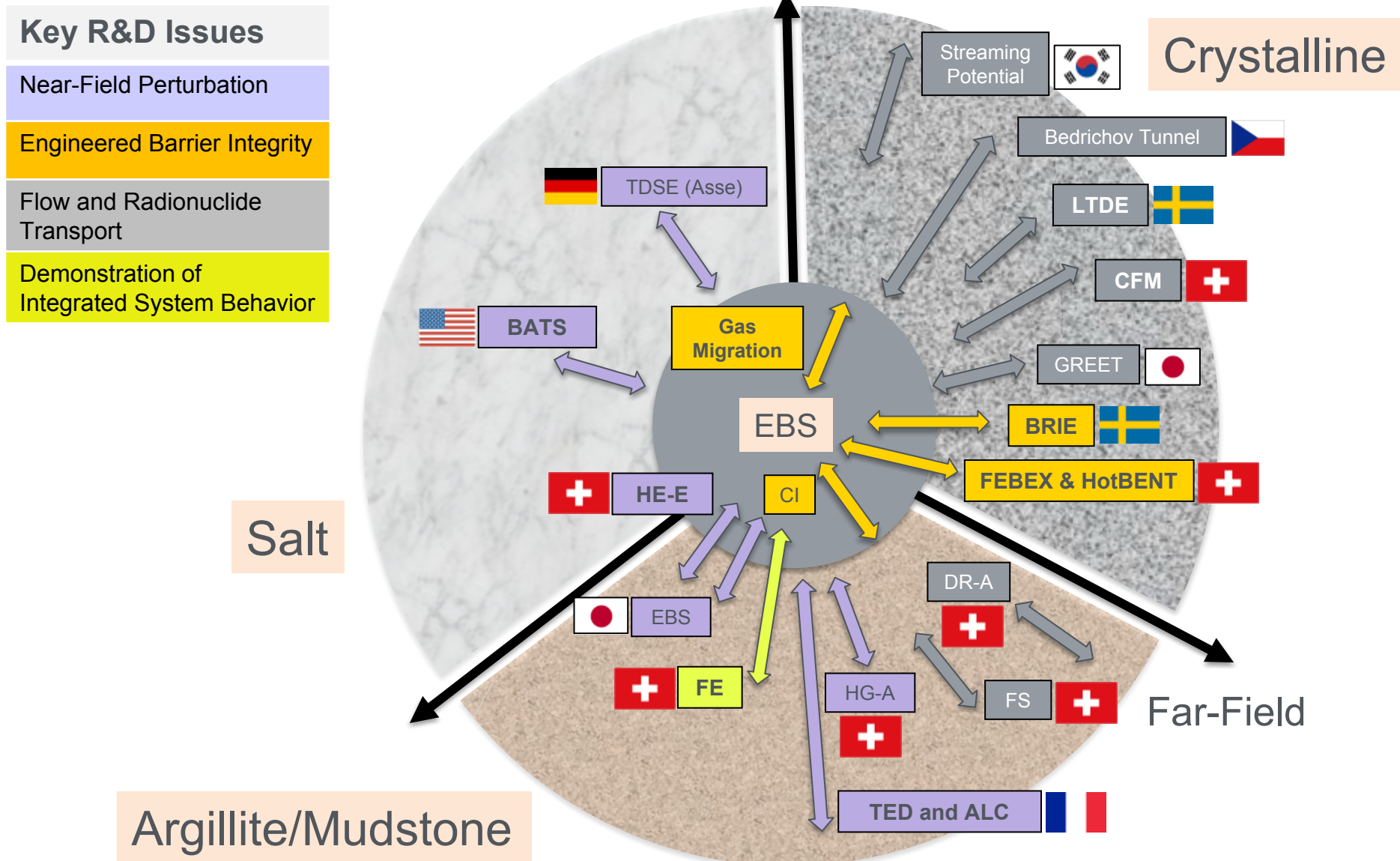
UZ = Unsaturated Zone  
DPC = Dual Purpose Canisters  
EBS = Engineered Barrier System  
GDSA = Geologic Disposal Safety Assessment



# Knowledge and Capability Gaps

- Gaps in understanding 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
  - Coupled processes
    - Chemo-mechanics
    - Thermal-Hydrologic-Mechanical-Chemical
    - Multi-phase flow
    - Multi-scale phenomenon
    - Linking microstructural scale to continuum scale

# International Portfolio in a Nutshell



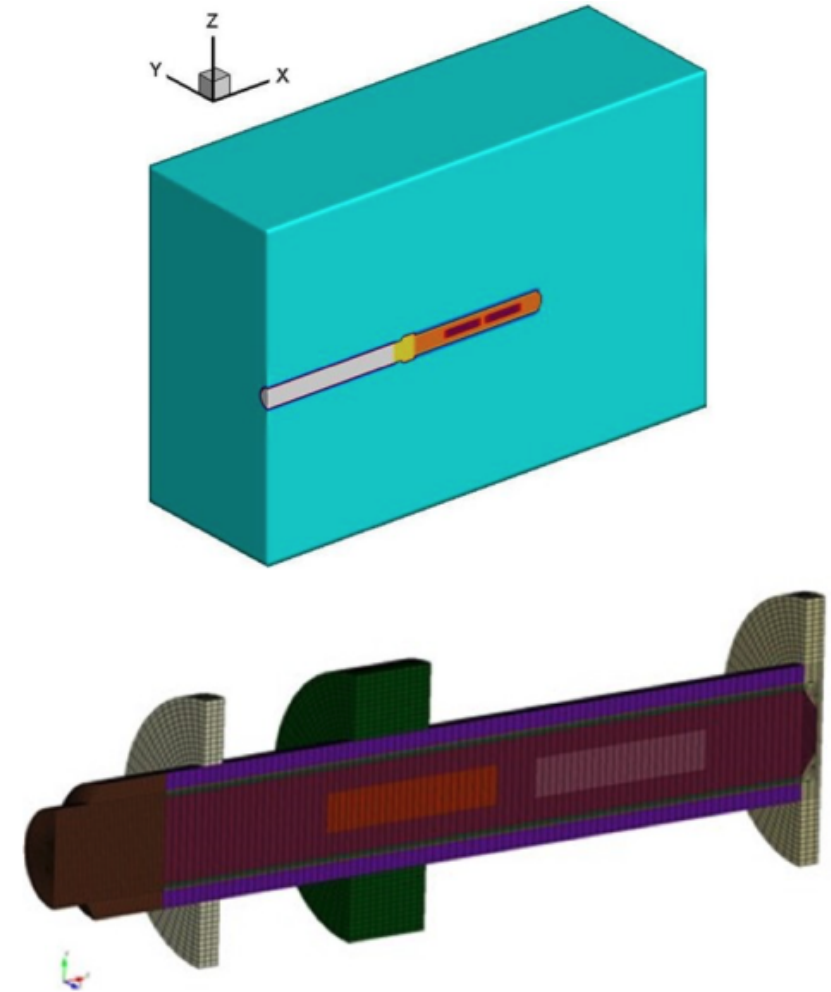
# Crosscuts with International Activities

- Engineered Barrier System Task Force Task 9 (completed March 2020)
  - 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



# Engineered Barrier Systems Task Force Task 9

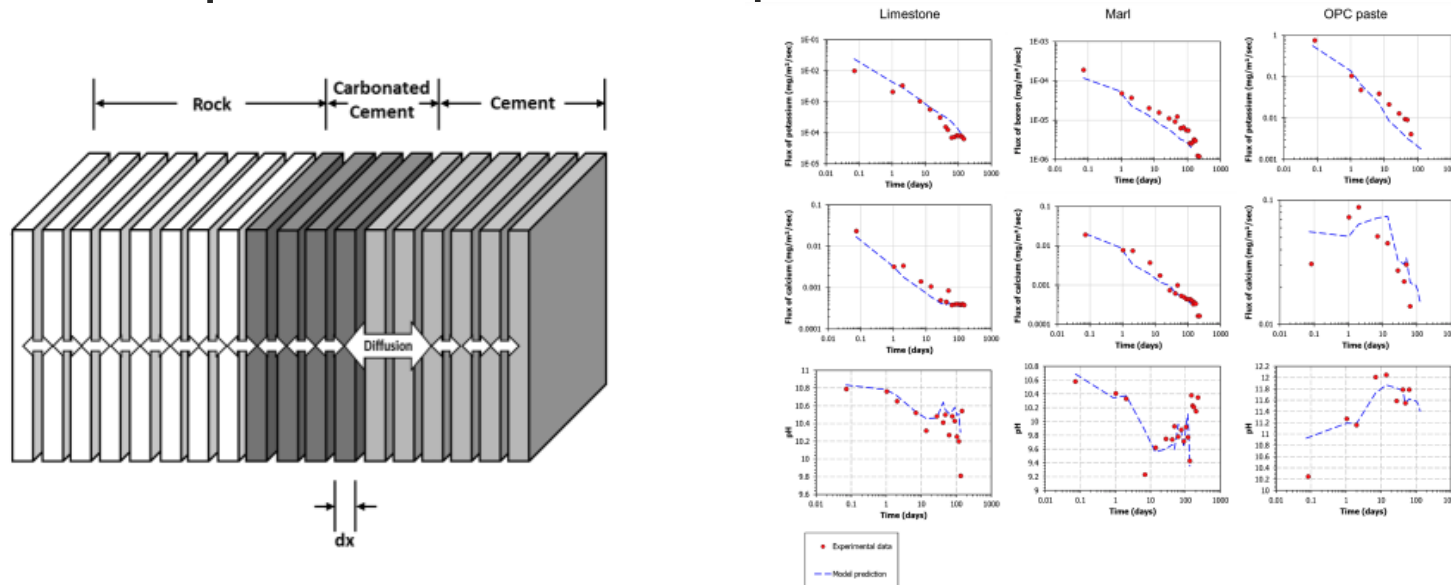
- Modelling teams simulate the FEBEX Test at the Grimsel Test Site in Switzerland
- 3-dimensional Thermal-Hydrologic Model using PFLOTRAN
- Good agreement with experimentally measured temperatures and liquid saturations
- Sensitivity study using DAKOTA-PFLOTRAN to examine model sensitivities, including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





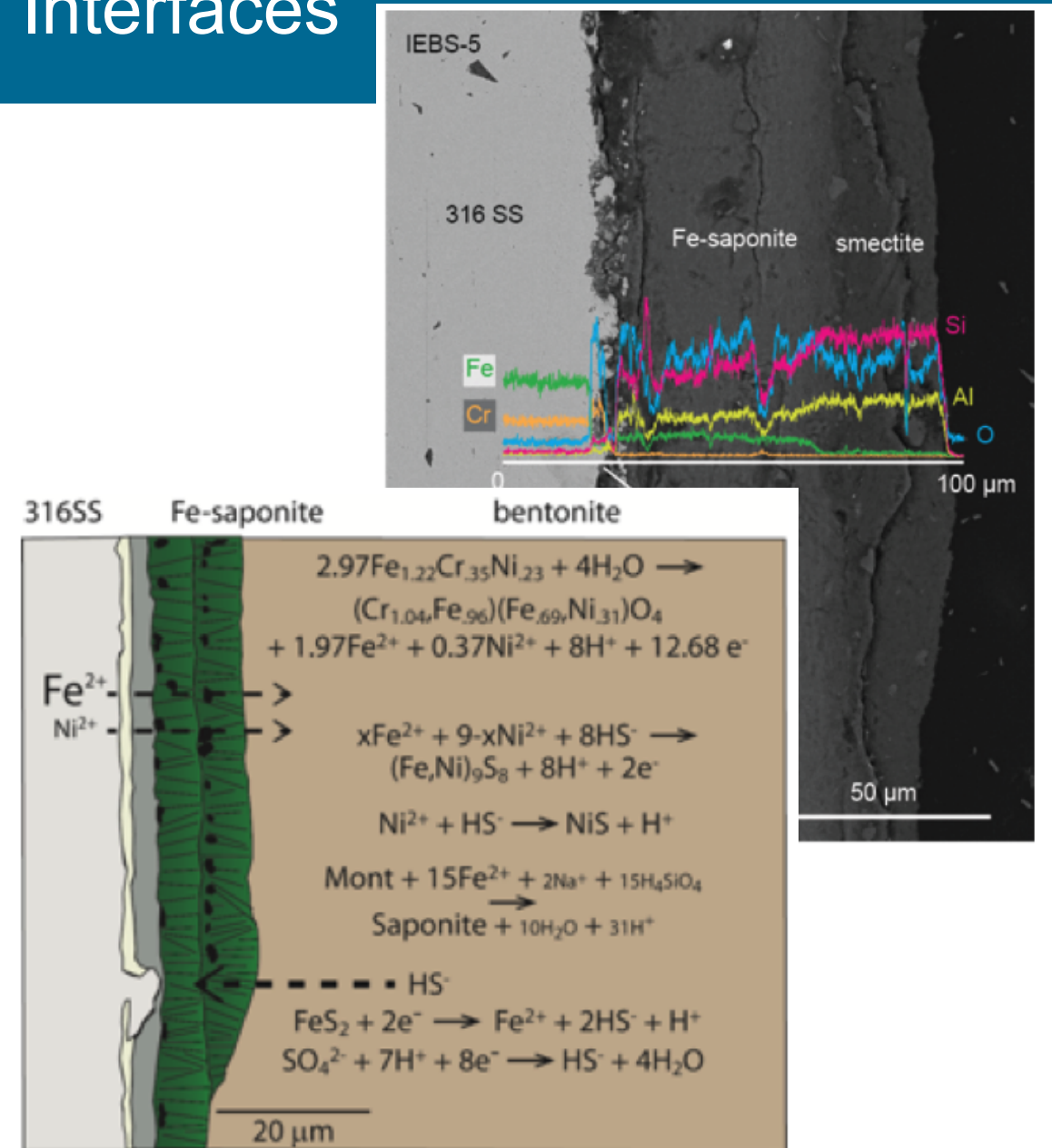
# Cement-degradation and Cement-Geomaterial Interactions

- 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

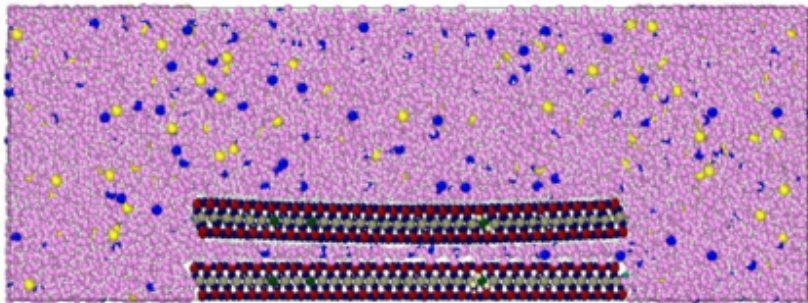
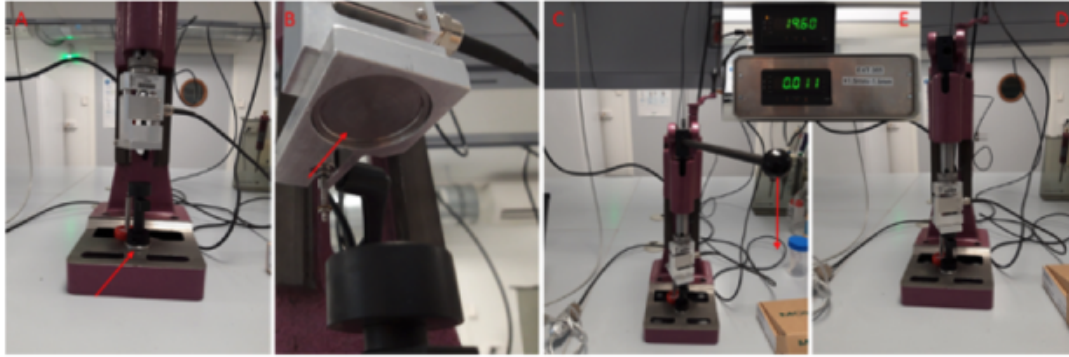
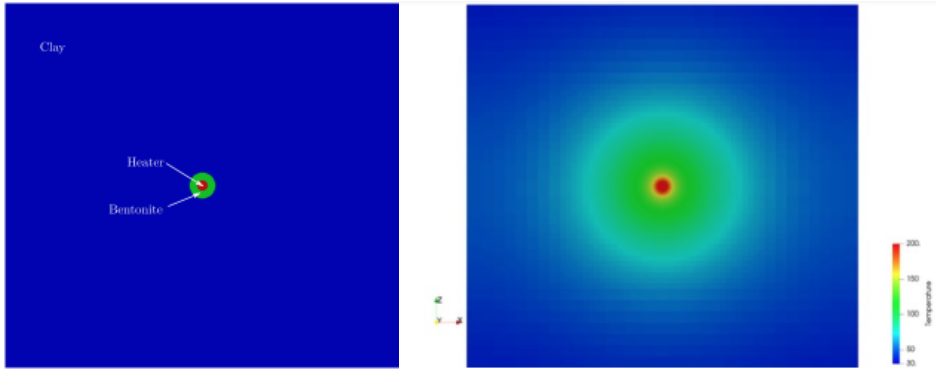


# Hydrothermal Alterations at Material Interfaces

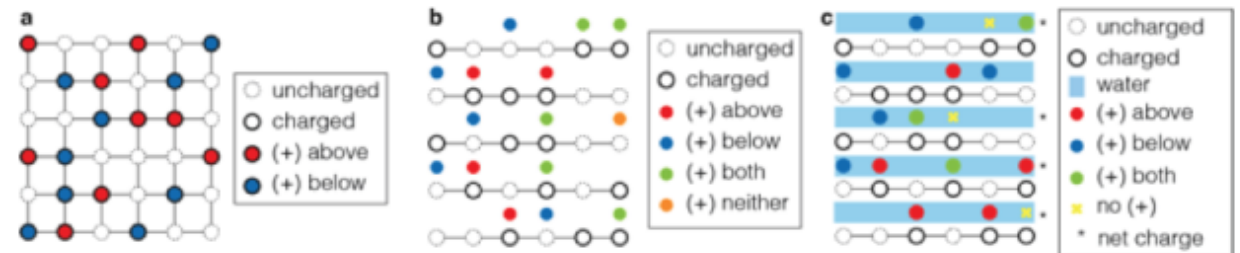
- Waste canister-buffer-host interactions investigated at hydrothermal conditions (e.g. steel-bentonite-granite in representative host pore solution)
- Recent tests have been also adding cementitious materials to the hydrothermal tests
- Post-test elemental fluid analysis and X-ray diffraction and electron 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



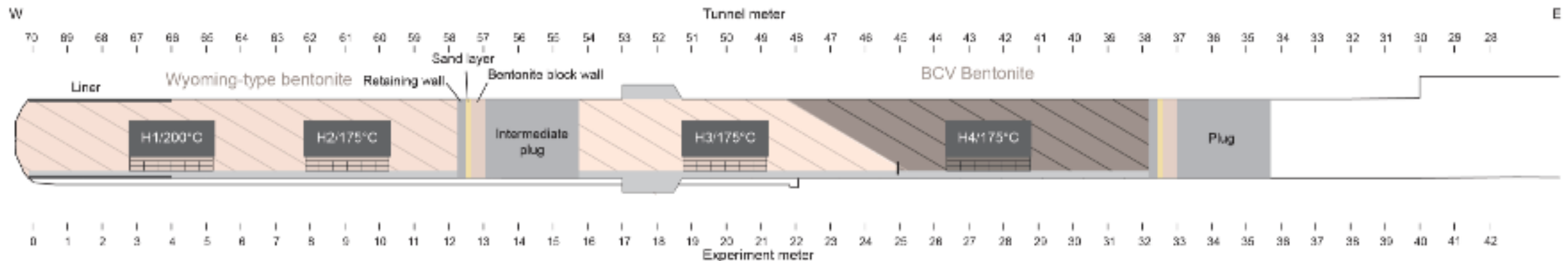
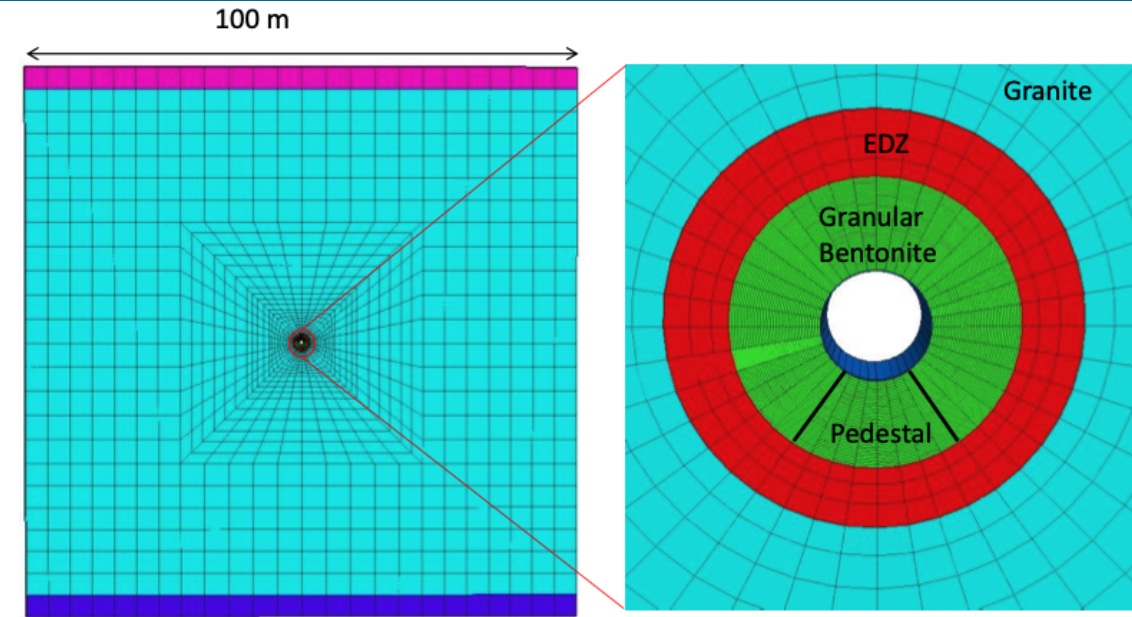
- Thermal-Hydrologic-Mechanical-Chemical modeling of buffer evolution using specialized constitutive models for clay swelling, esp. at high temperatures
- Uranium Sorption to bentonite to determine/improve distribution coefficients, so-called  $K_d$  values.
- Oedmetric swelling tests coupled with molecular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





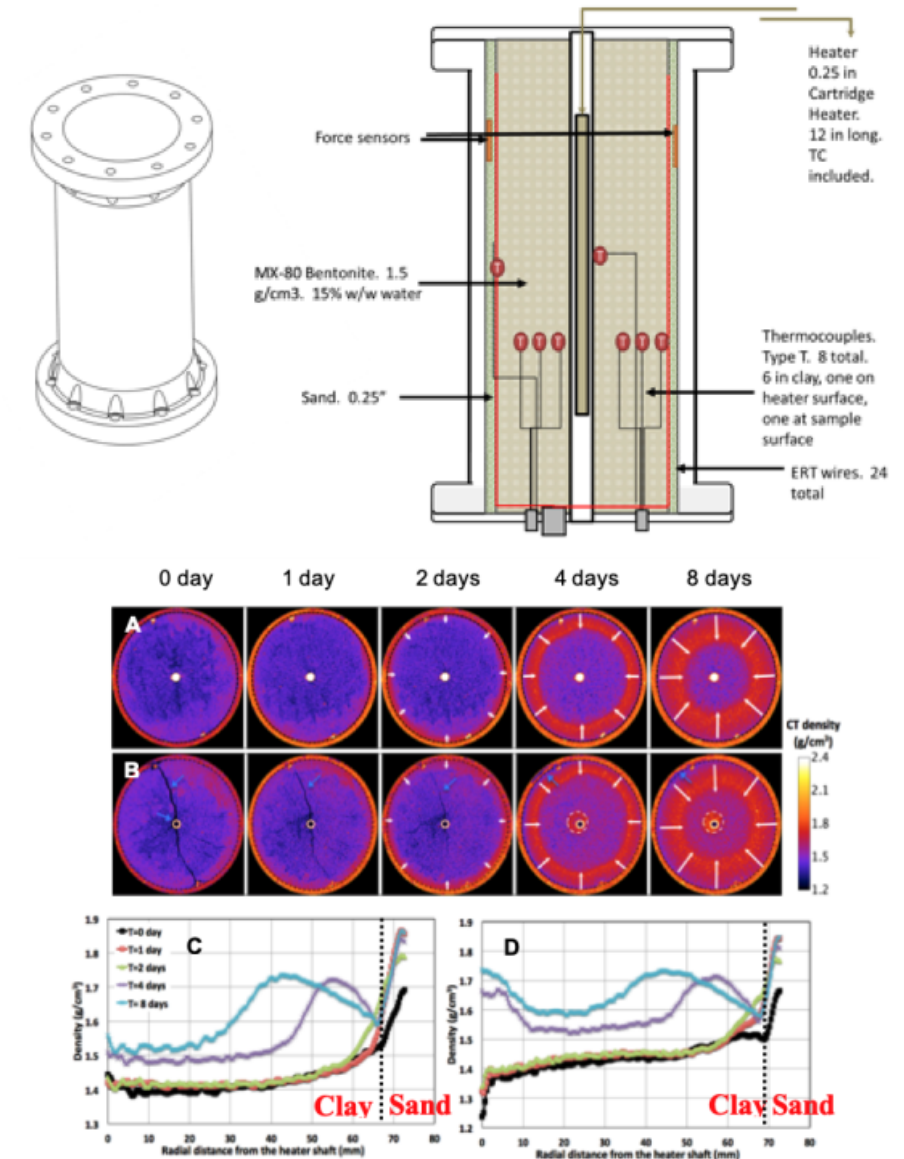
# Hot BENT and the LBNL Hot BENT Column Test

- 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.



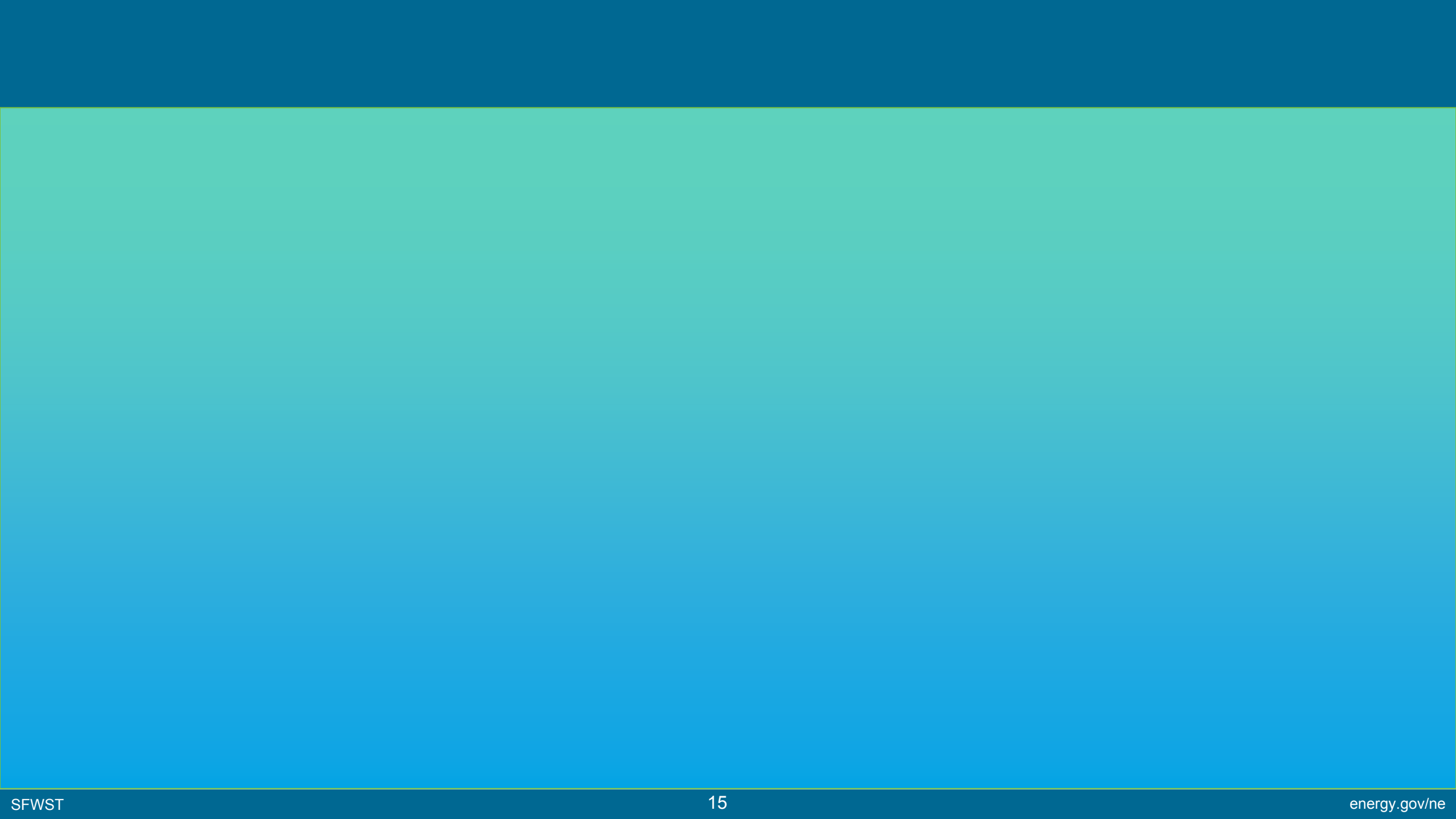
# Hot BENT and the LBNL Hot BENT Column Test

- In June 2019, hydration was started in both columns, and heating was applied to one column
- In FY19–20, columns were monitored continuously for hydration, temperature distribution, effluent chemistry, and density changes
- Effluent chemistry showed differences between 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



# Conclusions

- Knowledge and Capability Gaps
- Research Priorities
- Summary of current EBS Research in the the EBS
  - Drift-scale coupled process models (TH, THM, THMC)
  - Cement-degradation and Cement-Geomaterial Interactions
  - Hydrothermal Alterations at Material Interfaces
  - Bentonite Studies
    - THMC models for swelling
    - Uranium sorption
    - Oedometric Swelling tests
    - High temperature studies (e.g. HotBENT)





Back Up Slides

# Knowledge and Capability Gaps

- scale

- Gaps in modeling capability
  - Cement models for evolution plugs and liners
    - chemo-mechanical coupling
    - Fracture models
  - Bentonite buffer
- Address "multidisciplinary research needs" if any
- May be >1 slide! But not too much greater or you will be talking too long.

# How are EBS Knowledge Gaps Prioritized?

## **DOE SFWST Campaign R&D Roadmap Update**

### **Fuel Cycle Research & Development**

*Prepared for  
U.S. Department of Energy  
Spent Fuel and Waste Science and  
Technology Campaign*

*S. D. Sevougian, P. E. Mariner,  
L. A. Connolly, R. J. MacKinnon  
Sandia National Laboratories*

*R. D. Rogers, D. C. Dobson, J. L. Prouty  
Nuclear & Regulatory Support Services, LLC*

July 22, 2019  
M2SF-19SN010304042, Rev. 1  
SAND2019-9033 R



Cross-Cutting R&D Issue	Priority Score
DESIGN CONCEPT DEVELOPMENT	High
DISPOSAL SYSTEM MODELING	High
OPERATIONS-RELATED RESEARCH AND TECHNOLOGY DEVELOPMENT	Low
KNOWLEDGE MANAGEMENT	Medium
SITE SCREENING AND SELECTION TOOLS	Medium
EXPERIMENTAL AND ANALYTICAL TECHNIQUES FOR SITE CHARACTERIZATION	Medium
UNDERGROUND RESEARCH LABORATORIES	Medium
R&D CAPABILITIES EVALUATION	Medium

# High Priority Knowledge Gaps

Table 3-5. High Priority R&D Activities.

High Priority R&D Activities	
A-08	Evaluation of ordinary Portland cement (OPC)
C-15	Design improved backfill and seal materials
C-16	Development of new waste package concepts and models for evaluation of waste package performance for long-term disposal
D-01	Probabilistic post-closure DPC criticality consequence analyses Task 1 - Scoping Phase Task 2 - Preliminary Analysis Phase Task 3 - Development Phase
D-03	DPC filler and neutron absorber degradation testing and analysis
D-04	Coupled multi-physics simulation of DPC postclosure (chemical, mechanical, thermal-hydraulic) including processes external to the waste package.
D-05	Source term development with and without criticality
E-09	Cement plug/liner degradation
E-11	EBS High Temp experimental data collection- To evaluate high temperature mineralogy /geochemistry changes.
E-14	In-Package Chemistry
E-17	Buffer Material by Design
I-04	Experiment of bentonite EBS under high temperature, HotBENT
I-06	Mont Terri FS Fault Slip Experiment
I-08	DECOVALEX-2019 Task A: Advective gas flow in bentonite
I-12	TH and THM Processes in Salt: German-US Collaborations (WEIMOS)
I-13	TH and THM Processes in Salt: German-US Collaborations (BENVASIM)
I-16	New Activity: DECOVALEX Task on Salt Heater Test and Coupled Modeling
I-18	New Activity: Other potential DECOVALEX Tasks of Interest: Large-Scale Gas Transport
P-12	WP Degradation Model Framework
S-01	Salt Coupled THM processes, hydraulic properties from mechanical behavior (geomechanical)
S-03	Coupled THC advection and diffusion processes in Salt, multi-phase flow processes and material properties in Salt
S-04	Coupled THC processes in Salt, Dissolution and precipitation of salt near heat sources (heat pipes)
S-05	Borehole-based Field Testing in Salt

E-09	Cement plug/liner degradation
E-11	EBS High Temp experimental data collection- To evaluate high temperature mineralogy /geochemistry changes.
E-14	In-Package Chemistry
E-17	Buffer Material by Design
I-04	Experiment of bentonite EBS under high temperature, HotBENT
I-06	Mont Terri FS Fault Slip Experiment
I-08	DECOVALEX-2019 Task A: Advective gas flow in bentonite
I-12	TH and THM Processes in Salt: German-US Collaborations (WEIMOS)
I-13	TH and THM Processes in Salt: German-US Collaborations (BENVASIM)
I-16	New Activity: DECOVALEX Task on Salt Heater Test and Coupled Modeling
I-18	New Activity: Other potential DECOVALEX Tasks of Interest: Large-Scale Gas Transport

# Crosscuts with International Activities

High Impact R&D Topics	High-Priority R&D Activities	Medium-High-Priority R&D Activities
High Temperature Impacts	D-1, D-4, I-4, I-6, I-16, E-11, S-5	I-2, I-3, I-7, E-10
Buffer and Seal Studies	I-4, E-9, E-17, A-8, C-15	I-2, I-3, I-7, A-4, C-6, C-8, C-11
Coupled Processes (Salt)	S-1, S-3, S-4, I-12, I-13	I-14, S-2, S-7, S-8, S-11
Gas Flow in the EBS	I-6, I-8, I-18	I-9, P-17
Criticality	D-1, D-3, D-4, D-5	
Waste Package Degradation	C-16, P-12	E-4, E-6
In-Package Chemistry	E-14	E-2, E-20, P-15, P-16
Generic PA Models		P-1, P-2, P-4, P-11, P-13, P-14
Radionuclide Transport		C-11, C-13, C-14, P-15, P-16
DFN Issues		I-21, C-1, C-17
GDSA Geologic Modeling		O-2, O-3
THC Processes in EBS		E-3

# Medium-High Priority Knowledge Gaps

<b>E-02</b>	SNF Degradation testing activities
<b>E-03</b>	THC processes in EBS
<b>E-04</b>	Waste Package Degradation Model (mechanistic)
<b>E-06</b>	Waste Package Degradation Testing
<b>E-10</b>	High-Temperature Behavior
<b>E-20</b>	Colloid source terms
<b>I-02</b>	FEBEX-DP Modeling: Dismantling phase of the long-term FEBEX heater test - Modeling
<b>I-03</b>	FEBEX-DP Experimental Work: Dismantling phase of the long-term FEBEX heater test

# Priority R&D

- Process understanding
- Model development
- [Technology development, e.g. Dobson et al.] ??
- address gaps
- Include international and GD SA
- Include host-rock processes
- Include EBS processes that are highly relevant to this host rock.
- Should be multiple slides! But you will still have to pick and choose!



# Priority R&D – A Forward Look

- Longer range possibilities
- Look at 5-year plan, 3-5 year category for ideas.