SAND2018-5457PE

Spent Fuel and Waste Science and Technology

Disposal in Argillite R&D International Collaborations: FEBEX-DP & DECOVALEX2019

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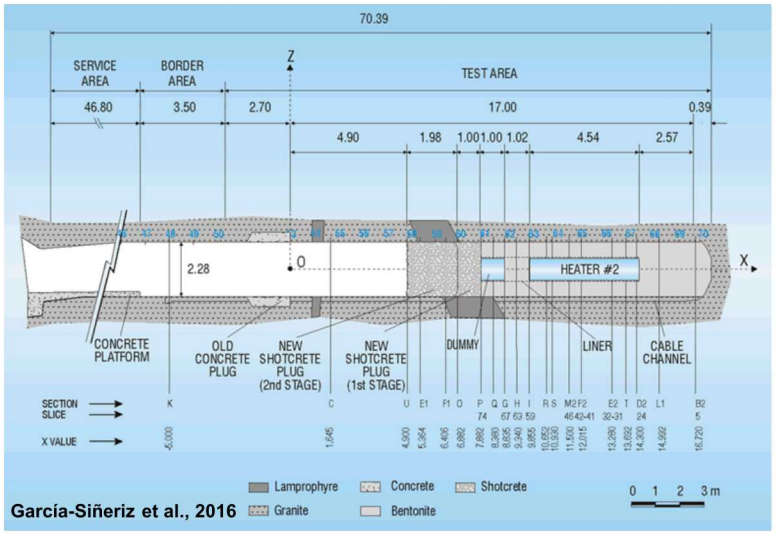
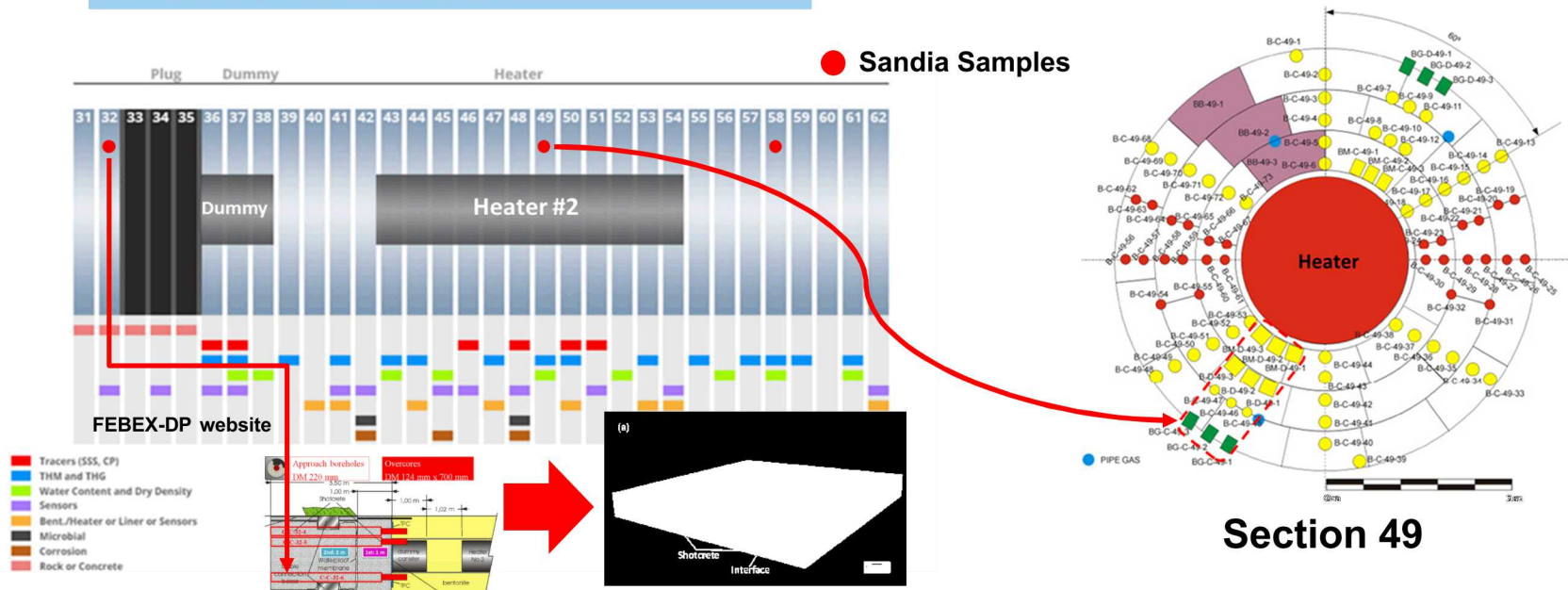
FEBEX-DP: Section 49 – Sample Characterization Studies

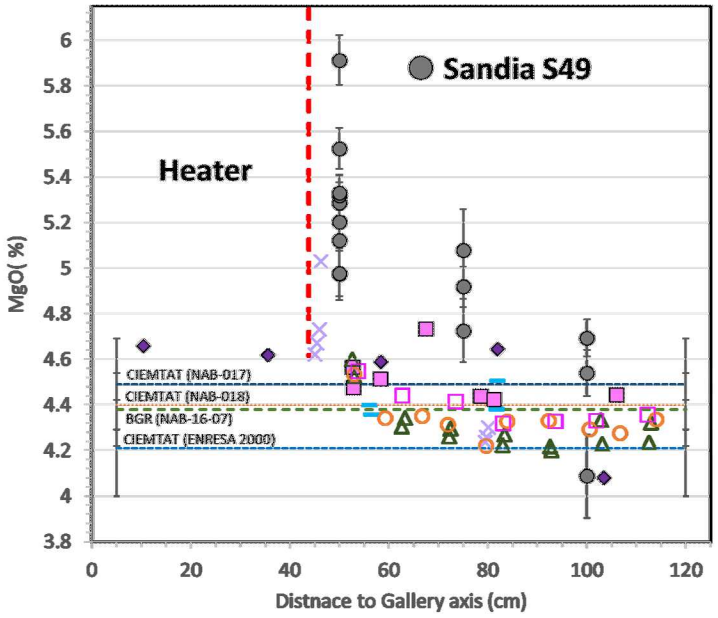


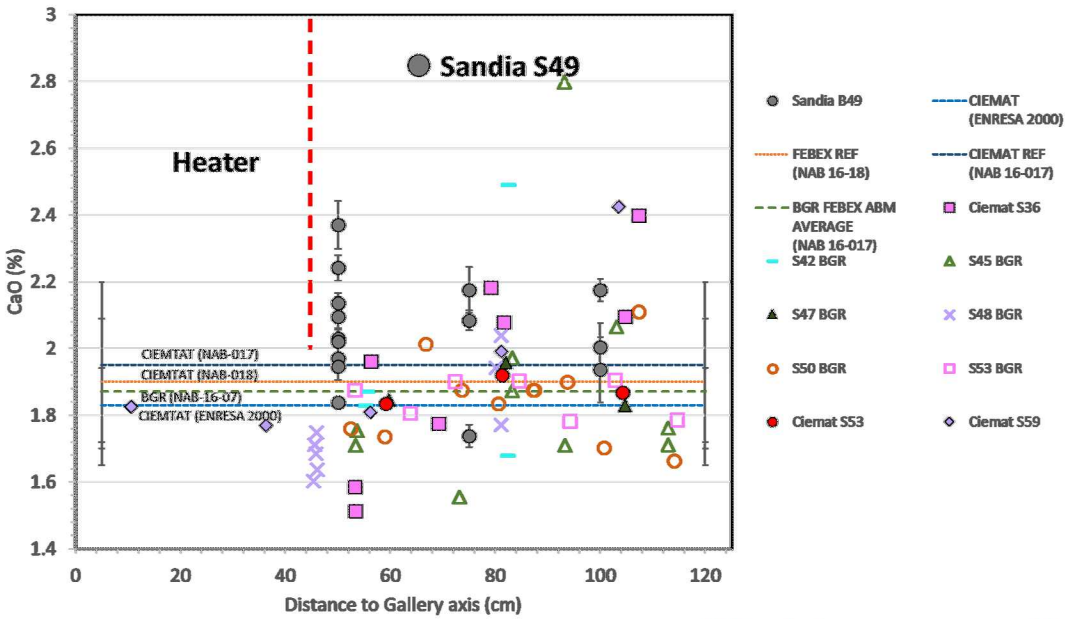
García-Siñeriz et al., 2016

- **FEBEX-DP**
  - Section 49 samples (near longitudinal central area of heater)
  - Bentonite samples from close to the heater towards the outer parts of the barrier
- **X-Ray Fluorescence (XRF) bulk composition, SEM-EDS, X-Ray Diffraction (XRD), Thermogravimetric analysis (TGA)**



Bulk Bentonite XRF Analyses (I)

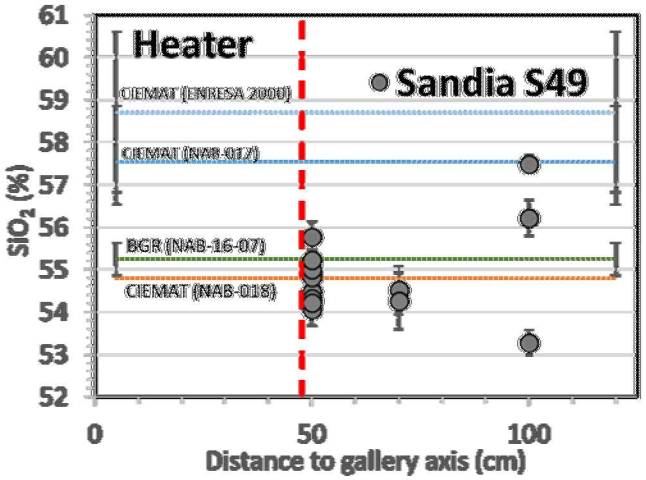


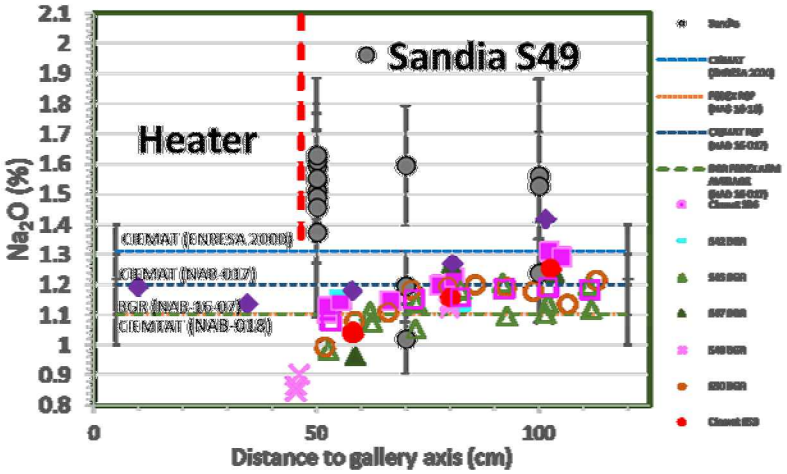


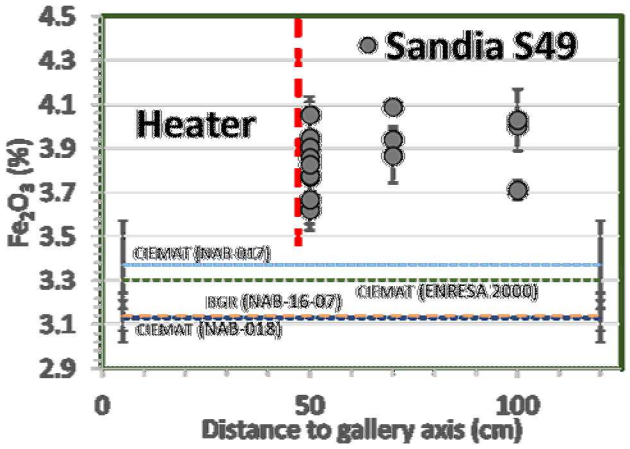
Work in progress!!!

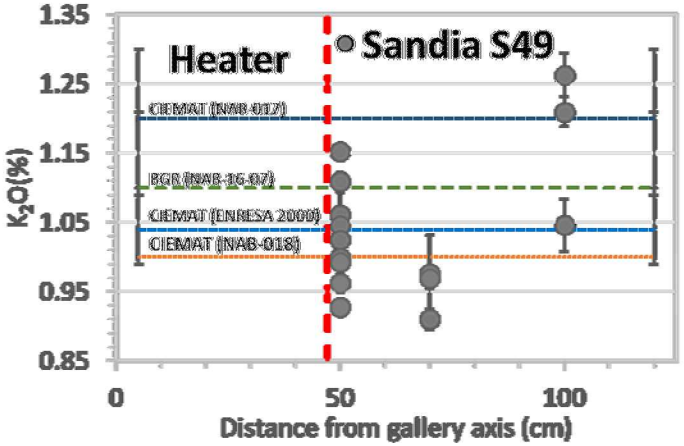
- Mg enrichment towards the heater surface
- Bulk MgO content far from heater nominally within the bounds of other lab analyses
- Overall, CaO content is relatively variable close to the heater surface
- Mg enrichment(?):
  - Enhanced Mg exchange with temperature?
  - SEM-EDS didn't show newly-formed Mg-bearing phases within the clay matrix
  - NEXT STEP: Conduct further SEM-EDS and XRD studies on all samples & compare

Bulk Bentonite XRF Analyses (II)





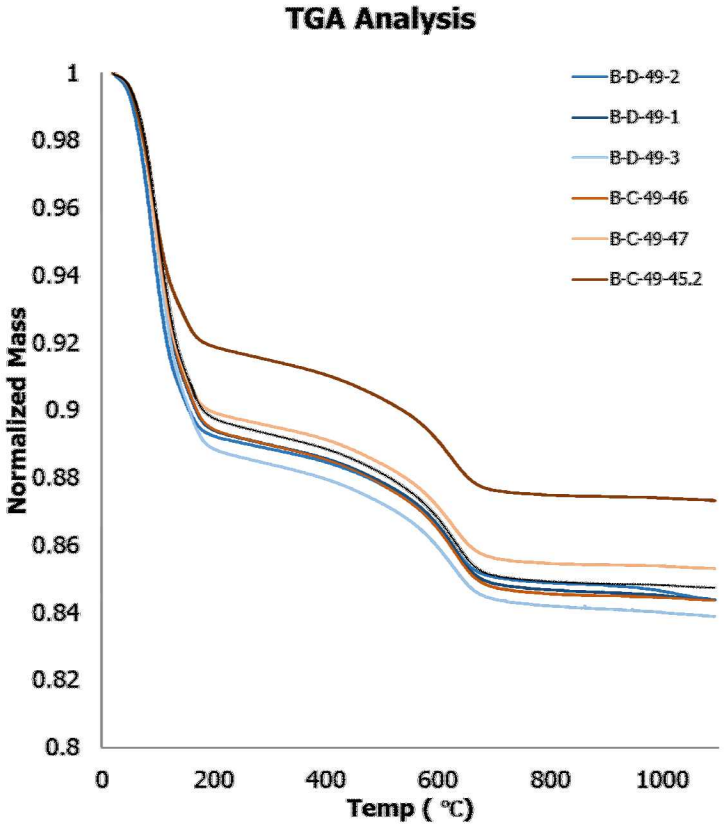


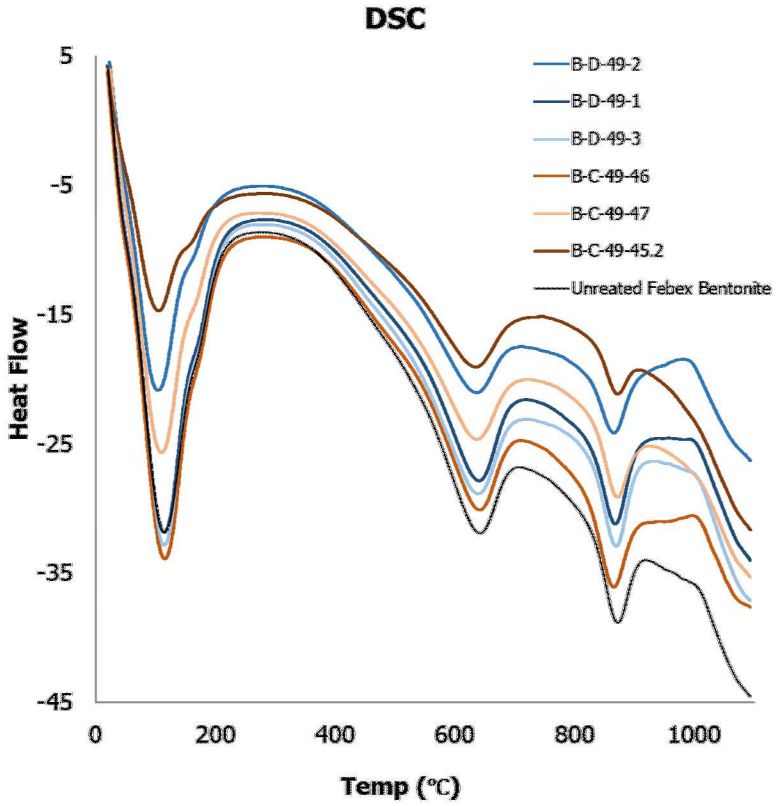


- Large uncertainties on Na_2O content – Issues with detection limits
- Slightly enriched in Fe_2O_3 relative to reference bentonite compositions
- Fe_2O_3, SiO_2, & K_2O fall within the range of reference bentonite compositions

Work in progress!!!

Thermogravimetric (TGA) & Differential Scanning Calorimetry (DSC) Analyses

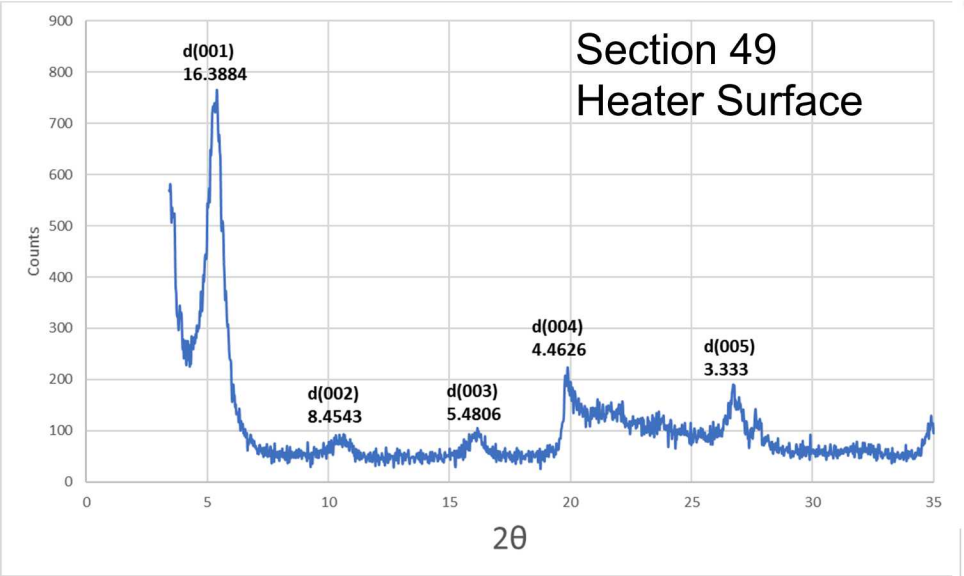


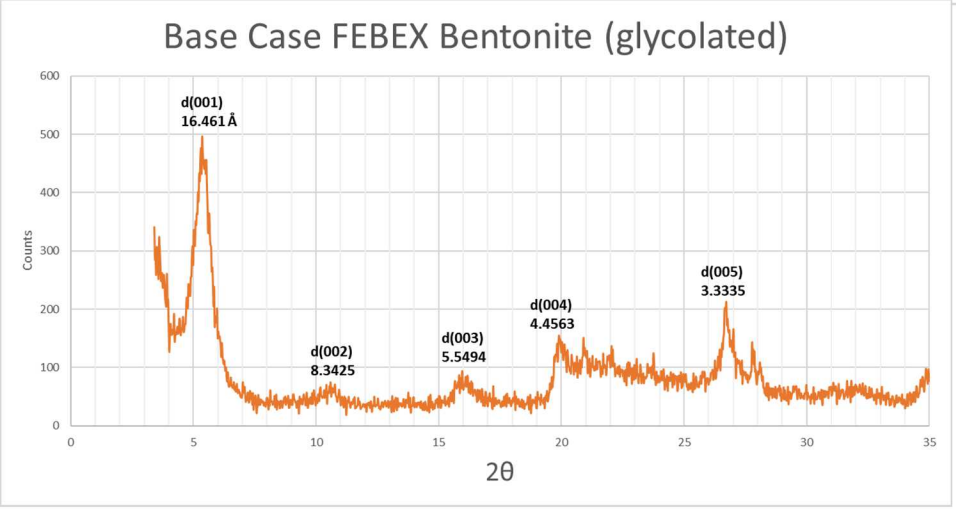


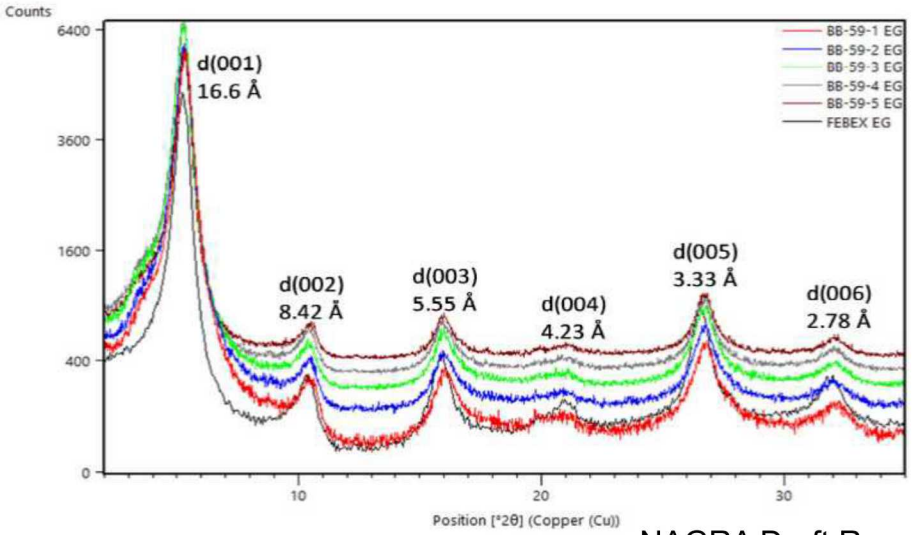
- Differences in TGA & DSC profiles with sample locations
- TODO / IN PROGRESS:
  - Profile(s) evaluation relative to FEBEX reference bentonite
  - Evaluate water content

Work in progress!!!

X-Ray Diffraction (XRD) Analyses





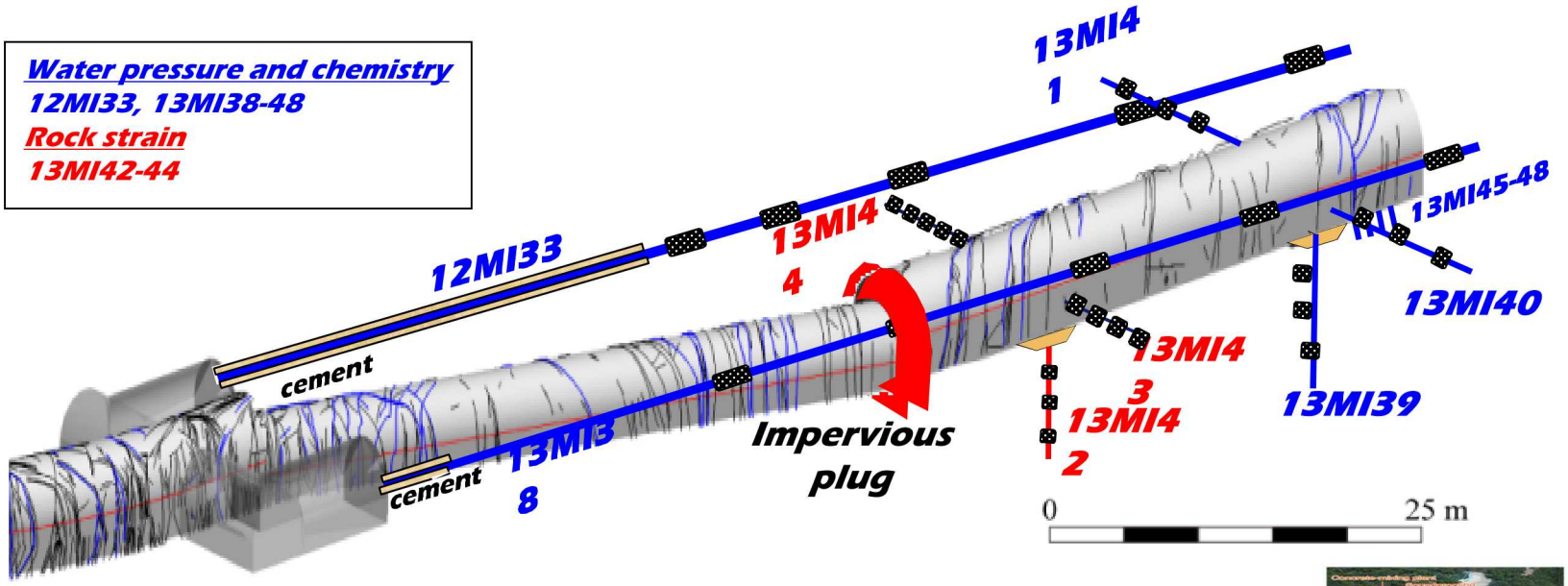


NAGRA Draft Report

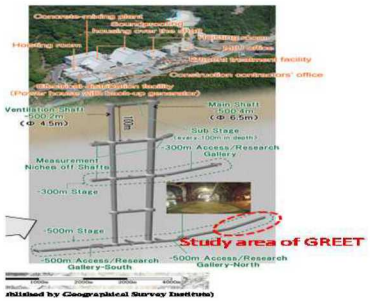
- Overall, XRD profiles show close similarities with those reported by FEBEX-DP project
- **TODO:**
  - XRD analyses of samples away from heater
  - Evaluate d(001)-spacings as a function of distance from heater surface

Work in progress!!!

DECOVALEX19: Closure Test Drift (CTD) Geochemistry



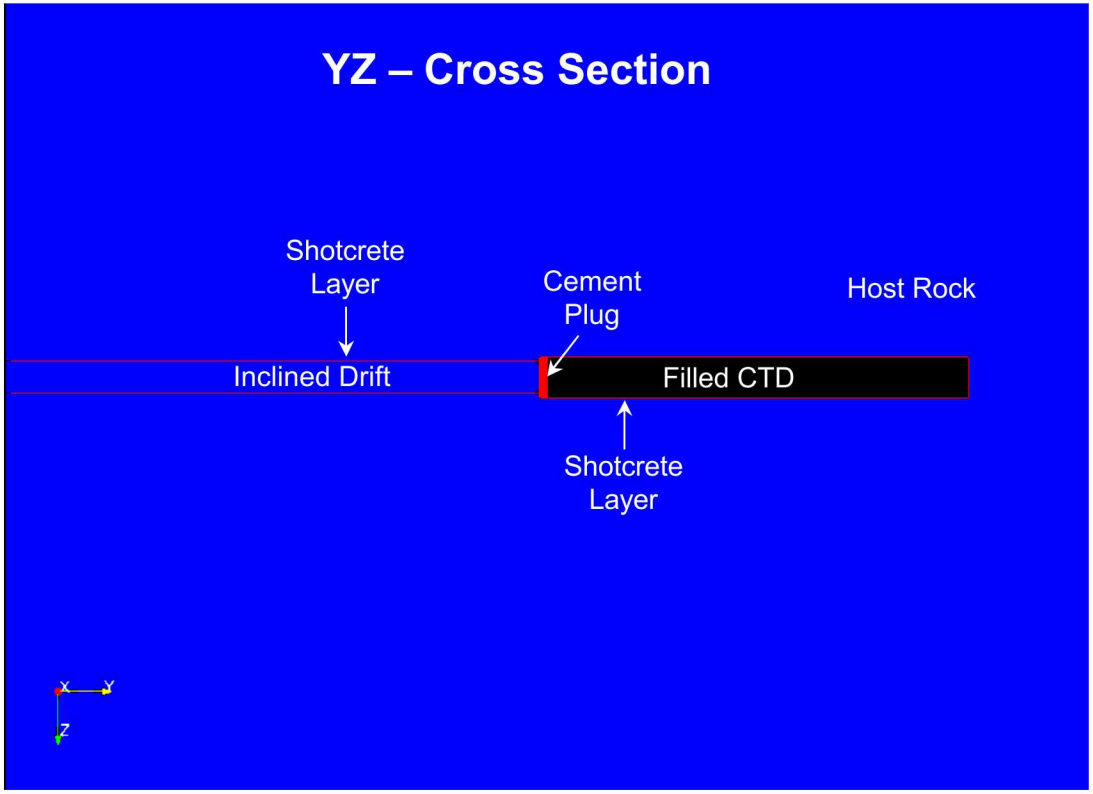
Schematic figure courtesy of Dr. Teruki Iwatsuki (JAEA)



- Step 2b Preliminary Reactive Transport Simulations
- Preliminary geochemical predictions at 12MI33 monitoring zones
- Preliminary (blind) predictions of filled CTD water chemistry
- PFLOTRAN simulation code
- Current mesh doesn't capture rock fracture effects
- Assuming shotcrete layer (0.1 m thick) covering CTD walls

Work in progress!!!

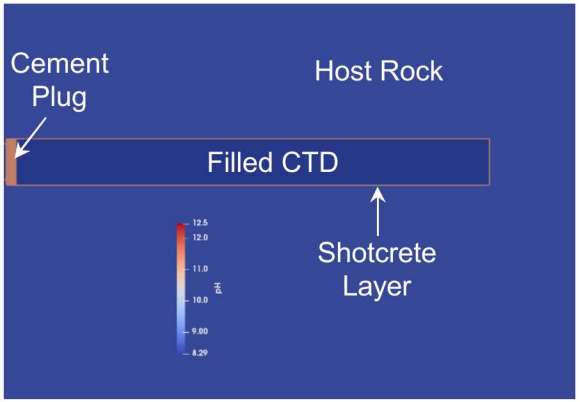
DECOVALEX19: PFLOTRAN Reactive Transport (RT) Model Domain



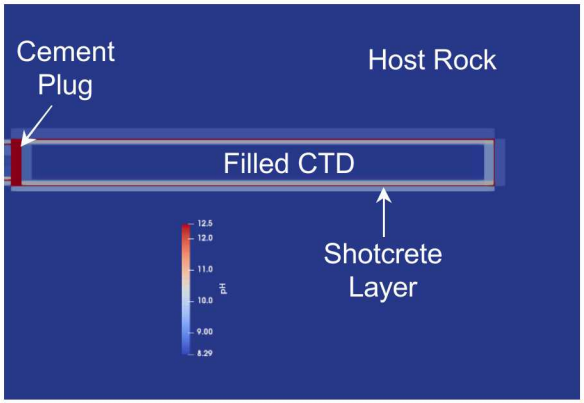
- PFLOTRAN Reacting Transport Simulation
  - 3D structured mesh
  - Focused on filled CTD with dilute groundwater
  - Starting pH 8.3
  - Shotcrete: generic OPC (no brucite)
  - Diffusion only problem
  - 400 days simulation

DECOVALEX19: PFLOTRAN 3D Reactive Transport (RT) Model (I)

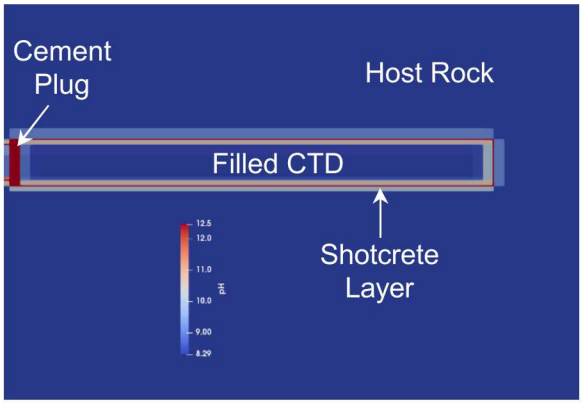
Filled CTD → Blind Prediction + Prelim. Results



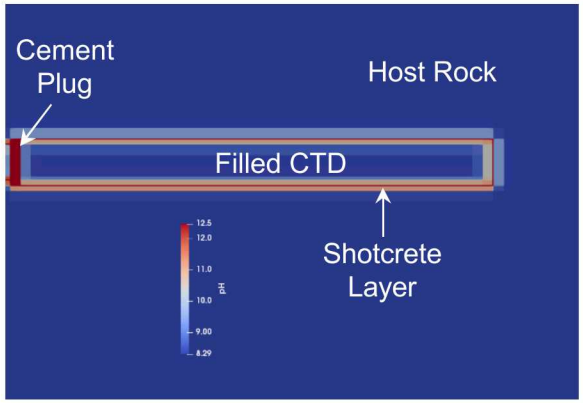
0 days



70 days



150 days

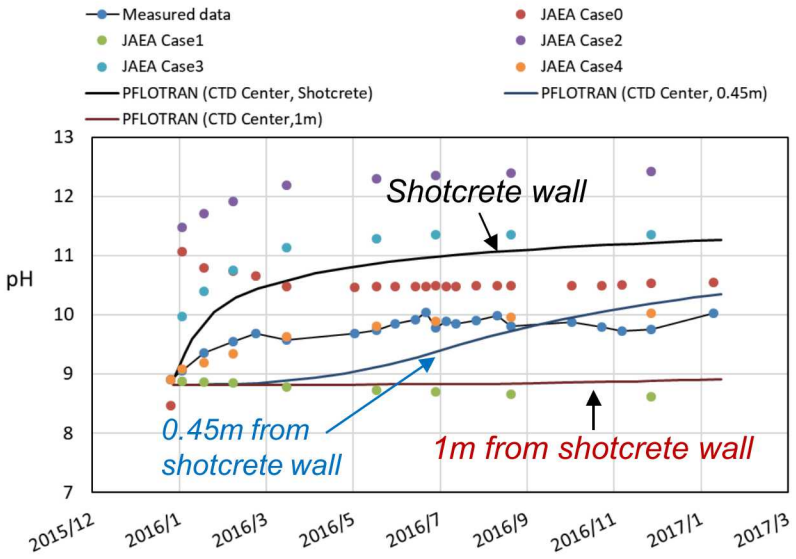


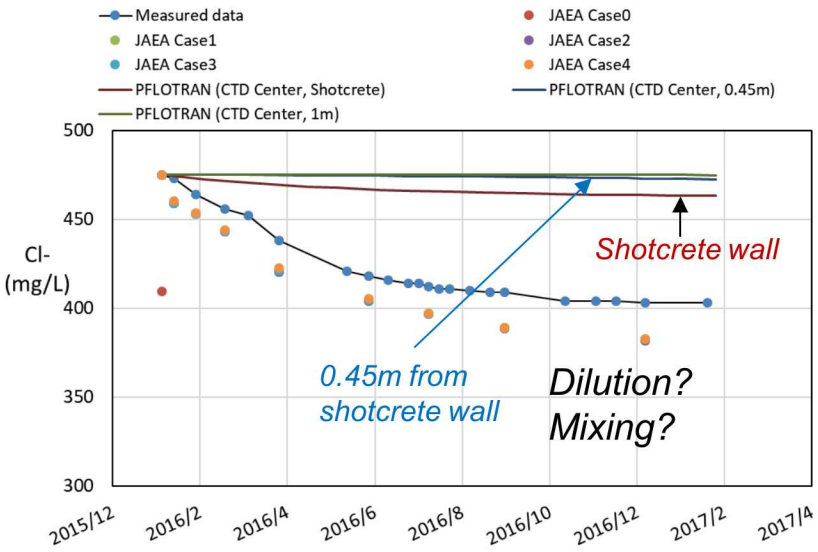
310 days

WORK IN PROGRESS!!!

- Reaction Front Simulation
  - pH increase with time within CTD and around the shotcrete lining
  - pH remains relatively unchanged around tunnel central region
- Questions?
  - pH deviations from measured
  - Diffusion coefficient effects
  - Kinetic rate parameters
  - Why the CTD region near the cement plug doesn't experience higher pH?

DECOVALEX19: PFLOTRAN 3D Reactive Transport (RT) Model (II)





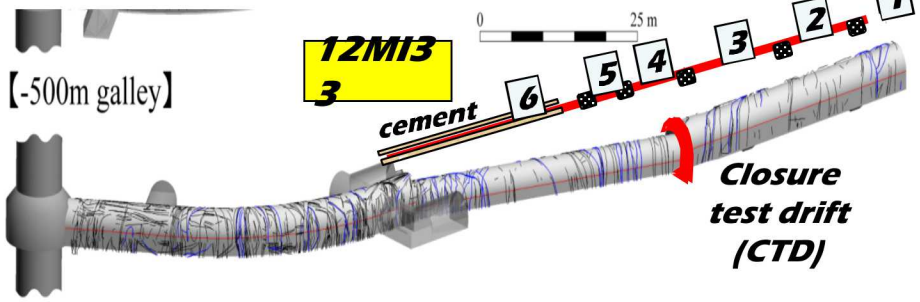
Filled CTD → Blind Prediction + Preliminary Results

■ Filled CTD RT Simulation Summary

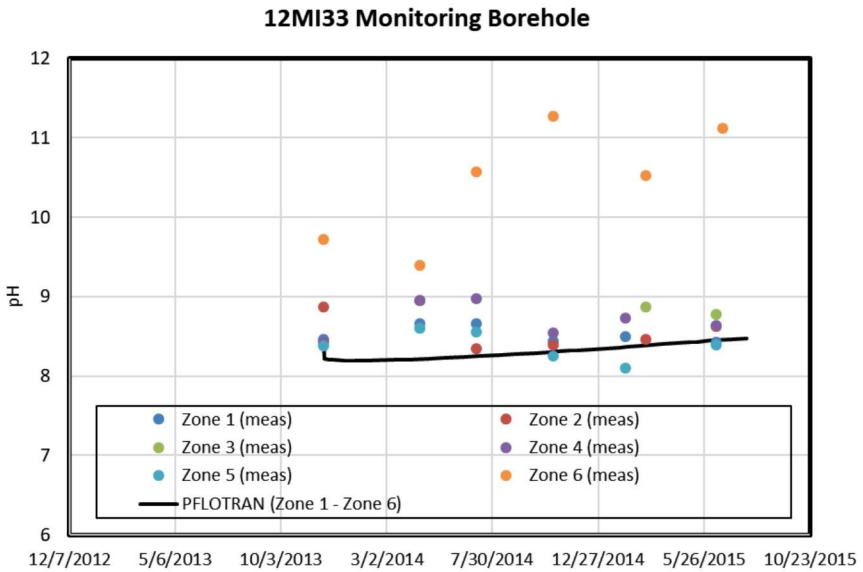
- Increase in pH with time → still far from measured pH data at 1m within the CTD
- Small decrease in [Cl-] concentration → much smaller than that of measured data
- **Next step:** Resolve discrepancies with measured data
  - Evaluation of transport and kinetic rate parameters
  - Update shotcrete composition
  - Eh (ORP) predictions → PFLOTRAN comparisons with measured data

WORK IN PROGRESS!!!

PFLOTRAN 3D Reactive Transport (RT) Model (III) – 12MI33 Borehole Zones



WORK IN PROGRESS!!!



12MI33 Borehole Zones → Predictions & Comparisons To Measured Data

- PFLOTRAN RT Simulations 12MI33 Borehole Zones Summary:
  - Overall, PFLOTRAN RT model predictions for pH are within the band of measurements (except Zone 6)
  - Marked Deviations from measurements in **Zone 6:**
    - **Close proximity to cement – expected higher pH's**
    - **Need to explore hydrologic effects in this zone**
    - **Water mixing effects?**

Effect on Repository Performance or Safety Case Confidence

- *DECOVALEX19 (Task C) and FEBEX-DP provide unique data sets and samples to study barrier interactions and their degradation, for example:*
  - *Effects of chemical interactions between percolating water and liner/seals in the vicinity of the excavated disturbed zone (EDZ)*
  - *Evolution of in-drift chemistry*
  - *Engineered barrier interactions and degradation in response to thermal loads*

Task #	Task Name/ (and Work Package number -- if needed or helpful for more specificity)	Brief Task Description including Relevance (and/or input) to PA/GDSA (nPA = not direct input to PA)	Personnel/Lab	Type of Activity L = Literature review M = Modeling T = Testing or Experimental	Code (if applicable)	Importance to Safety Case (ISC) (H, M, or L -- see ISC table definitions) (Identify applicable Safety Case element from the provided figure)	Current "State of the Art" Level (SAL = 1, 2, 3, 4, or 5 -- see SAL table definitions) (Give brief update to applicable state-of-the-art "discussion(s)" shown in UFD Roadmap App. A, i.e., those discussion(s) for the highest scoring related FEPs)	Short-term (1 yr) R&D Priority Scores & Brief FY19 Work Scope Proposal (Priority Score = H, M, or L, based on combined ISC and SAL -- see PS table definitions) (Also give Roadmap Score for related FEP)	Long-term (2-5 yrs) R&D Priority Scores & Brief FY19-23 Work Scope Proposal (Priority Score = H, M, or L, based on combined ISC and SAL) ("Long-term" is most applicable to SAL = 5 issues) (Also give Roadmap Score for related FEP)	Related UFD Roadmap Issue(s)/FEP(s), and associated UFD Roadmap priority scores* (Find highest scoring related FEP in App. B of UFD Roadmap)	Other Notes/Comments (e.g., type of linkage to PA-GDSA; inputs required and/or linkages to other models and experiments)
36a	FEBEX-DP: Dismantling phase of the long-term FEBEX heater test	• Evaluate post-test state of FEBEX barrier clay and interactions at EBS interfaces • Effects of dryout and mineral dehydration on backfill/buffer • Characterization (compositional, mineralogical) of FEBEX-DP (heated) bentonite and interactions with cement barrier	C. Jove-Colon, SNL L. Zheng, LBNL Caporuscio, LANL	T	N/A	M-H	5	M-H	M-H	• Primary FEPs 2.1.04.01, 2.1.05.01 score = 3.5; 2.2.08.07 score = 2.82; 2.1.07.09 score = 2.56	• Analysis of FEBEX-DP samples will provide insights on clay buffer degradation and interactions at EBS interfaces to inform modeling approaches.
41	DECOVALEX-2019 Task C: GREET (Groundwater REcovery Experiment in Tunnel) at Mizunami URL, Japan	• Geochemistry: Evaluate groundwater chemistry in a crystalline repository and the effect of repository construction • Utilize fracture data for validation of fracture models in crystalline rock • Evaluate reactive transport processes at the filled CTD & cement interactions	Y. Wang Jove-Colon T. Hadgu, SNL	T, M	PFLOTRAN, EQ3/6, DFN, FCM	H	5	H	H	• Primary FEP is 2.2.05.01 (crystalline) score = 3.74; applicable FEP 2.2.09.51 (crystalline); 2.2.08.04 (crystalline) score = 3.23; 2.2.09.02 (crystalline) score = 5.86;	• The DECOVALEX-2019 project Task C will provide comprehensive geochemical and fracture characterization of host-rock at various locations and times. • Experimental and field test results (groundwater recovery, monitoring) will provide key information about groundwater chemical evolution. • Coupling effects of fracture with reactive transport, fluid mixing?

Integration with GDSA/PA and/or the Safety Case (Disposal in Argillite R&D)

- **Understanding thermal effects on bentonite barrier to evaluate constrains on the extent of the *sacrificial zone* away from the heater. This could place constrains in EBS design according to thermal loads**
  - Inform PA on the effects of clay barrier degradation → Chemical, swelling inhomogeneities → porosity, permeability changes
- **3D Simulations of liner/barrier interactions and transport to evaluate performance**
  - Chemical effects on fluid chemistry with time → To provide PA with more realistic representations of barrier chemical and transport properties for RN migration
  - Cement/fluid interactions and in-drift water chemistry

Future Outlook and Accomplishments

- **Future Outlook:**

  FEBEX-DP:

  - Evaluate thermal effects on clay chemistry (e.g., Mg enrichment in FEBEX-DP samples close to heater surface)
    - Comprehensive characterization of clay phase in bentonite as a function of sample location
  - Illitization studies on FEBEX-DP samples (in conjunction with crystalline work package)
  - TGA/DSC analyses of bentonite with distance from heater surface
  - 3D simulation of unsaturated flow and reactive transport in response to heating and resaturation

  DECOVALEX19:

  - Sensitivity analysis (SA) to evaluate simulations predictions & measurements
  - Extend PFLOTRAN reactive-transport (chemistry) CTD simulations to cases of fracture media
  - Update shotcrete phase assemblage and composition consistent with JAEA analyses

- **Accomplishments:**
  - FEBEX-DP
    - Textural and compositional characterization of cement-clay interfaces (e.g., X-ray tomography, micro-XRF compositional mapping at interfaces, (m)SEM-EDS
  - SKB EBS BRIE & FEBEX: Bentonite hydration data to constrain clay hydration thermodynamic modeling

Questions?

Aknowledgements

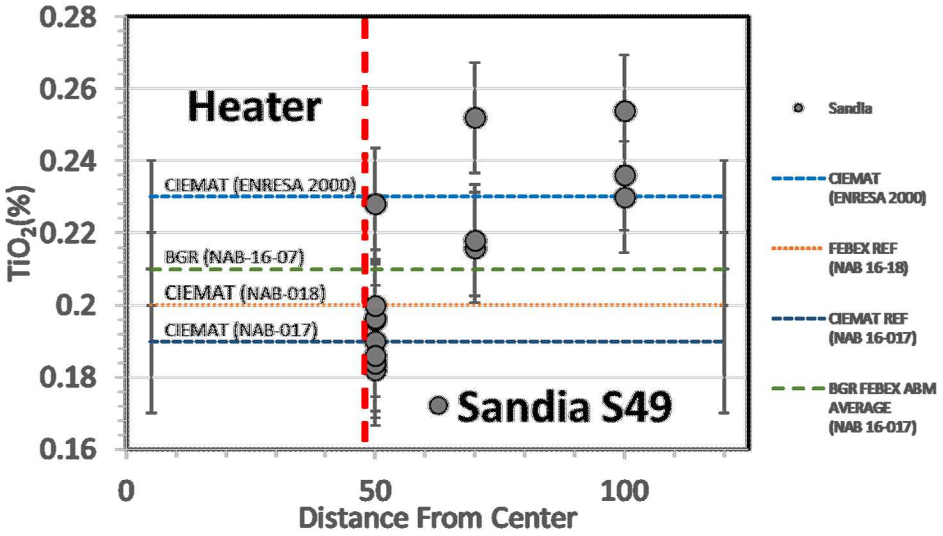
- This work supported by the DOE-NE Spent Fuel Waste Science and Technology campaign, Fuel Cycle Technologies R&D program.

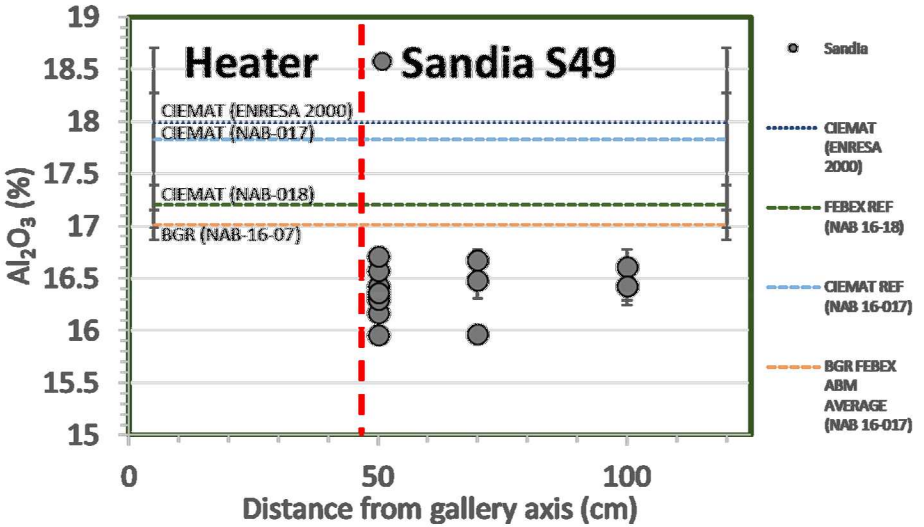
Backup Slides

Integration with International

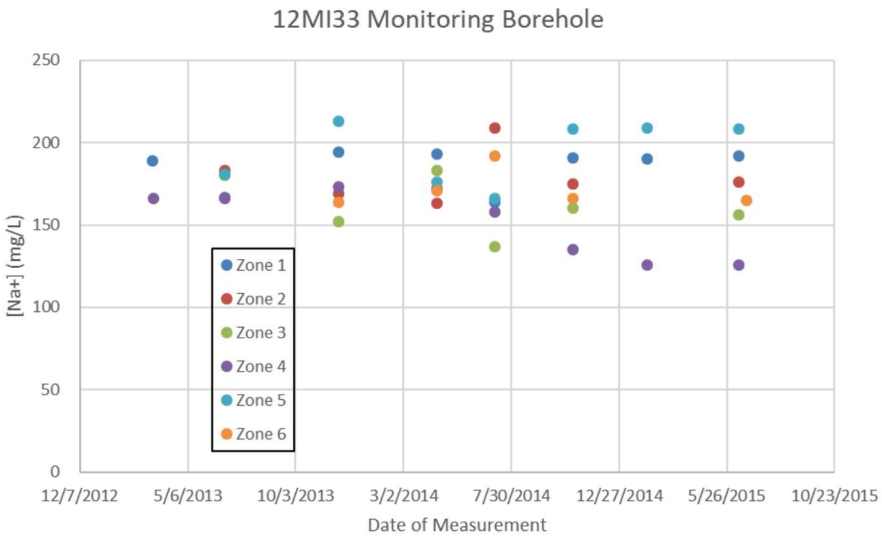
- **Understanding thermal effects on bentonite barrier to evaluate constrains on the extent of the *sacrificial zone* away from the heater. This could place constrains in EBS design according to thermal loads**
  - Inform PA on the effects of clay barrier degradation → Chemical, swelling inhomogeneities → porosity, permeability changes
- **Model Validation → 3D reactive transport simulations of liner/barrier interactions and transport to evaluate performance**
  - Chemical effects on fluid chemistry with time → To provide PA with more realistic representations of barrier chemical and transport properties for RN migration
  - Cement/fluid interactions and in-drift water chemistry

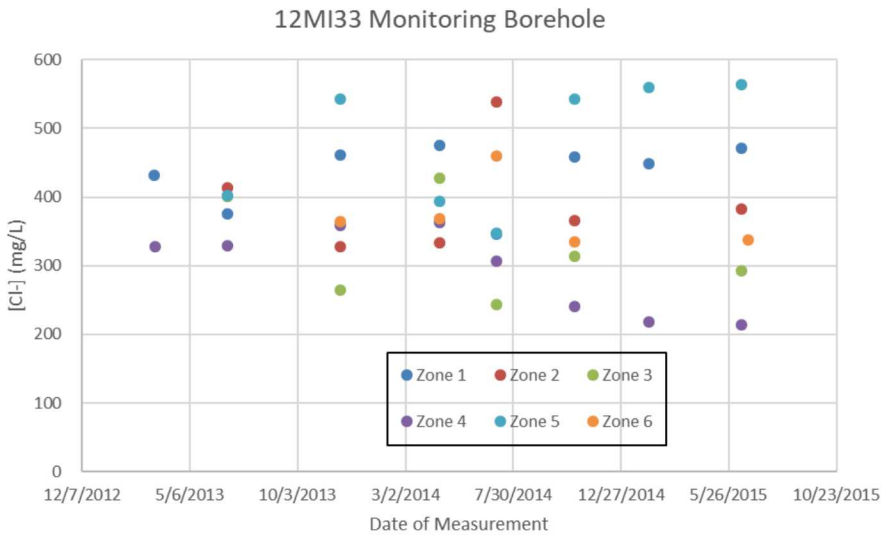
Bulk Sample XRF Analyses (III)





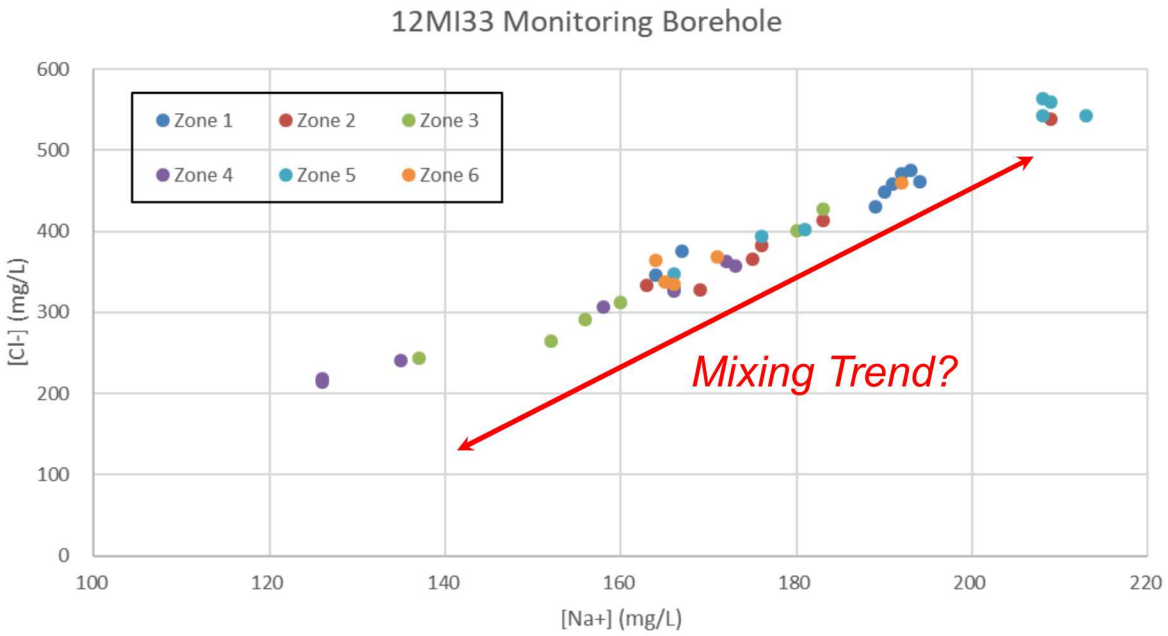
DECOVALEX19: Preliminary Analysis of Geochemical Trends – Monitoring Borehole 12MI33





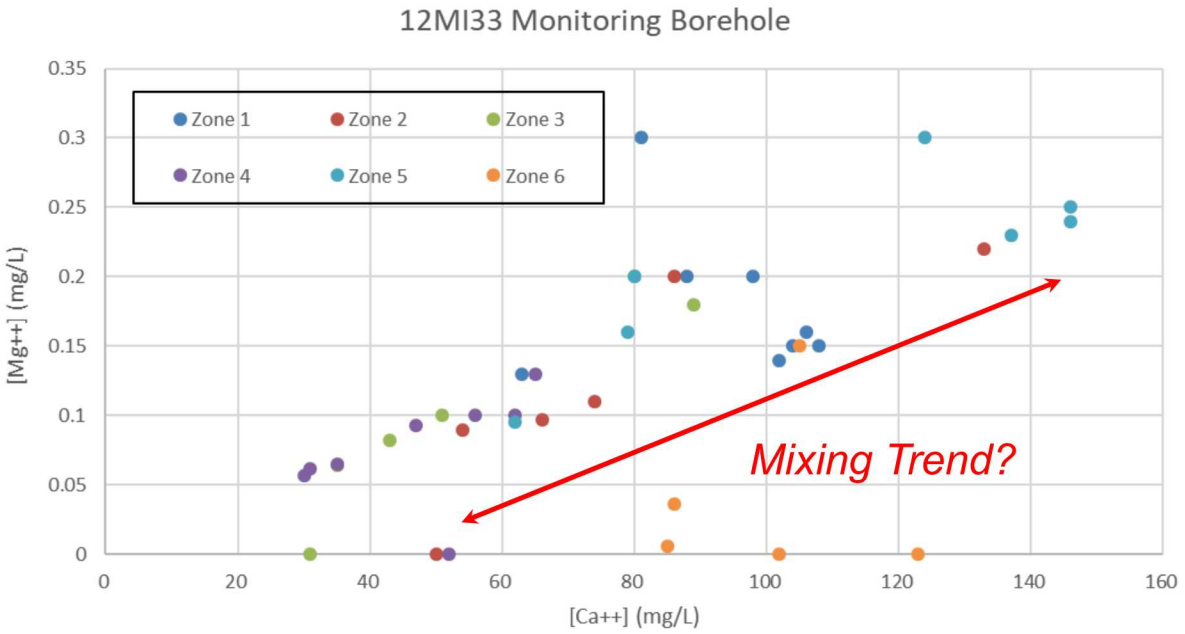
- *Some spreading of the data with time*
- *Mixing events???*

12MI33 Monitoring Borehole: [Cl-] vs. [Na+] Correlation



- Linear trend suggest mixing between two(?) waters
  - Relatively large spread in measured [Cl-] & [Na+]
  - Dilution events?
  - Potential water compositions neighboring these zones???
- **TODO:**
- Simple test: EQ3/6 model of water mixing/dilution?
  - Assess end-member water chemistries
- PFLOTRAN RT Simulation
  - Hydrologic effects
  - Analyze variability in solute concentration for each zone

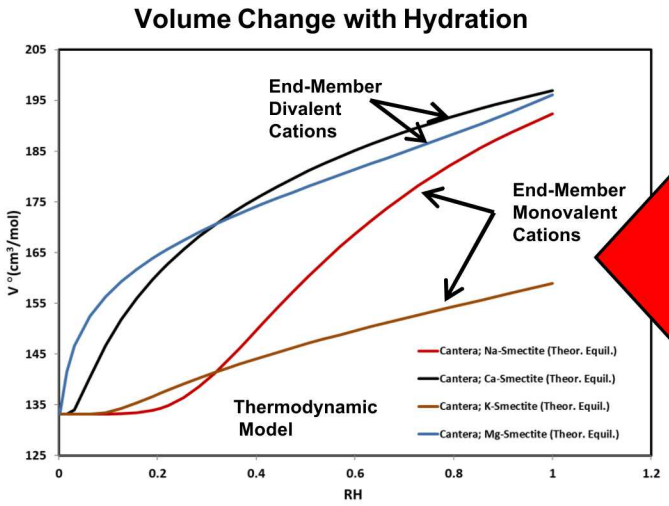
12MI33 Monitoring Borehole: [Mg++] vs. [Ca++] Correlation

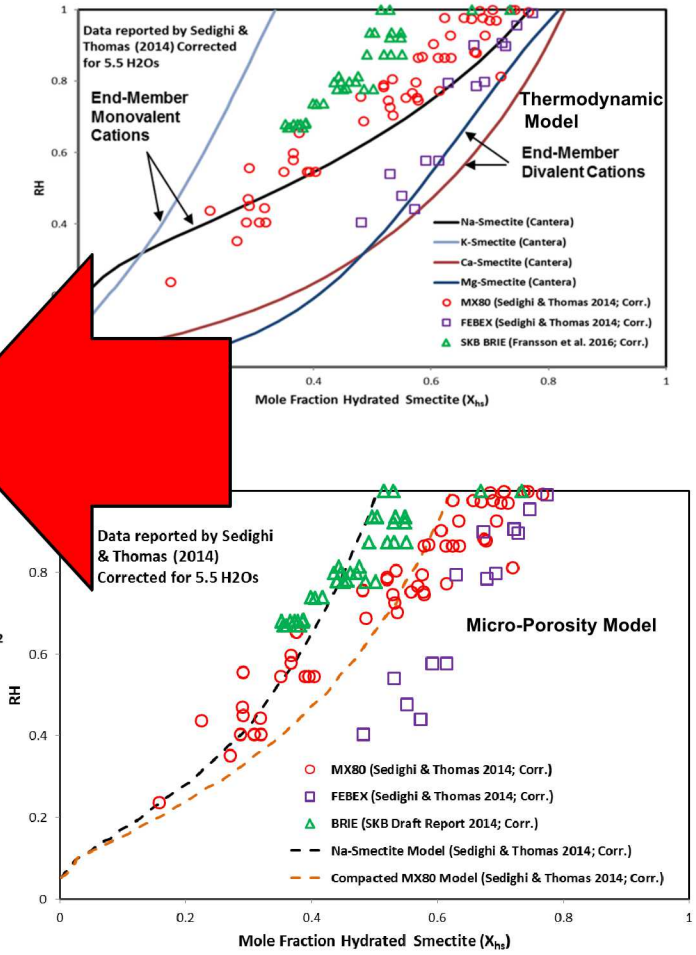


- Similar trend to that of [Na+] vs [Cl-]
- Data is more scattered:
  - Hydrologic effects
  - Solute concentration variability
- Next Step:
  - EQ3/6 water mixing simulation approach?
  - Which water compositions to consider?

Clay Hydration Modeling and Micro-Porosity Evolution: Model Comparison with Data

- Relationships between clay composition and swelling behavior
- Data retrieval from URL and laboratory experiments
  - FEBEX
  - Bentonite H_2O retention (SKB TF BRIE)
  - Bentonite MX80
- Trends for monovalent and divalent cationic composition consistent with thermodynamic model predictions for clay hydration





DECOVALEX19: Summary of Modeling Activities

- **PFLOTRAN 3D Reactive Transport (RT) simulations were conducted for DECOVALEX Task C, Step2a-b**
  - *Leveraged high performance computing (HPC) capability of PFLOTRAN*
  - *Simulations encompassed predictions at observations points corresponding to 12MI33 monitoring zones and filled CTD center*
  - *Shotcrete layer (generic OPC) in tunnel(s) was included in model domain*
    - **TODO NEXT:** Utilize shotcrete composition provided by JAEA
- **Discrepancies between blind predictions and measured values:**
  - ***TODO NEXT:***
    - *Analysis of RT simulation parameters (gauged by measurements)*
    - *E.g., solubility / dissolution rate parameters of constituent phases*
    - *Initial volume fraction of phase constituents*
    - *Eh, solute concentrations, etc.…*
  - **Evaluate potential water mixing at 12MI33 monitoring zones:**
    - PFLOTRAN and EQ3/6 modeling codes
    - Target potential water compositions???

EC Project: BEACON (Bentonite Mechanical Evolution)

- **Goals**
  - "To develop and test the tools necessary for the assessment of the mechanical evolution of an installed bentonite barrier"
  - "To verify the performance of current designs for buffers, backfills, seals and plugs"
  - "Enhanced, robust and practical numerical tools, firmly grounded on a good conceptual understanding, that have the required predictive capabilities concerning the behaviour of engineered barriers and seals"
  - "A complete experimental database for the need of the assessment models"
  - EC Project, 25 Partners; Coordinated by SKB