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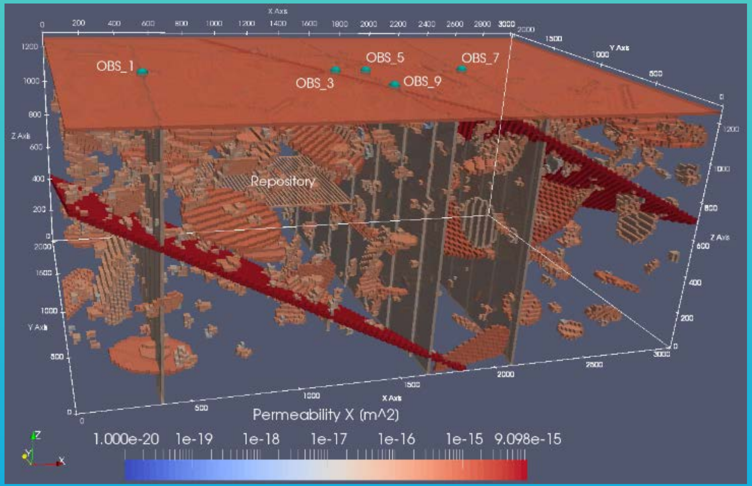

Coupled THMC Processes under High Temperature in Bentonite Buffer: Laboratory Experiments, Field Tests, and Modeling

U.S. Nuclear Waste Technical Review Board
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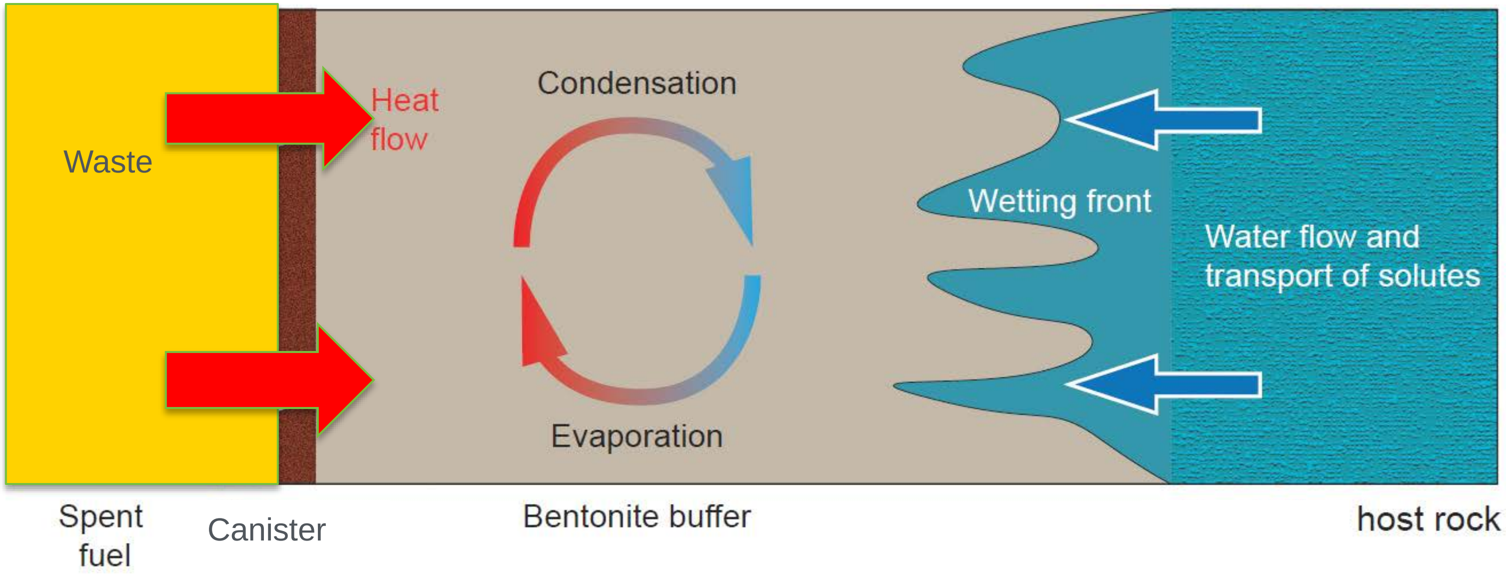
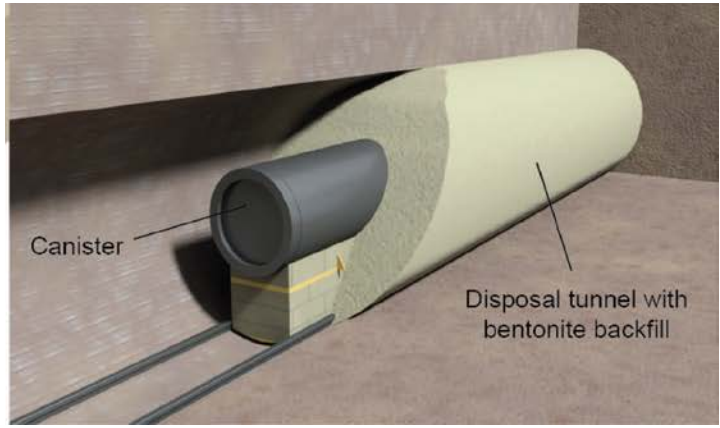
Processes Involved in Bentonite Evolution (1)

To ensure favorable features of the bentonite in the long term, understanding and modeling of early-time thermal, hydrological, mechanical and chemical (THMC) perturbations is critical:

- **Thermal process:** Heat emission from waste and transport through bentonite buffer
- **Hydrological process:** Partially saturated bentonite becomes fully saturated after transient de-saturation and re-saturation
- **Mechanical process:** Stress evolution, possibly leading to damage
- **Chemical process:** solute transport, radionuclide migration and mineralogical change

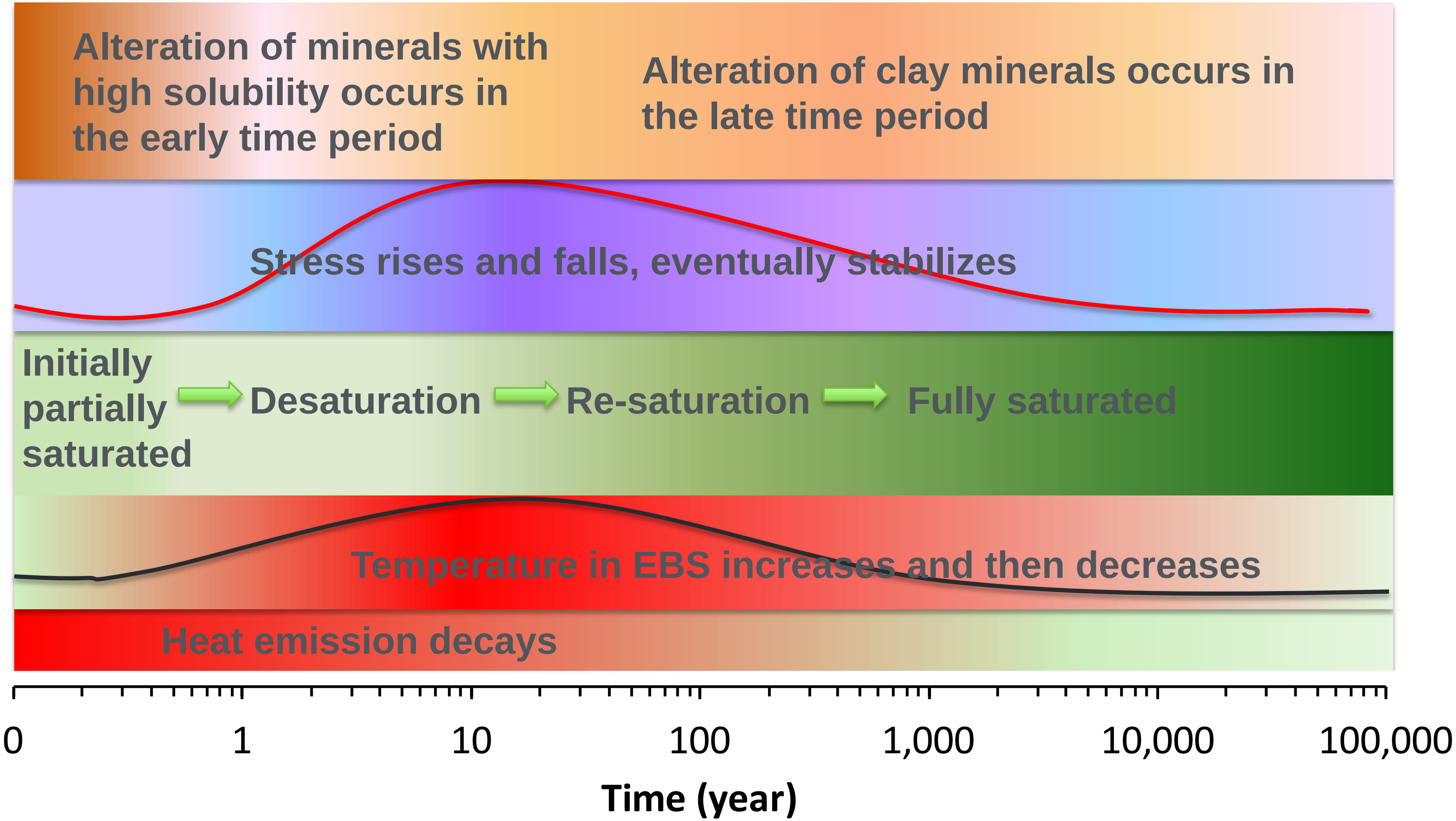


(Modified from Leupin et al, 2014)



Processes Involved in Bentonite Evolution (2)

THMC processes are coupled and evolve temporally and spatially



Alteration of minerals with high solubility occurs in the early time period

Alteration of clay minerals occurs in the late time period

Stress rises and falls, eventually stabilizes

Initially partially saturated → Desaturation → Re-saturation → Fully saturated

Temperature in EBS increases and then decreases

Heat emission decays

To Build a Reliable Process Model, We Need to Know—

Processes model is the foundation of performance assessment model. To build such models, we need to know:

- **What are the key processes that have to be included in the model?**
- **Do we have reliable constitutive relationships and parameters to describe THM processes?**
  - Porosity and permeability changes
  - Stress evolution
- **Do we have reliable chemical models and parameters to describe chemical processes?**
  - Evolution of pore-water geochemistry in bentonite
  - Mineralogical changes in bentonite
  - Retardation capability
  - Interactions between canister/bentonite/host rock

Studies had focused on the THMC process under 100 ^{o}C

What If the Temperature is Higher (200 ^{o}C)?

Benefit

- Support Dual Purpose Canister disposal as it can lead to higher temperatures in the engineered and near-field natural barrier system
- Open the possibility of raising thermal limit of 100 ^{o}C for small PWR canisters
- Expanding the knowledge and data base to build the confidence

Key knowledge gaps to be narrowed

- When bentonite evolves from partial saturation to full saturation at temperatures up to 200 ^{o}C, how does bentonite change hydrologically and mechanically (e.g., boiling temperatures, high pore pressure, high stress, gas transport, etc.)?
- What are the mineralogical alterations of bentonite in the short-term and long-term (e.g., illitization and loss of swelling capacity)?
- Are the models (including processes, constitutive relationships and parameters) developed for 100 ^{o}C suitable for high temperature conditions?

Using generic models, laboratory experiments and field tests to address these questions

An Interactive and Iterative Approach

Goal

- Better understanding
- Reliable process model
- Gear toward performance assessment model

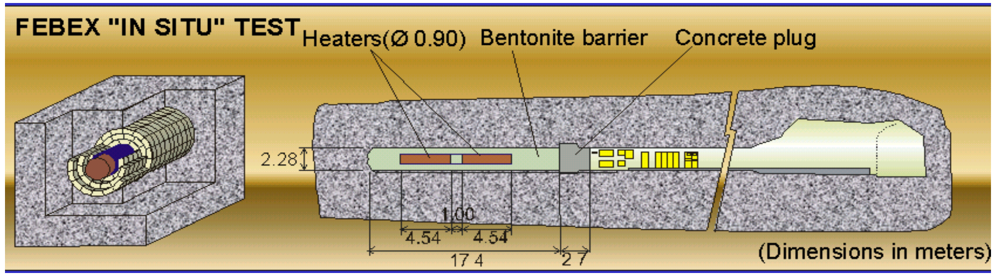
Approach

- Interaction between modeling and test
- Gradually increase the level of complexity test
- From low temperature to high temperature
- Synergy among multiple modeling/test efforts
- Revisit/revise the model

Experience Gained from Low Temperature THMC Test and Model (1)

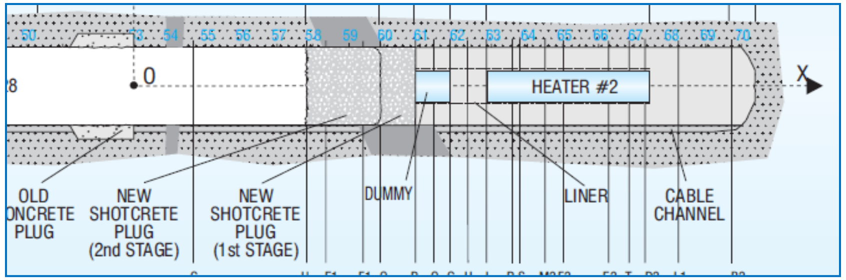
An *in situ* test

The full-scale *in situ* test is located in Grimsel, Switzerland, heating started in 1997 at 100 ^{o}C, as part of FEBEX (Full-scale Engineered Barrier Experiment) *(ENRESA, 2000)*.



In 2015, Dismantling of Heater #2

In 2002, Dismantling of Heater #1



Extensive laboratory tests were carried out to characterize THMC properties of bentonite, concrete, steel liner and granite.

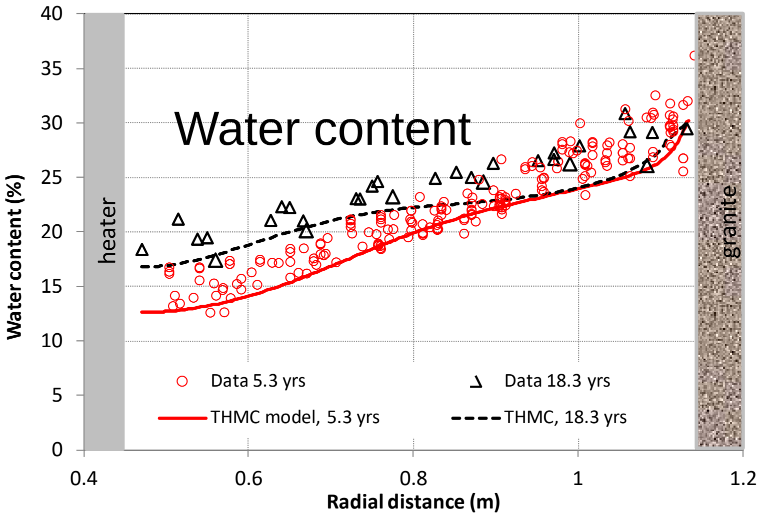
Experience Gained from Low Temperature THMC Test and Model (2)

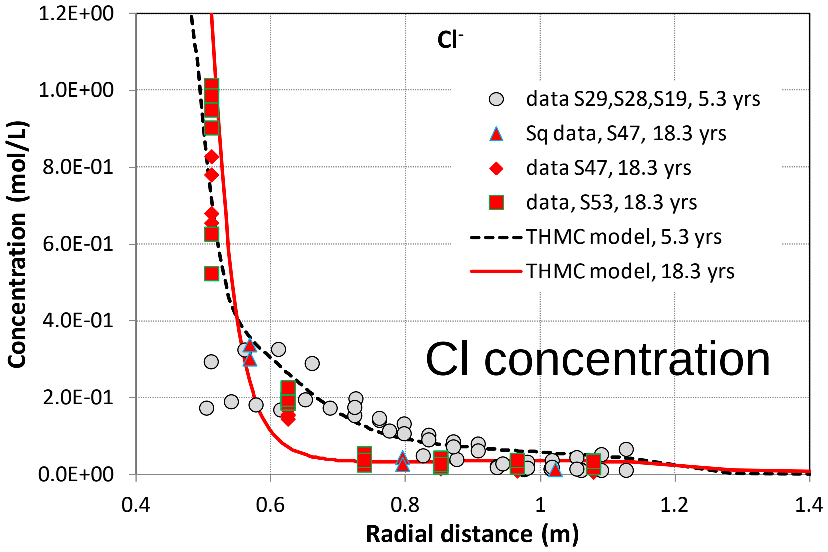
THMC modeling

Developing the model

- **Thermal model:** Heat convection and conduction
- **Flow model:** Two-phase (gas and water) flow
- **Mechanical model:** Poro-elastic using state surface approach
- **Chemical model:** Aqueous complexation, surface complexation, cation exchange and minerals dissolution/precipitation
- **Key coupled processes** needed to reproduce data: vapor diffusion, porosity and permeability change due to swelling, thermal osmosis

Testing the model with THMC data



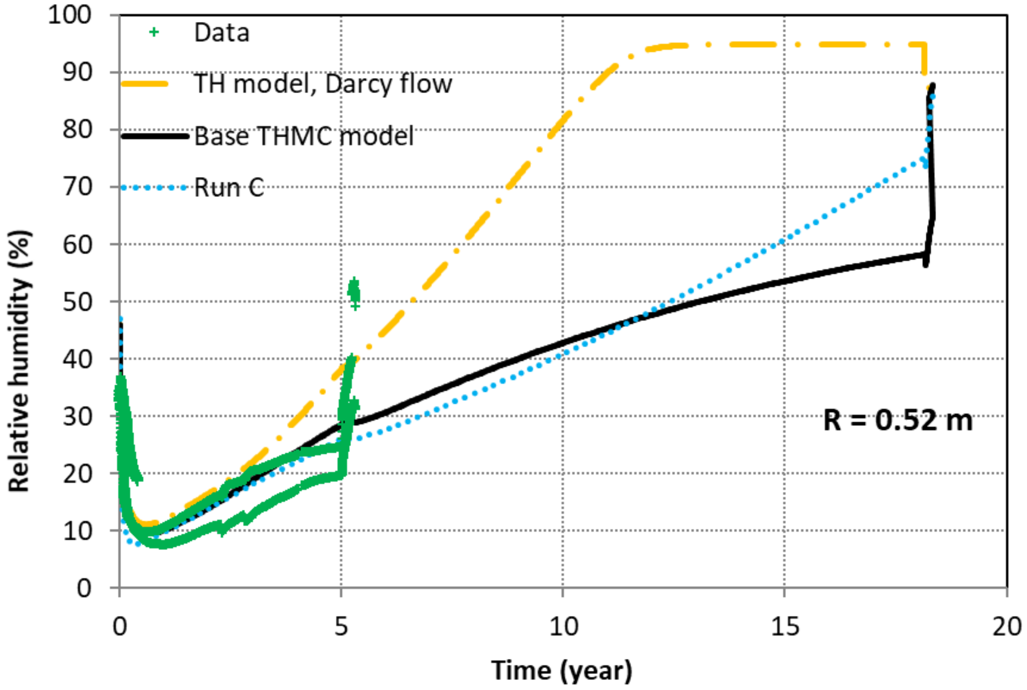


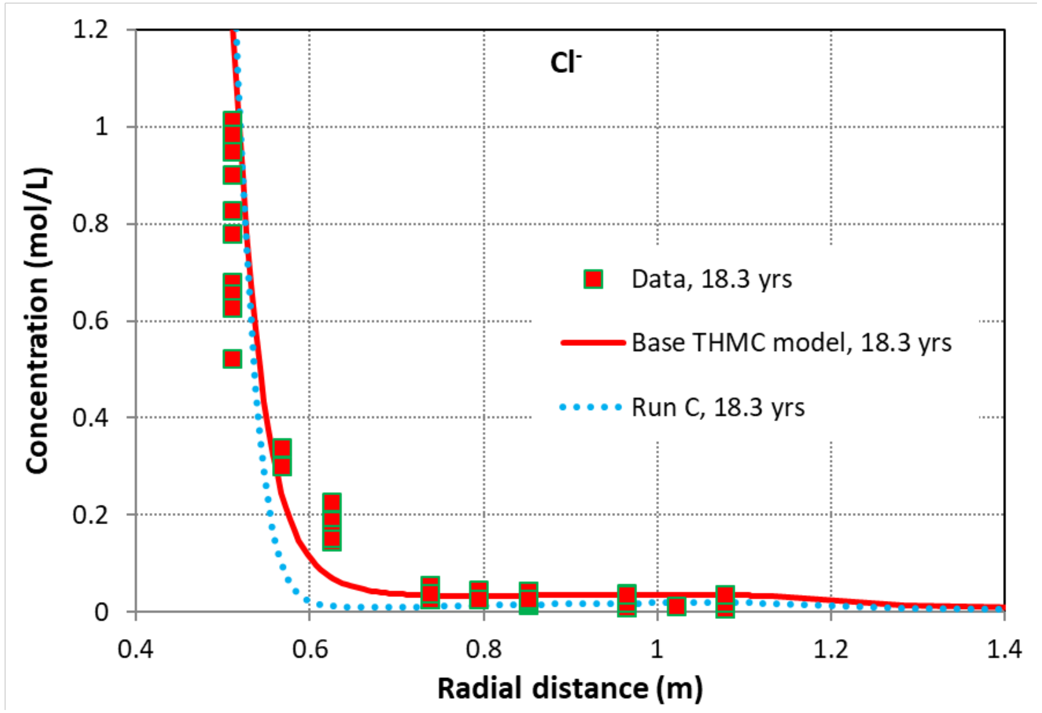
Zheng et al. 2019

Experience Gained from Low Temperature THMC Test and Model (3)

THMC modeling

- Complex model vs limited data
- Deficiency of some models were not revealed by short-term data
- Long-term measurements and multiple types of data are critical for reducing uncertainty and delineating right conceptual model and parameters





Zheng et al. 2019

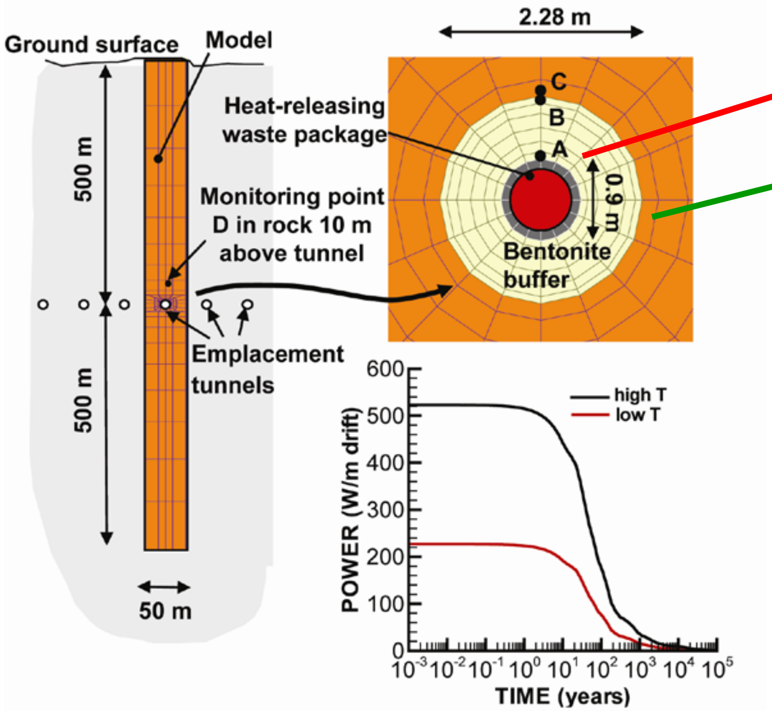
Experience Gained from Low Temperature THMC Test and Model (4)

Understanding deepened and modeling capabilities improved

- **Processes needed for modeling bentonite THM evolution:**
  - Thermal conduction and convection
  - Multiphase flow
  - Poro-elasticity
  - Porosity and permeability changes due to swelling
- **About geochemical evolution:**
  - Ion concentrations in pore water are high near the heater, which were largely shaped by transport processes, but also affected by minerals and cation exchange
  - Alterations to carbonate minerals and gypsum happened in the entire bentonite barrier
  - Alterations to clay minerals were moderate and mostly occurred near the heater, which cannot be verified by the data that have large measurement uncertainties
- **Key to increase the robustness of our predictive models for bentonite:**
  - long-term measurements
  - Multiple types of data

Exploration with Generic Models for High T (100 ºC vs 200 ºC)

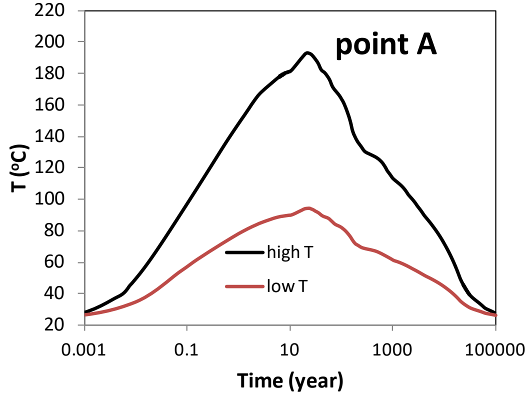
Model development



EBS Bentonite: Kunigel-VI or FEBEX bentonite

Clay formation : Opalinus Clay

Two cases for comparison: a “high T” case and a ”low T” case

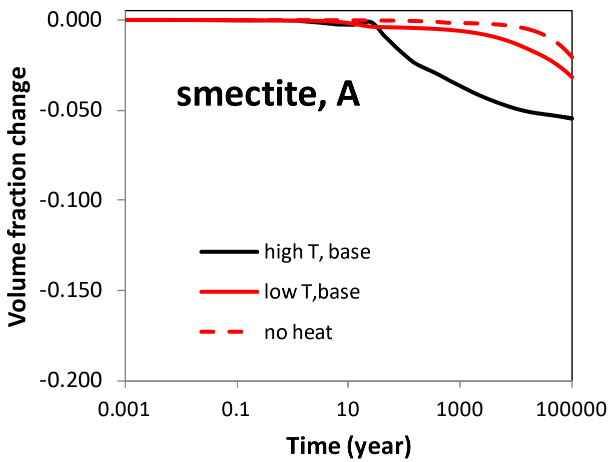


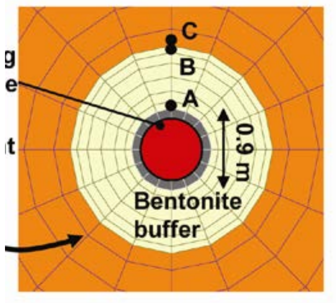
- Chemical model: aqueous complexation, minerals dissolution/precipitation and cation exchangeable
- Illitization was modeled as smectite dissolution and precipitation of illite:
  Smectite + $0.52H^+$ + $0.63AlO_2^-$ + 0.6K = illite + $0.26H_2O$ + $0.08Mg^{+2}$ + $0.33Na^+$ + $0.5SiO_2(aq)$
- The reaction rate was calibrated against data from Kinnekulle bentonite, Sweden *(Push and Madsen, 1995)*
- Mechanical-chemical coupling was formulated via an extended linear swelling model or Dual structural Expansive Clay Model (BExM)

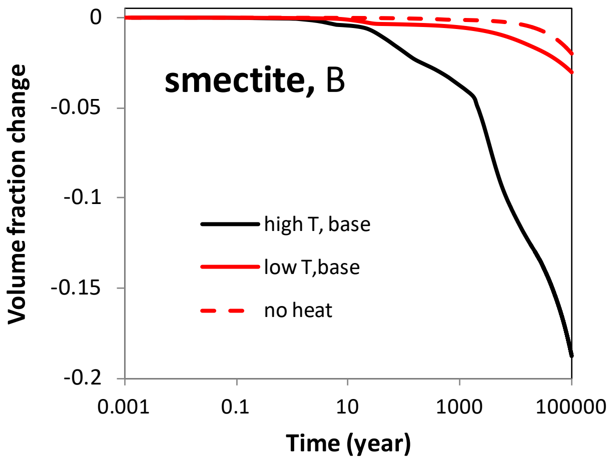
(Zheng et al., 2015; 2017)

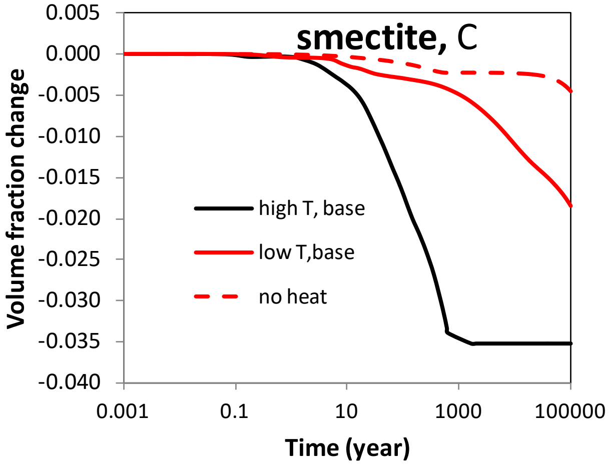
Exploration with Generic Models for High T (100 ^{o}C vs 200 ^{o}C)

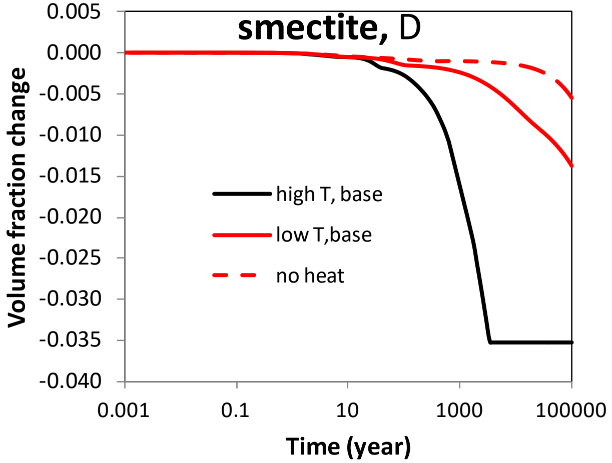
Example of key results: illitization occurs, temperature plays a key role and bentonite-host rock interaction is important









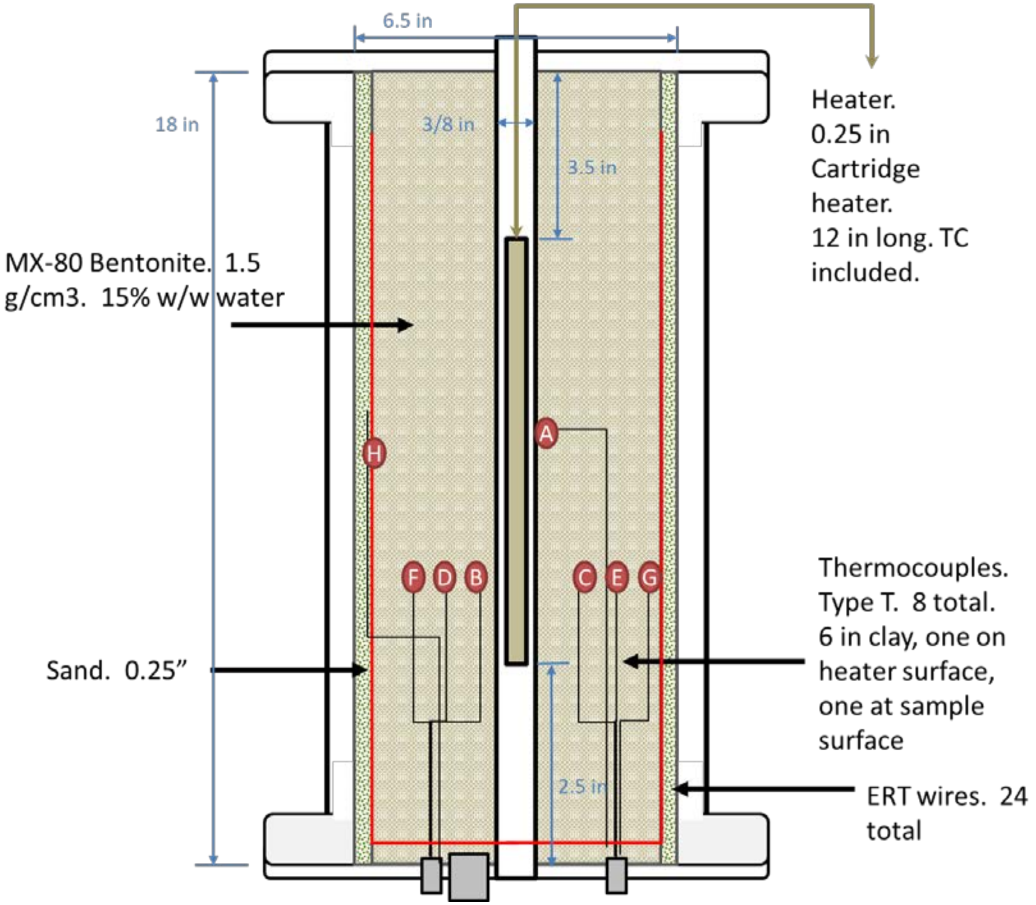


The temporal evolution of smectite volume fraction at points A, B, C, and D for Kunigel-VI bentonite.

At early times, dissolution of k-feldspar supplies K for illitization; after about 3000 years, illitization in host rock stops and K is transported into bentonite which leads to very different illitization at points A and B

Laboratory Tests and Modeling (1)

High temperature column experiment on bentonite



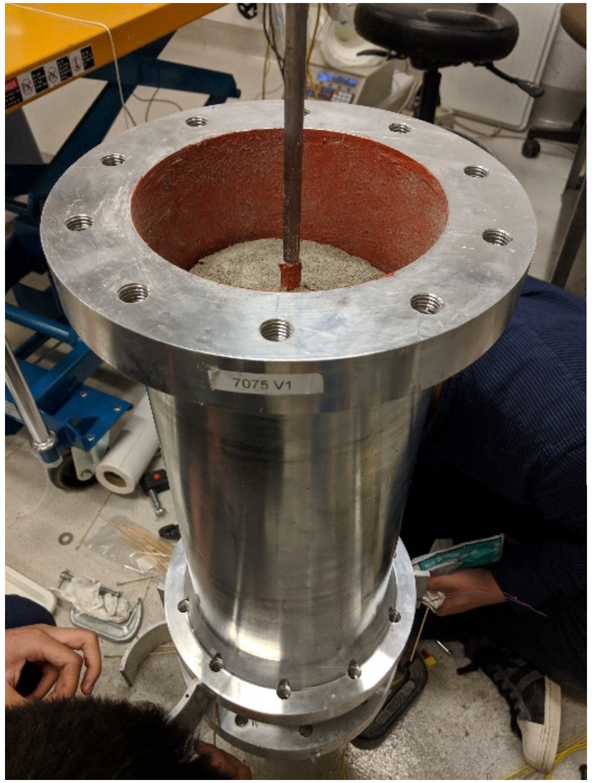
Heater.
0.25 in
Cartridge
heater.
12 in long. TC
included.

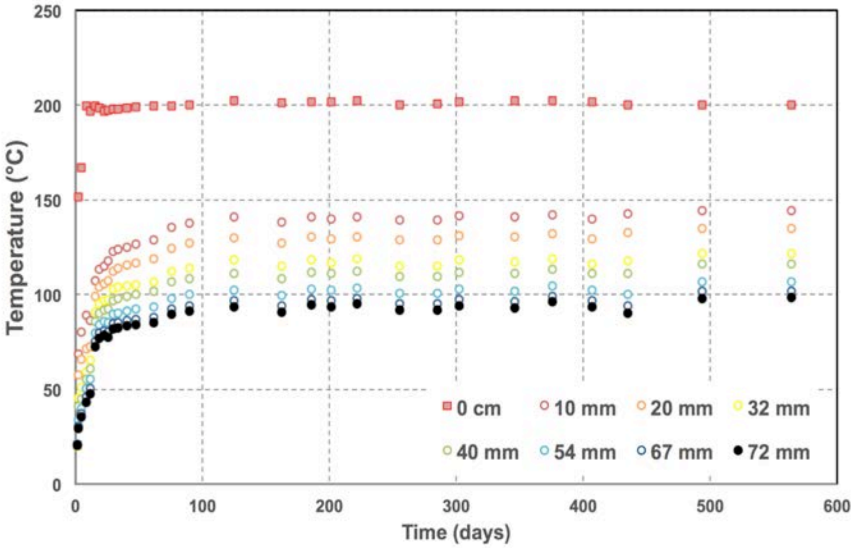
MX-80 Bentonite. 1.5
g/cm3. 15% w/w water

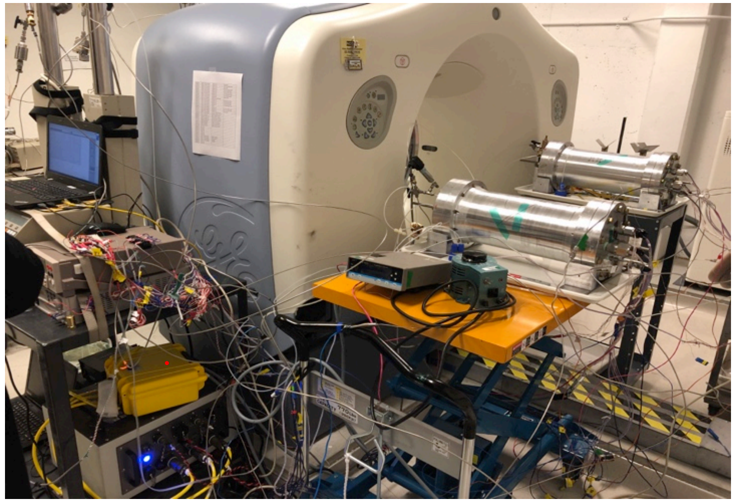
Sand. 0.25”

Thermocouples.
Type T. 8 total.
6 in clay, one on
heater surface,
one at sample
surface

ERT wires. 24
total



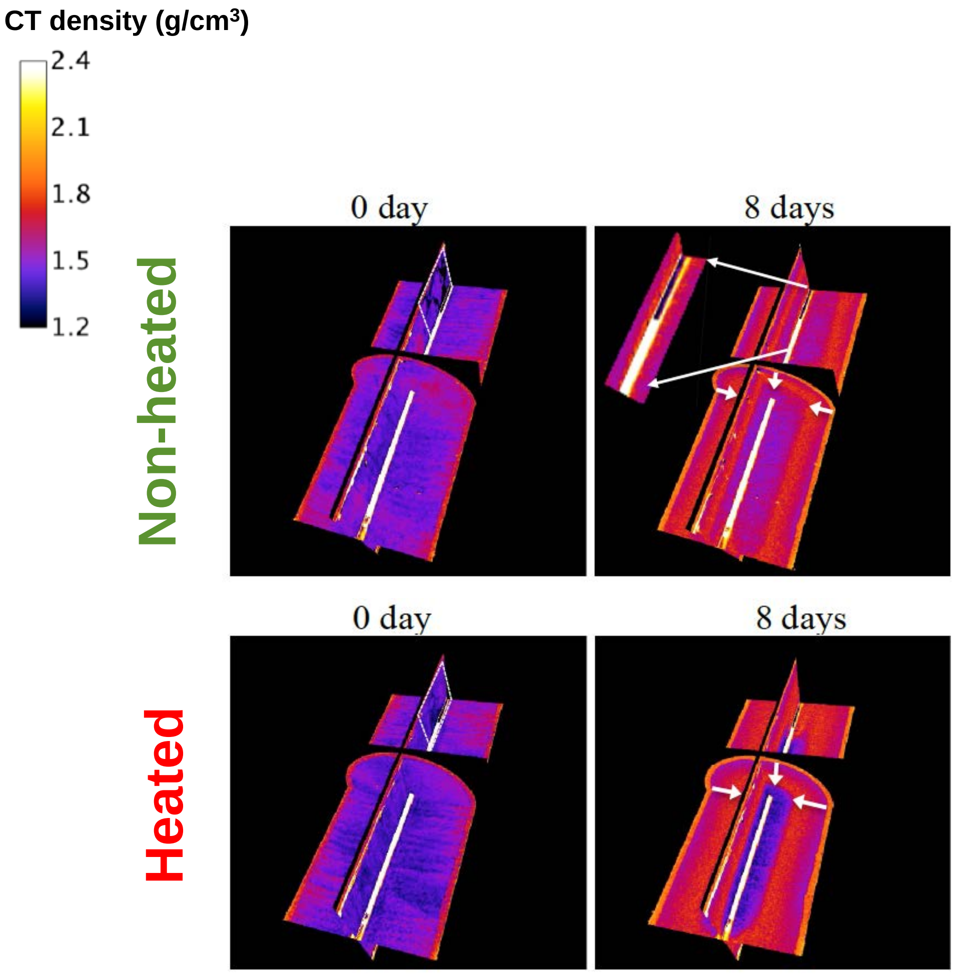


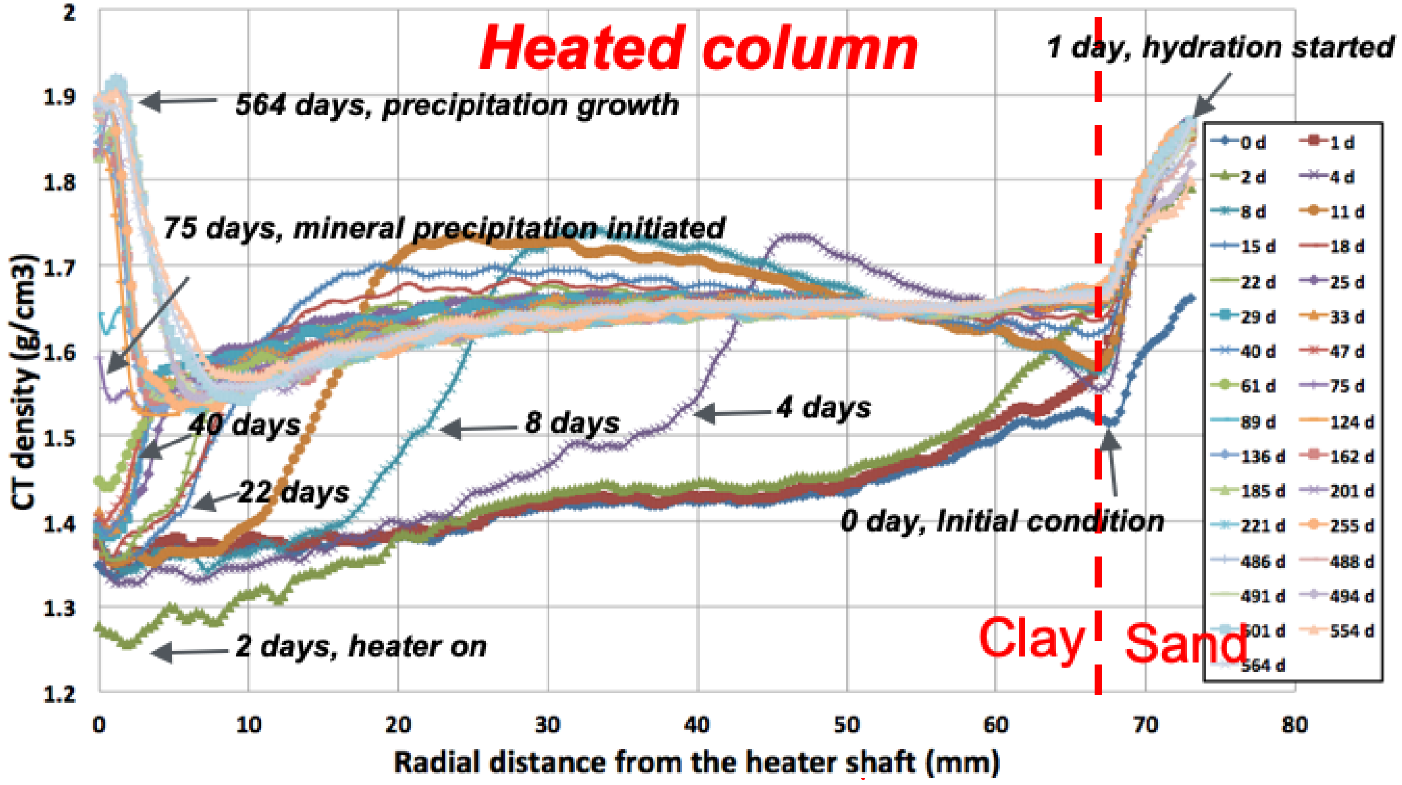


Average for inlet and outlet pressure has been 120 psi (8.3 bars). Flow is 0.11 mL/min.
After the bentonite was flooded for 1 day, heater was turned on at 150 ^{o}C.
After a week the temperature at the heater was maintained at 200 ^{o}C

Laboratory Tests and Modeling (2)

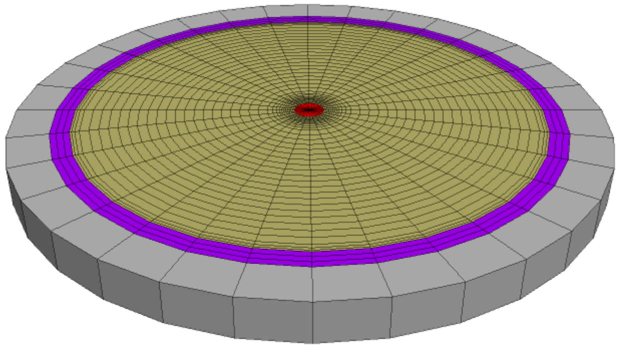
High temperature column experiment on bentonite: Hydration showed by CT scan



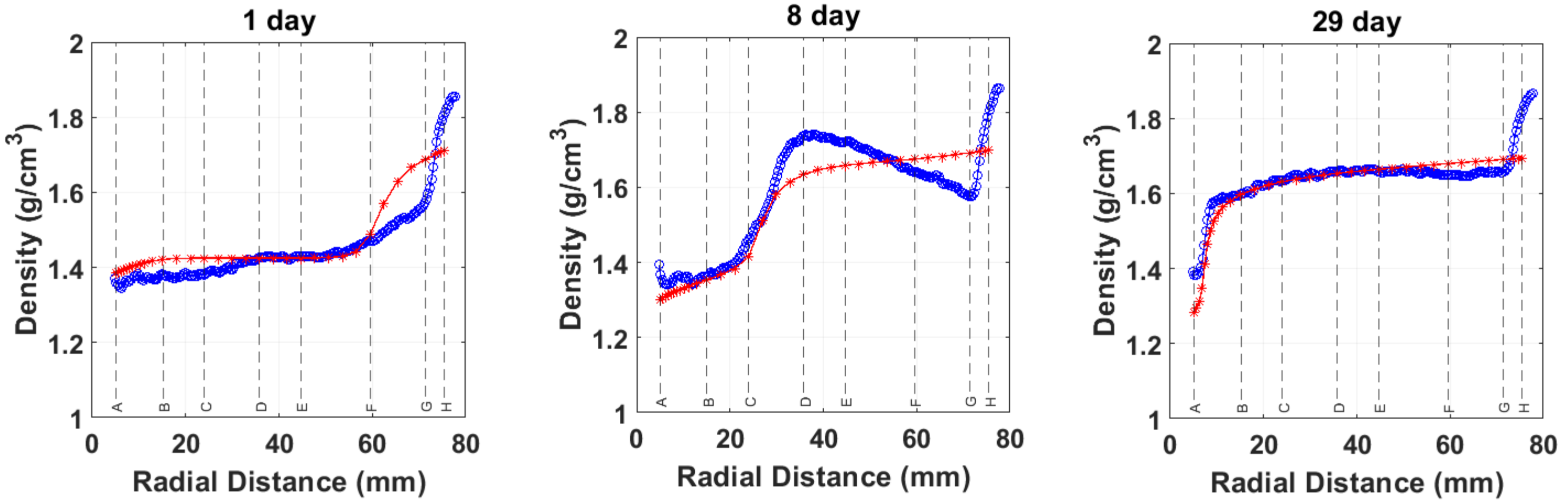


Laboratory Tests and Modeling (3)

Develop THM model



Geomechanics – 2D



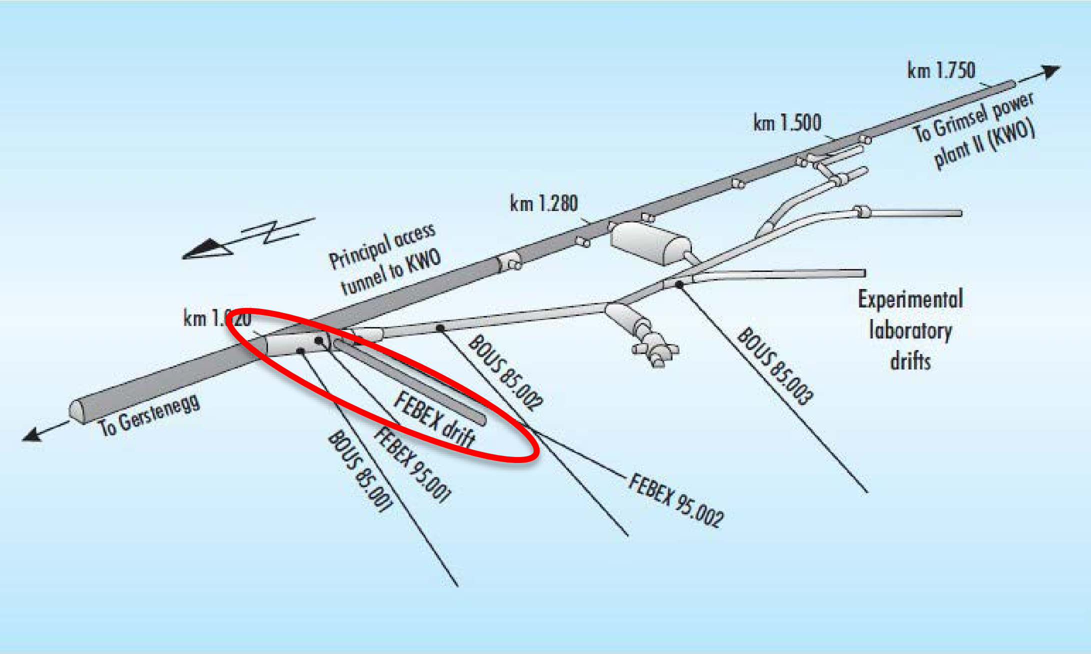
- Simulating the dynamic THM process is challenging
- Further refine of the mechanical model
- Temperature-dependent water retention curve
- Expansion to THMC model will be conducted after THM model is settled

HotBENT Field Experiment (1)

Location

Grimsel area (view to the west)

1 Grimsel Test Site 2 Lake Raeterichsboden 3 Lake Grimsel 4 Juchlistock

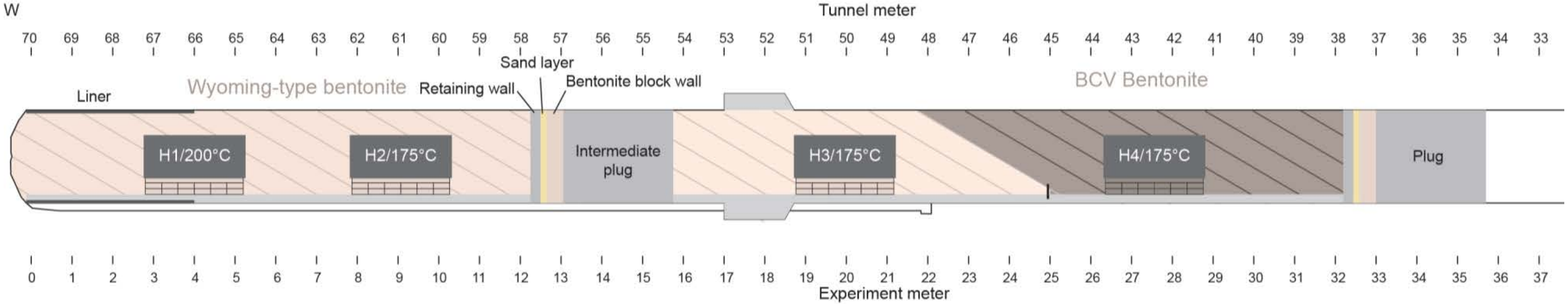


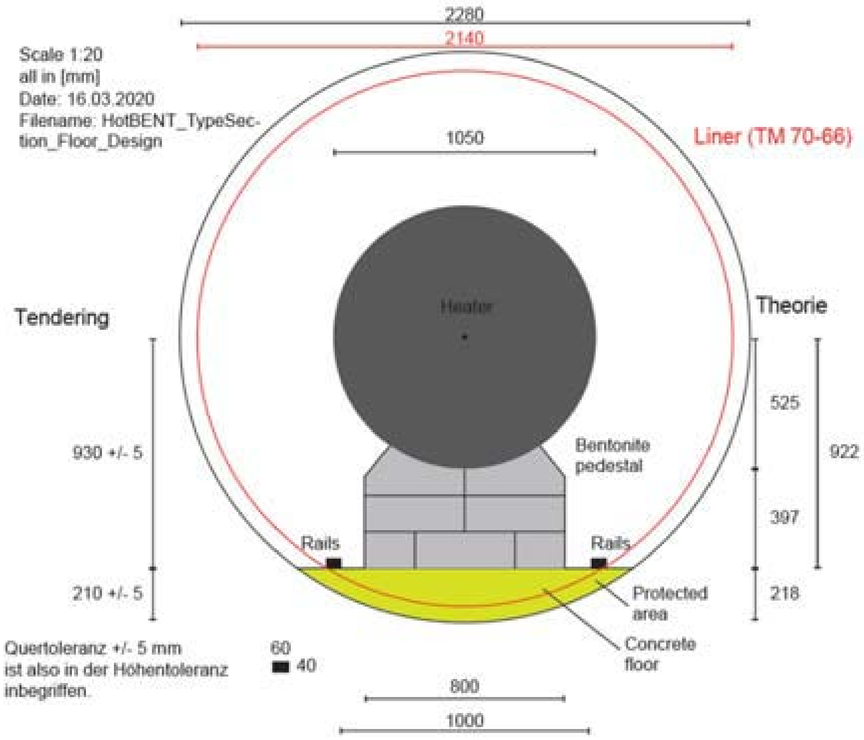
Participating organizations

NAGRA (Switzerland), **DOE(**USA**), NUMO (**Japan**), RWM (**UK**), SÚRAO (**Czech Republic), **NWMO (**Canada**), BGR (Germany); ENRESA (Spain), Obayashi (Japan)**

HotBENT Field Experiment (2)

Design



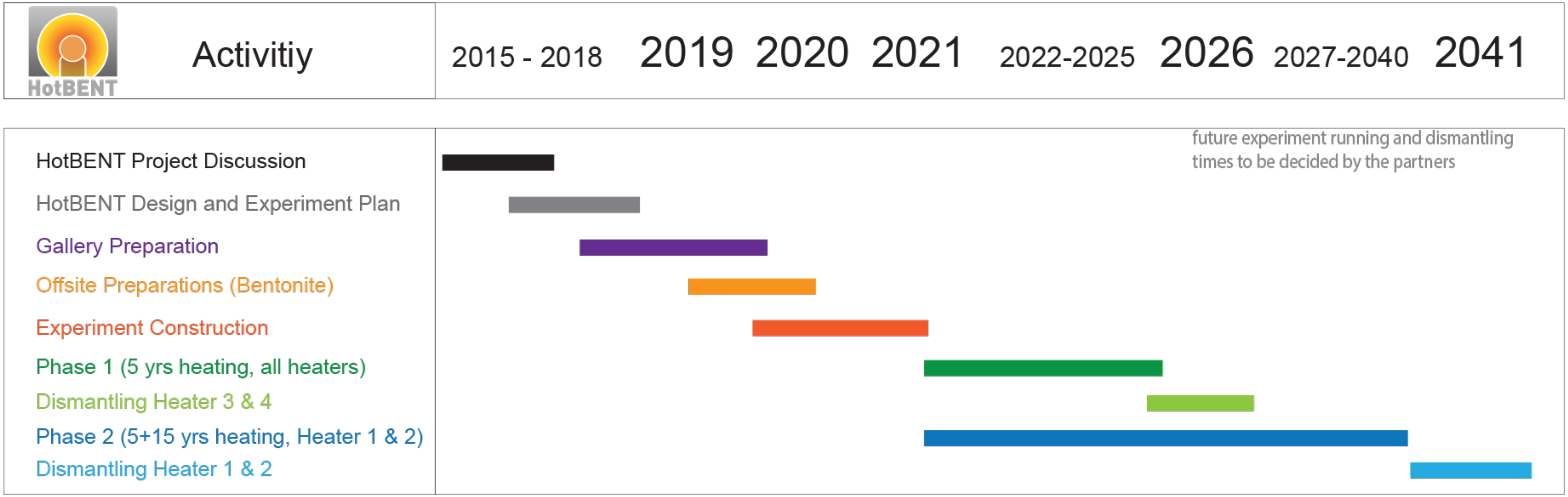


(Kober, 2020)

- **Four modules**
  - ✓ Differing in heating temperature, bentonite, time length and w/o concrete liner
- **Two experimental time lengths**
  - ✓ H3 and H4 will run for 5-10 years
  - ✓ H1 and H2 will run 15-20 years
- **Two bentonites**
  - ✓ Wyoming (MX-80)
  - ✓ BCV (Czech Republic bentonite)
- **Two shapes**
  - ✓ Pedestals for the heaters made of highly compacted blocks, dry density > 1.7 g/cm^3
  - ✓ Granulated Bentonite Mixture (GBM), dry density >1.45 g/cm^3

HotBENT Field Experiment (3)

Timeline



Activitiy

2015 - 2018 2019 2020 2021 2022-2025 2026 2027-2040 2041

HotBENT Project Discussion

HotBENT Design and Experiment Plan

Gallery Preparation

Offsite Preparations (Bentonite)

Experiment Construction

Phase 1 (5 yrs heating, all heaters)

Dismantling Heater 3 & 4

Phase 2 (5+15 yrs heating, Heater 1 & 2)

Dismantling Heater 1 & 2

future experiment running and dismantling times to be decided by the partners

HotBENT Field Experiment (4)

Installation


HotBENT

Operational overview 2021

Grimsel Test Site

GTS

HotBENT : Operational overview video:
https://grimsel.com/gts-projects/hotbent-high-temperature-effects-on-bentonite-buffers/hotbent-video

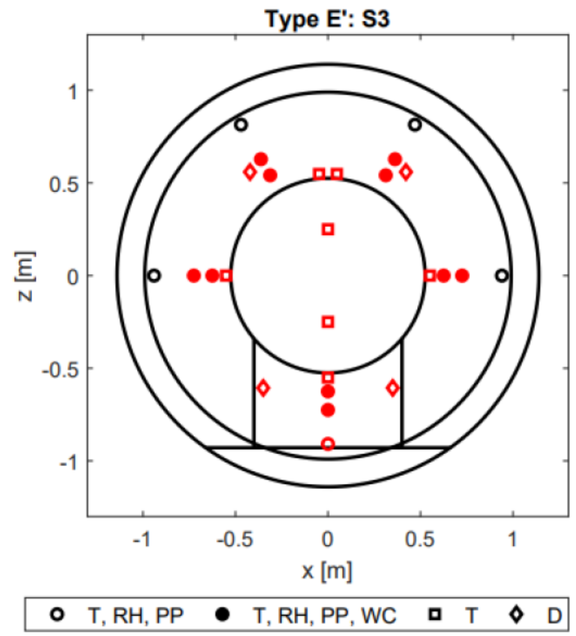
HotBENT Field Experiment (5)

Instrumentation

Lot 1

Section E'
Measurements of:

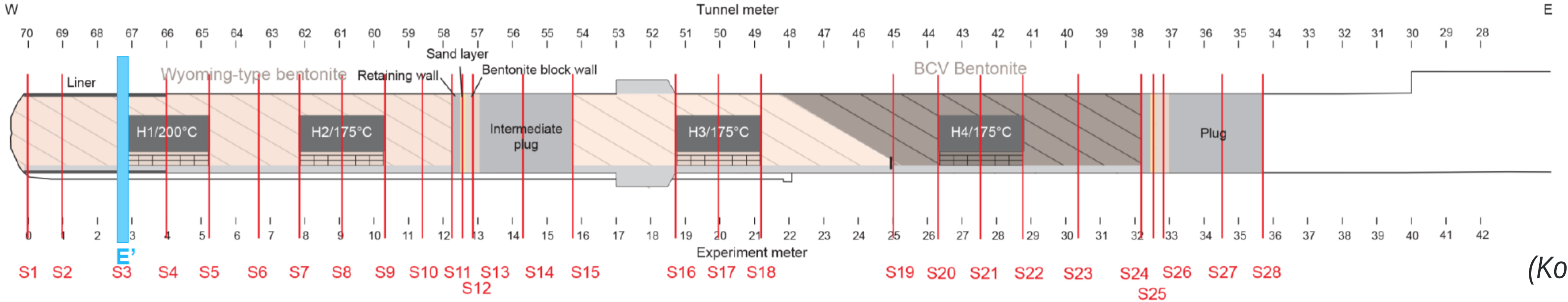
- Temperature (T)
- Pore pressure (PP)
- Relative humidity (RH)



Lot 6

Section E'
Measurements of:

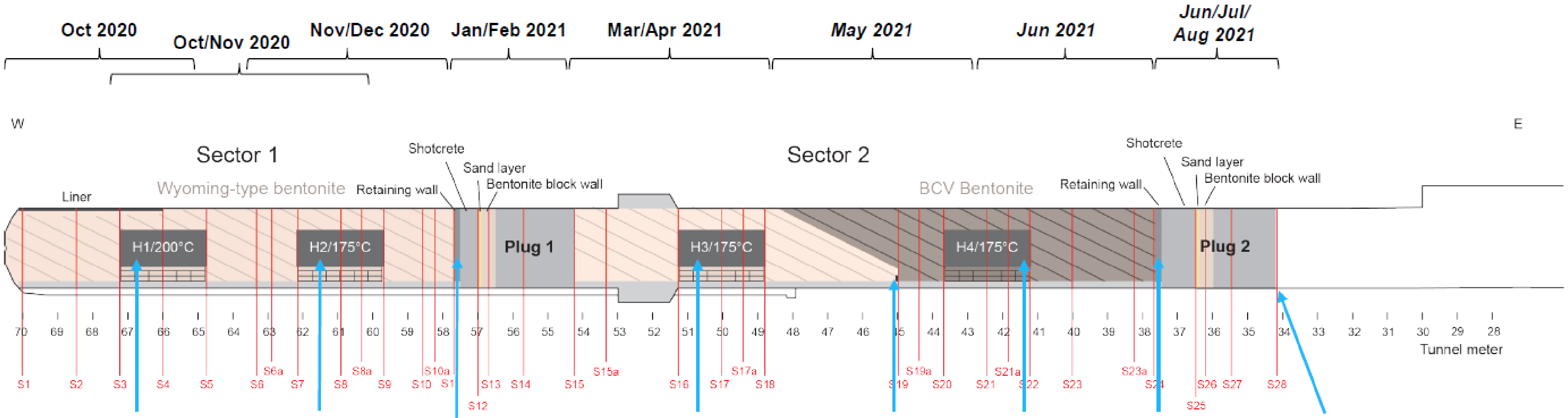
- Temperature (T)
- Pore pressure (PP)
- Relative humidity (RH)
- Total pressure (TP)
- Water content (WC)
- Displacement (D)



(Kober, 2020)

HotBENT Field Experiment (6)

HotBENT emplacement -milestones



29 Oct 2020
(Heater #1
positioned)

26 Nov 2020
(Heater #2
positioned)

18 Dec 2020
(retaining wall
Sector 1 completed)
Retaining wall: 14-18.12.2020
Plug 1:
First shotcrete layer: 11./12.02.2021
Sand-layer/bentonite block wall: 15.-17.02.2021
Shotcrete layer 2-5: 18.-24.02.2021

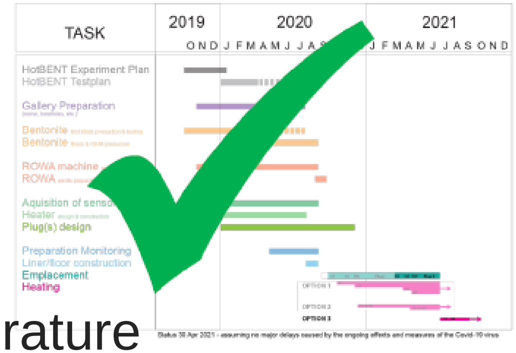
19 Apr 2021
(Heater #3
positioned)

04 May 2021
(end of Wyoming
bentonite)

21 May 2021
*(Heater #4
positioned)*

17 Jun 2021
*(retaining wall
Sector 2 completed)*

30 Aug 2021
Plug 2:
First shotcrete layer: 22.-23.07.2021
Sand-layer/bentonite block wall: 23.-25.08.2021
Shotcrete layer 2-5: 26.-30.08.2021

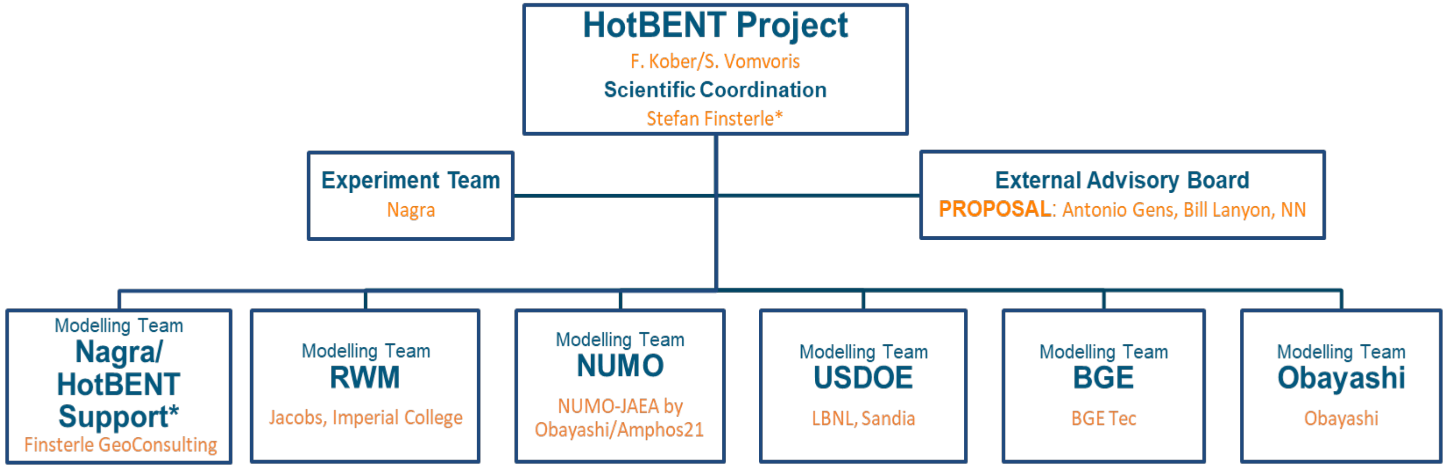


- Heating Started on Sep 9, 2021
- Heaters have been ramped up in steps.
- By June 2, all heaters reached their targeted temperature

HotBENT Modeling (1)

HotBENT modeling platform was established

- Overarching goal:
  - Assess with “initial” modelling the capability of various approaches based on existing laboratory data and simplified assumptions to capture the behavior of the system
  - Interpret the observed behavior based on limited calibration (data release cycles) and predict (including uncertainty) the evolution of the system
  - Predict the state and inform in advance of the partial (and at a later stage full) dismantling activities.



HotBENT Project
F. Kober/S. Vomvoris
Scientific Coordination
Stefan Finsterle*

Experiment Team
Nagra

External Advisory Board
PROPOSAL: Antonio Gens, Bill Lanyon, NN

Modelling Team
Nagra/ HotBENT Support*
Finsterle GeoConsulting

Modelling Team
RWM
Jacobs, Imperial College

Modelling Team
NUMO
NUMO-JAEA by Obayashi/Amphos21

Modelling Team
USDOE
LBNL, Sandia

Modelling Team
BGE
BGE Tec

Modelling Team
Obayashi
Obayashi

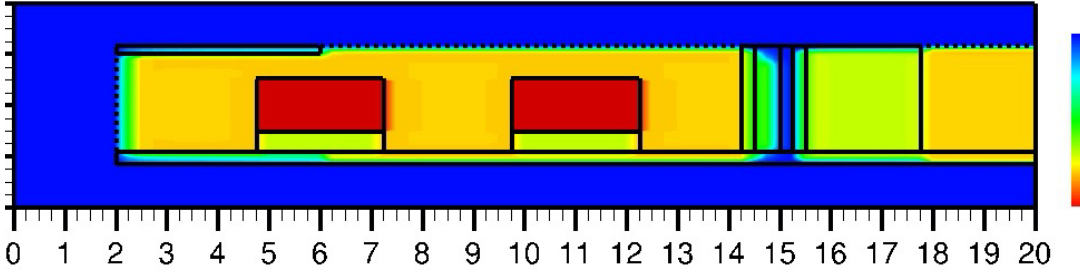
*following the discussion of the 2nd HMP Meeting (18/19 Jan 2022) **Design and Operational Model Support, Nagra interest (UQ, etc.)

SNL Modeling: THMC process at interfacial areas, e.g. metal corrosion at metal-buffer material interfaces

HotBENT Modeling (2)

Coupled THMC model

Goal: Increase the predictability of THMC evolution of bentonite under high temperature: focusing on Improved constitutive relationships under high T, long term geochemical evolution and UQ.



Ongoing:

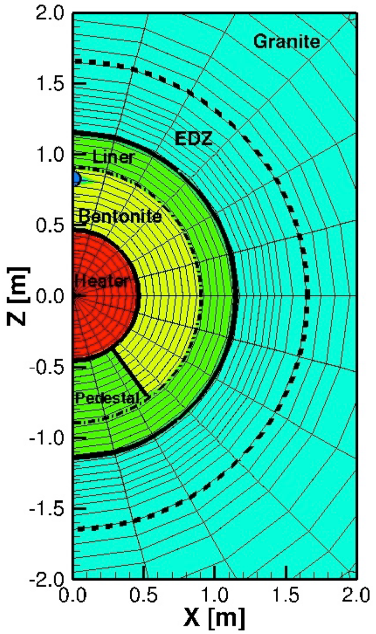
- 3-D TH model

Next steps:

- Expanding the 3-D TH model to THM model
- Make blind prediction of the 1-year response in the field test
- Refinement the model based on the goodness-of-fit of 1-year data
- Make long term prediction using the refined model
- Expanding the THM model to THMC model
- UQ for THMC model

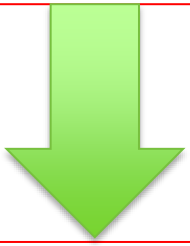
Code: TOUGHREACT-FLAC3D, sequentially coupled THMC code

Performance measure: use as much data as possible in bentonite and geosphere



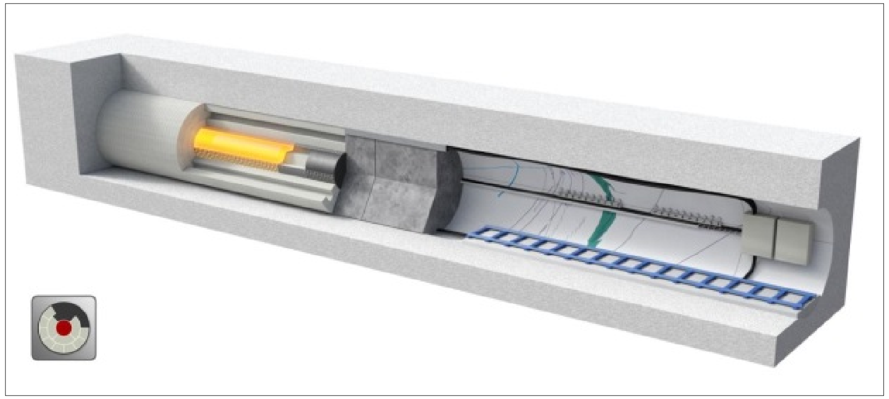
Integrating Coupled THMC models with Generic Disposal

- Developing advanced modeling tools
- Constructing multi-physics coupled process models
- Testing models with large scale experiments

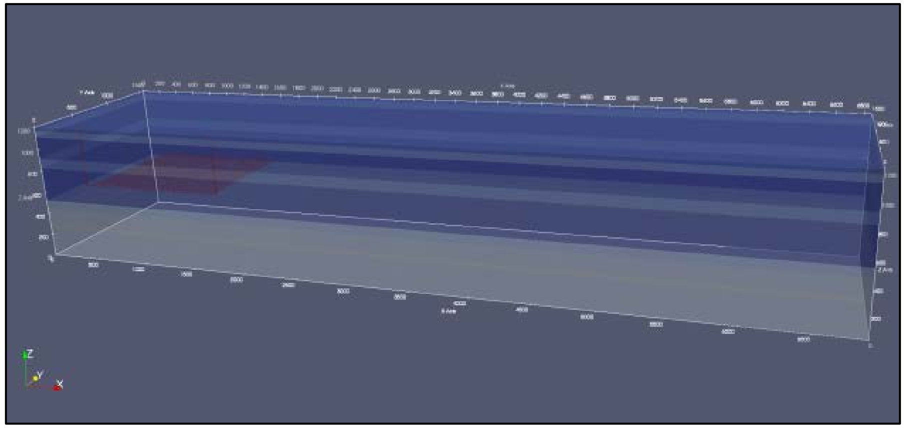


- Supplying generic Performance Assessment (PA) models with reliable conceptual model and parameters
- Providing generic PA models with well-tested constitutive relationships
- Integrating process models into PA

Field Experiments



Generic PA Modeling



Summary

- Understanding and modeling of THMC perturbations in bentonite buffer is critical for clay repository
- Experience was gained for THMC process under low temperature, but recent studies have been dedicated to high temperature conditions.
- Generic models, laboratory and field experiments and the corresponding modeling work have been conducted.
- Modeling and laboratory/field test are working iteratively and interactively to deepen understanding and improve modeling capability.
- Understanding of the alteration of bentonite buffer is enhanced and modeling capability is improved, which will be integrated into Generic Disposal Systems Analyses (GDSA) for performance assessment.

References

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