Engineered Barrier Systems R&D

Ed Matteo

Sandia National Laboratories

SAND2019-xxxx

SFWD

Spent Fuel & Waste Disposition

Annual Working Group Meeting
UNLV-SEB – *Las Vegas, Nevada*
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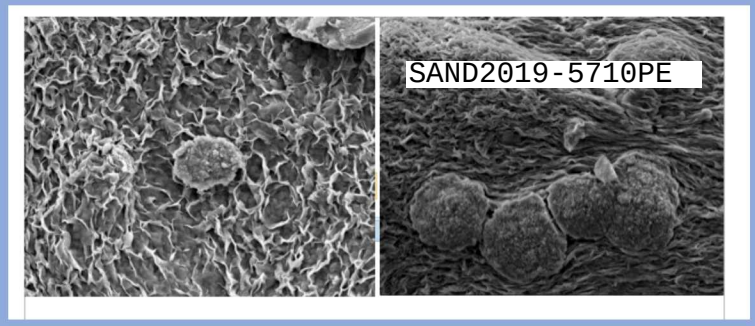
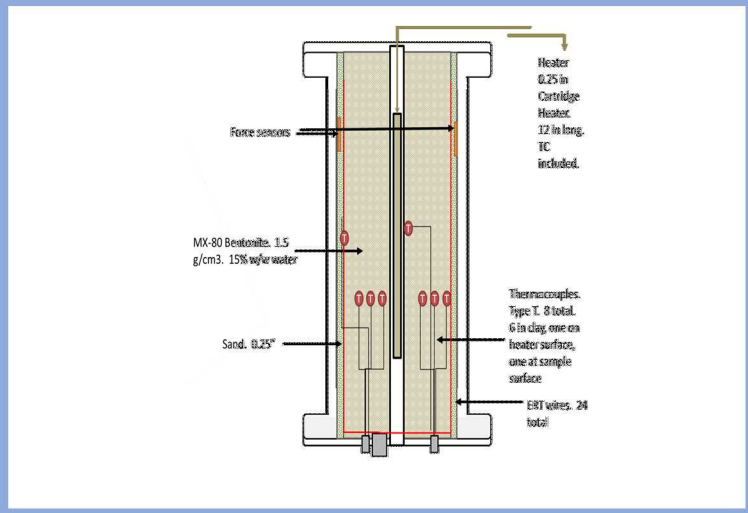
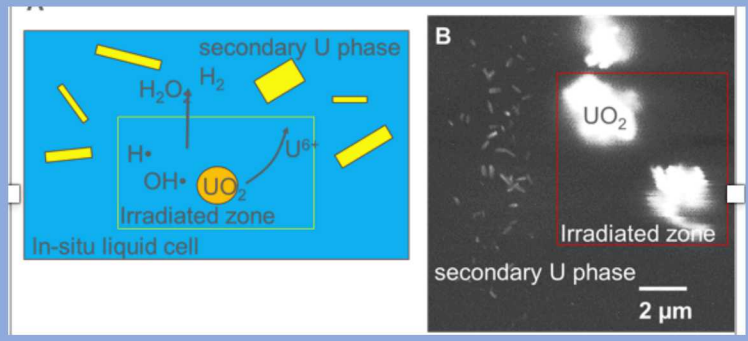






Overview of the…Overview

- EBS related talks at this meeting
- Highlights - Key Accomplishments in UFD/SFWD
- Technical accomplishments

EBS TALKS IN THE DR SESSIONS

- Argillite
  - Edgar Buck, PNNL: "In-situ Microscopy Observations of the Corrosion of Uranium Oxide"
  - Florie Caporuscio, LANL: "Engineered Barrier System (EBS) hydrothermal experiments for a Grimsel granodiorite host rock: Mineralogical evolution at repository pressures and temperatures"
  - Artis Migdissov, LANL: "Tetravalent uranium solubility and speciation under reducing conditions in sulfate-bearing aqueous solutions at temperatures up to 350 °"
- Crystalline
  - Patricia Fox, LBNL: U interaction w/ bentonite
  - Liange Zheng, LBNL: THMC modeling & integration w/ GDSA
    Liange Zheng, LBNL: FEBEX-DP and HotBENT
- Salt
  - Ed Matteo, SNL: "Engineered Barrier System Component of the BATS Test"

Key Accomplishments and Path Forward

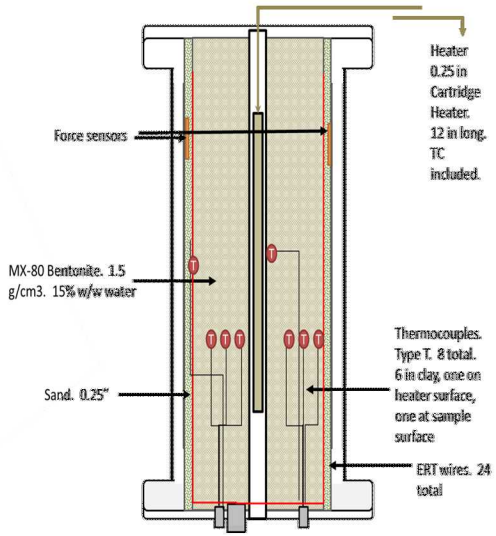
- EBS WP re-start in FY18
- Significant integration with International, Salt, Argillite, and Crystalline activities
- Papers, presentations, session chairs
- Moving forward:
  - continued integration with GDSA
  - International opportunities
    - FEBEX DP and HotBENT
    - DECOVALEX
    - KOMPASS/RANGERS - US/Germany Salt Collaborations

LBNL EBS R&D HIGHLIGHTS

- Understanding coupled THMC processes and improving modeling capability
  - Accomplishments
    - Improving parallel THMC code, TreactMech and comparing model results of TreactMech vs TOUGHREACT-FLAC, a first step towards developing surrogate models for integrating coupled processes model into GDSA
    - THC models to study the impact of bentonite/host rocks interaction on the transport of radionuclides within EBS using generic models (a journal article submitted Chemical Geology)
  - In the future
    - Exploratory high temperature THMC simulations for MX-80 bentonite
    - Fully coupled THMC model with transport of radionuclides
- Fundamental understanding coupled MC processes using microscopic experiment and modeling
  - Implement molecular-scale models to quantify the relative free energies of montmorillonite clay systems
  - Construct a specialized oedometer for measuring the swelling pressure of compacted clay and simultaneously measuring key aspects of the clay microstructure using synchrotron X-ray methods
  - Design and commission a new TXM at beamline 11.3.1 and provide proof-of-principle data on (1) the structural evolution of hydrated compacted bentonite under changing chemical conditions or (2) the deformation and fracture sealing of candidate repository rocks under stress over multiple time scales
  - Computational prediction of the retention of multi-nuclear radionuclide complexes
  - Experiments have been constructed and will produce data by the end of FY19

LBNL EBS R&D INTERNATIONAL HIGHLIGHTS

- Large scale *in situ* test
  - Accomplishments:
    - Understanding key THMC processes via model interpretation of FEBEX-DP data
    - Scoping calculations to support the design of HotBENT
  - In the future
    - Model interpretation of the chemical data at the interfacial area: granite/bentonite, canister/bentonite
    - 3-D THMC models for HotBENT
- Laboratory experiments
  - Accomplishment
    - Construct high temperature column test to supplement HotBENT
    - Conduct diffusion experiment with FEBEX bentonite and reference bentonite (pure smectite)
  - In the future
    - Prediction of the THMC evolution of the high temperature column test
    - Model interpretation of the diffusion experiment



High T column test at LBNL

LANL UPDATES (1/3)

1) Hydrothermal experiments in crystalline rock.
   - Grimsel Granodiorite/ bentonite clay/Grimsel groundwater
   - Temperature = 250 C, pressure = 150 bar
   - Clay / zeolite transformations
   - Steel corrosion

2) Speciation of U(IV) in sulfate-bearing solutions
   - UO2 pellets / sulfate solution replicating Grimsel groundwater
   - Very reducing conditions (Co/CoO, Ni/NiO)

LANL Updates (2/3)

Hydrothermal experiment Mineralogy summary

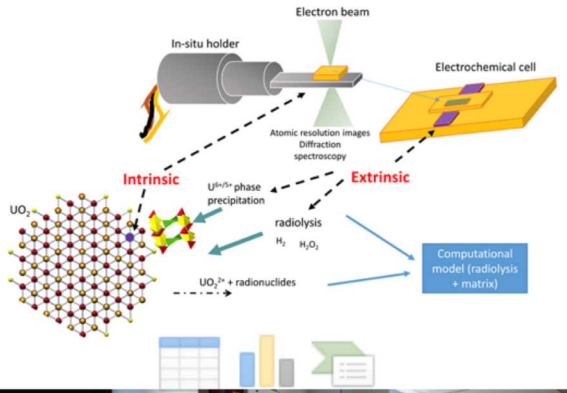
- Lack of illite growth, however growth of muscovite.
- Tobermorite present / no zeolites formed. Due to bulk chemistry.
- Steel interface with bentonite still creates Fe-saponite.
- Authigenic mineralogy different from argillite host rock. Perhaps due to host rock / groundwater chemistry differences, investigation ongoing.
- Future experiments 1) six month run, 2) addition of cement to starting materials

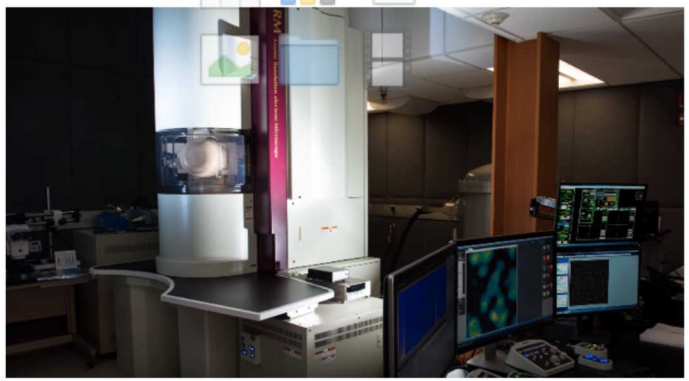
LANL Updates (2/3)

- 250, 300, 350 C experiments have been completed.
- 200 C experiments are in progress.
- thermodynamic constants and species stoichiometry have been derived.
- Dependent on pH – temperature U(IV) solubility ranges from 10s of ppb to low ppm concentration
- Draft manuscript prepared for submission to GCA

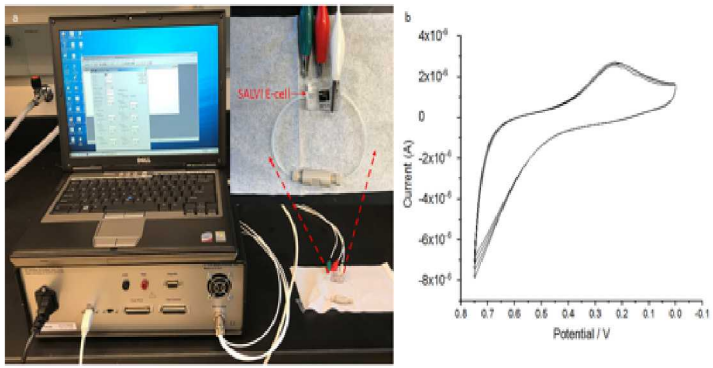
PNNL Updates (1/2)

- To investigate the corrosion of UO2 corrosion *in situ* in the Scanning Electron Microscope (SEM) and Transmission Electron Microscope (TEM).
  - Using the System for Analysis at the Vacuum Liquid Interface (SALVI) electrochemical cell (E-cell).
  - Using Protochips Electrochemical In-situ TEM Stage
- To provide real-time and *in-operando* monitoring of UO2 stability and morphological change and to study the UO2 corrosion process at the microscale and using CryoEM to monitor progress.
- The results will be utilized to support the Mixed Potential Model that has been developed for the repository program.

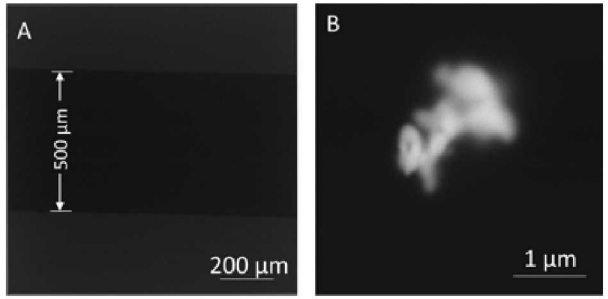




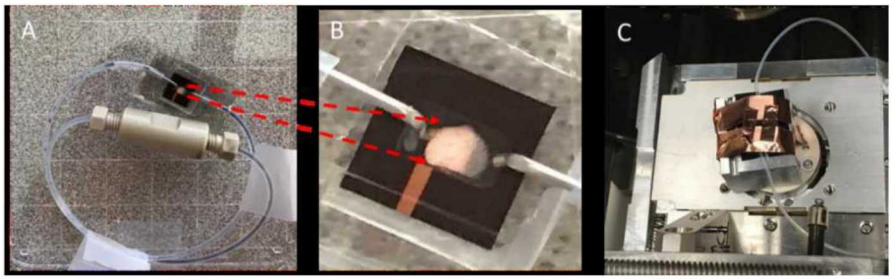
PNNL Updates (2/2)



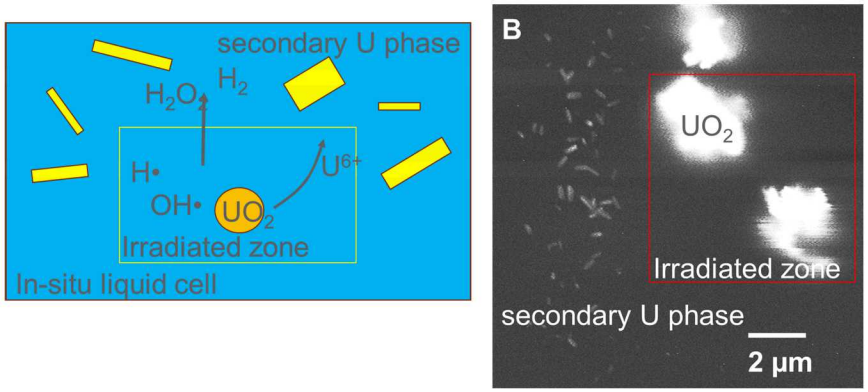
(a) In operando SEM setup showing the SALVI E-cell (insert) connected with an electrochemical station purchased by the project; and (b) cyclic voltammograms acquired using this setup.



The BSE image of the SAVLI microchannel imaged under low magnification and a BSE image of a UO_2 particle in the channel in the low vacuum mode.



SALVI cell in the SEM



Bromine effects on radiolysis in the EM

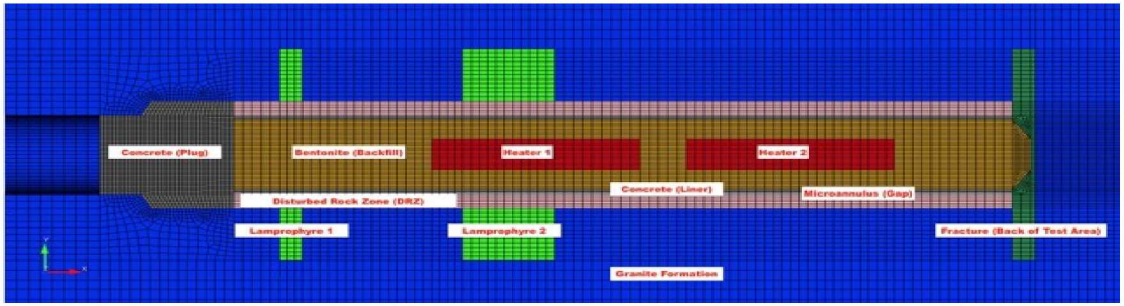
- **Irradiation of the UO_2 leads to dissolution and then precipitation of studtite distant from the source of irradiation**

SNL Updates (1/2)

- Thermal-hydrology modeling for disposal of spent nuclear fuel in crystalline host roc
  - Sensitivity analysis by varying parameters such as: waste type, host rock properties, buffer properties.
  - So far, effect of host rock permeability has been completed. The results show that rock permeability has a significant effect on vapor migration.
- Thermal analysis for disposal of dual-purpose canisters in a generic repository
  - Thermal-only semi-analytic analysis of DPC's in a generic repository.
    - 37-PWR 60 GW-d/MT and 150 years out of reactor
  - Backfill thermal conductivity has a greater effect on waste package surface temperature than waste package and drift spacing. The results also showed that limiting temperatures would require use of engineered buffer material to increase thermal conductivity.
- Novel Anionic Sorbents (crosscuts with Crystalline DR)
  - Paper/presentation in IHLRWM
  - Journal paper in progress

SNL UPDATES (2/2)

- SKB EBS Task Force - Task 9
  - Task 9 is focused on modeling of FEBEX In-situ
  - TH and THM modeling using PFLOTRAN and COMSOL
- Cement leaching modelling and experiments
  - In collaboration with Vanderbilt and NRCN (Israel)
  - Benchmarking between Leach XS and PFLOTRAN for modelling cement leaching
- Crosscut with Salt DR - German Collaborations in EBS for Salt
  - Host KOMPASS - salt reconsolidation
  - RANGERS - seal design and performance



PRIORITIES

	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

Questions?

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