Used Fuel Disposition Campaign

International Collaboration: SKB EBS Task Force – General Overview

Carlos F. Jové Colón (SNL)

Las Vegas, Nevada – June 7 – 9, 2016

SAND2016-5553 PE

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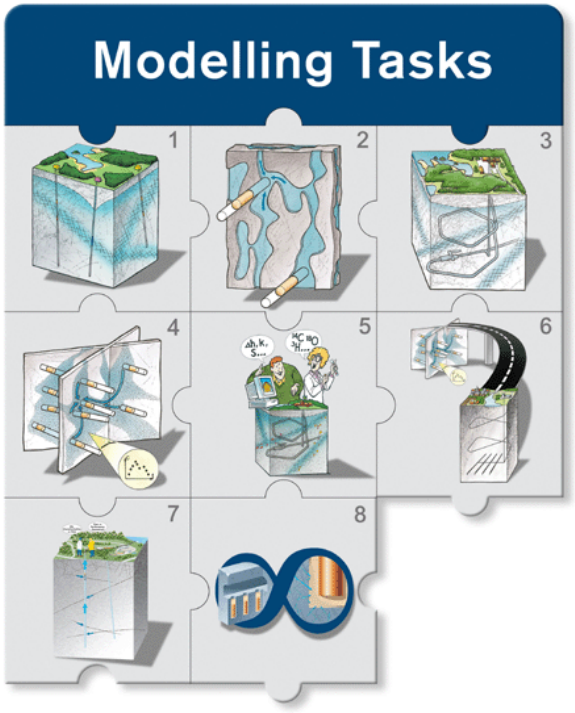
Used Fuel Disposition

SKB-Task Force

Engineered Barrier System (EBS); Modeling of Groundwater Flow and Transport of Solutes (GWFTS)

Scope: *The Task Force selects specific experiments made or to be performed by the Äspö Hard Rock Laboratory (HRL) for modeling by more than one team participating in the Task Force (TF). Selection of experiments must be performed in consultation with the Äspö HRL.*

Task 1 - The LPT2 experiments, evaluation modeling
Task 2 - Äspö field tracer experiments, design modeling
Task 3 - The Äspö tunnel experiment, predictive/evaluation modeling
Task 4 - Tracer Retention and Understanding Experiments - TRUE-1, predictive modeling
Task 5 - Integration of hydrogeology and hydrochemistry
Task 6 - Performance Assessment (PA) Modeling Using Site Characterization Data (PASC)
Task 7 - Reduction of Performance Assessment uncertainty through site scale modeling of long-term pumping in KR24 at Olkiluoto, Finland
Task 8 - Interface Engineered and Natural Barriers
Task 9 - Develop models that in a more realistic way represent solute transport and retardation in the natural rock matrix.



Source: SKB TF Documentation

- Tasks 1 through 7 → Completed
- Task 8(a,b,c,d,e) → Task 8 still ongoing!!!
- Task 9 → Proposal Stage

SKB-Task Force
Engineered Barrier System (EBS)

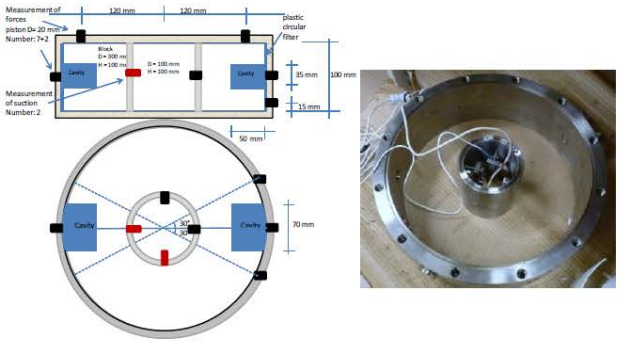
- OBJECTIVE: "Development of general and effective tools for the advanced coupled THMC analysis of buffer and backfill behavior"
- THM:
  - Verify the capability to model THM processes in unsaturated and saturated bentonite clay backfill materials
  - Validation and development of material models and simulation codes by numerical THM modeling of laboratory and field tests
  - Evaluate the influence of parameter variations, parameter uncertainties and model imperfections
- TF Goal:
  - Support the long term work for making it possible to predict the normal THM evolution of the buffer and backfill in the repository
  - Evaluate barrier interactions with rock, canister, and other EBS components.
  - Evaluate THM evolution in possible abnormal scenarios that may occur

Source: SKB TF Documentation

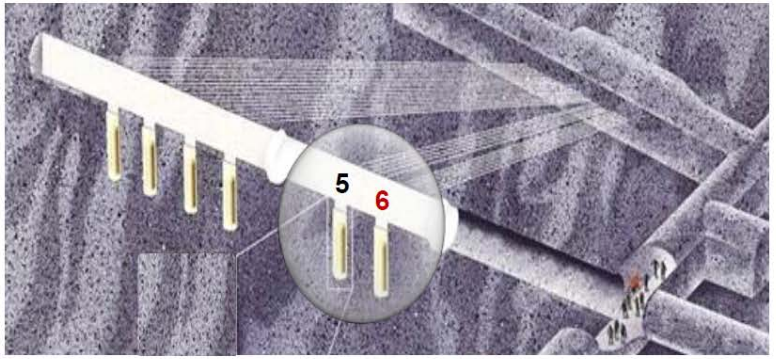
SKB-Task Force

Engineered Barrier System (EBS)

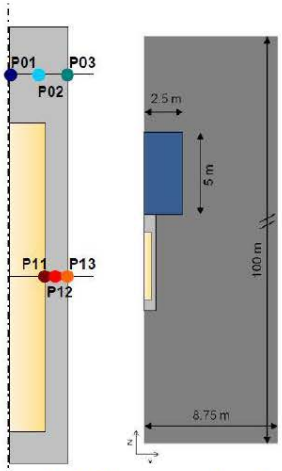
- Current THM Tasks



Homogenisation



Prototype



Sensitivity analysis

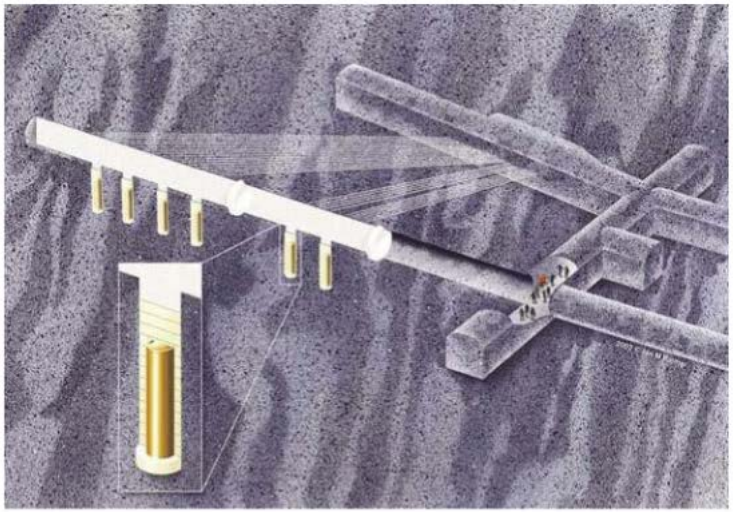
Task 8 (BRIE)
Interaction natural/engineered barrier

Source: SKB TF Documentation

SKB-Task Force
Engineered Barrier System (EBS)

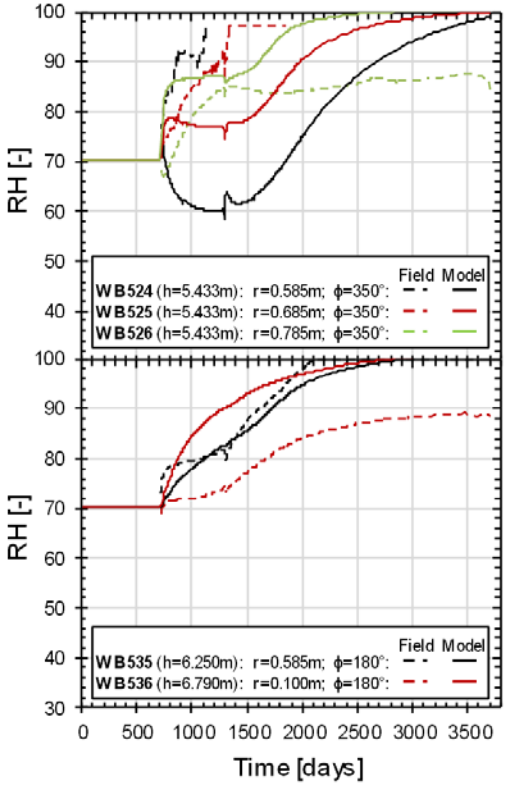
- THM – Prototype
  - *The goal is to predict the final state of the buffer in the deposition holes in the outer (now excavated) section (DH5 & DH6)*

The prototype repository: Äspö, 450 m deep



Source: SKB TF Documentation

TH model with Code_Bright

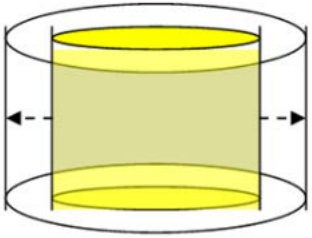


SKB-Task Force

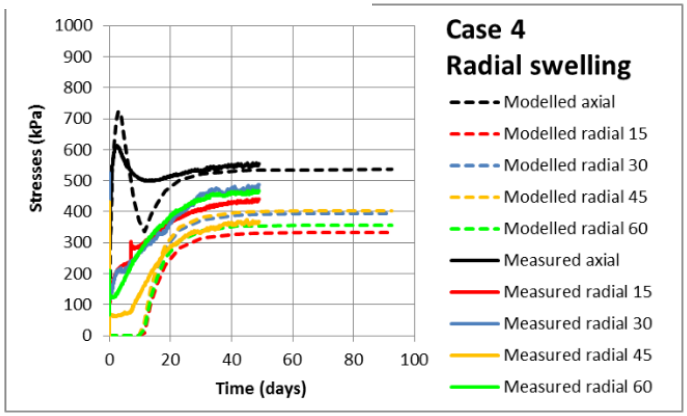
Engineered Barrier System (EBS)

- THM – Homogenization
  - *Gaps, holes or inhomogeneous density distributions may prevail in the buffer or backfill material*
  - *How well can the bentonite self-seal and homogenize these anomalies?*
  - *Development, calibration and verification of material models and modeling techniques!*

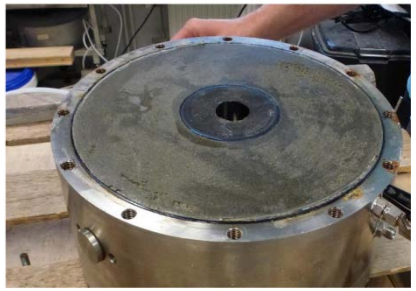
Small scale swelling test: radial swelling

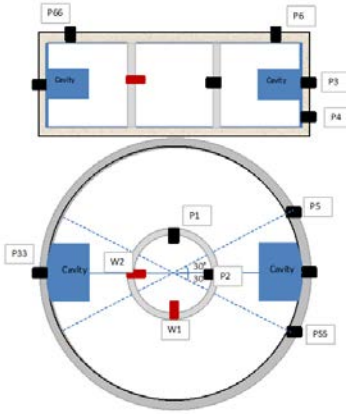


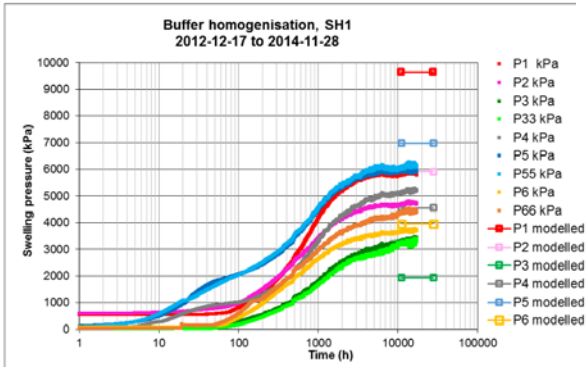
Models from Clay Technology



Large scale homogenization test







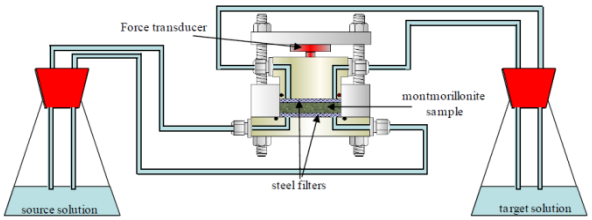
Source: SKB TF Documentation

SKB-Task Force
Engineered Barrier System (EBS)

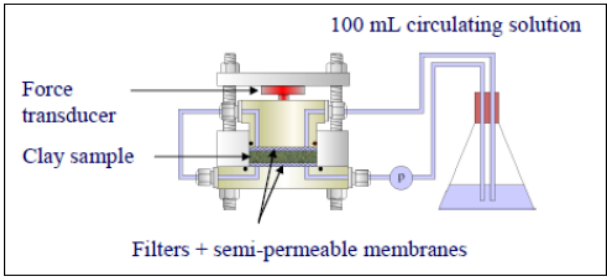
- THC – benchmarks for modeling

Five experimental benchmark data sets:

Benchmark 1: Salt diffusion in montmorillonite

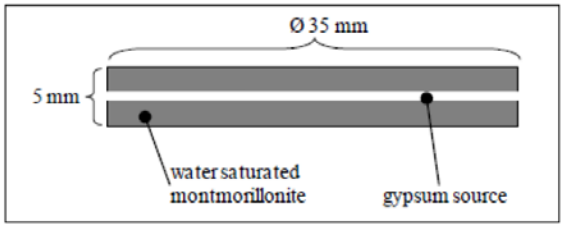


Benchmark 3: Ca/Na ion exchange in montmorillonite



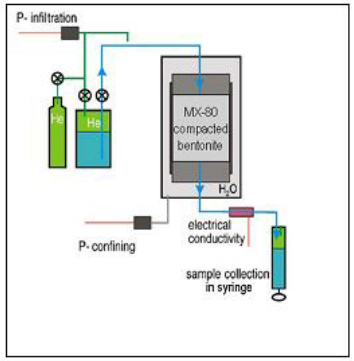
- **SKB TF Benchmark data and documentation available through web-based access**
- **Code/model development?**
- **Evaluate porosity concepts**
- **Clay-solution interactions**
- **Effects on bentonite swelling**

Benchmark 2: Gypsum dissolution in Na-and Ca-montmorillonite

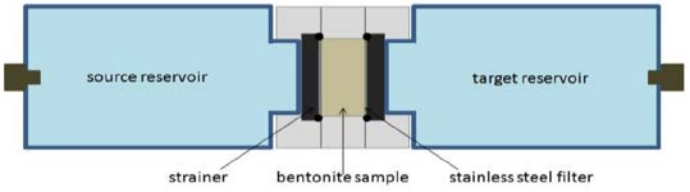


Source: SKB TF Communication "Chemistry issues" Dr. Urs Mäder, University of Bern

Benchmark 4: Multi-Component (adv-diff) transport experiment in MX-80 comp. bentonite



Benchmark 5: Diffusion of anions (Cl, Se, I) through compacted bentonite



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International Collaboration: SKB EBS Task Force – Potential Activities of Interest to UFD R&D

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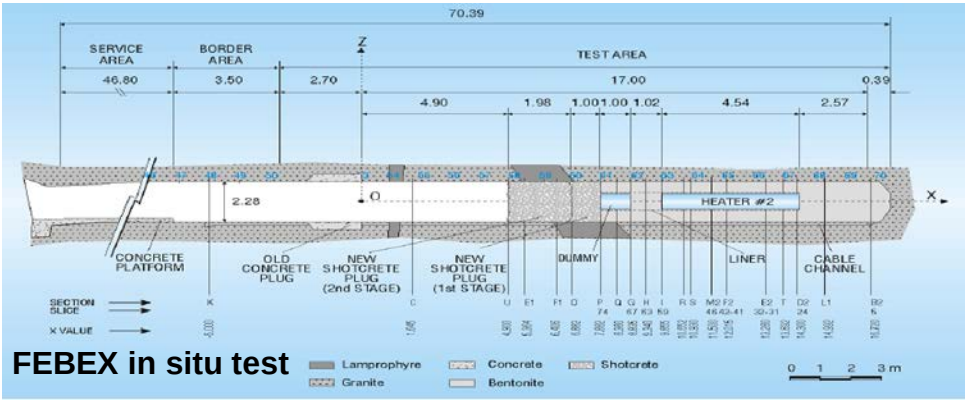
NNSA National Nuclear Security Administration

SKB TF: Proposed New Tasks

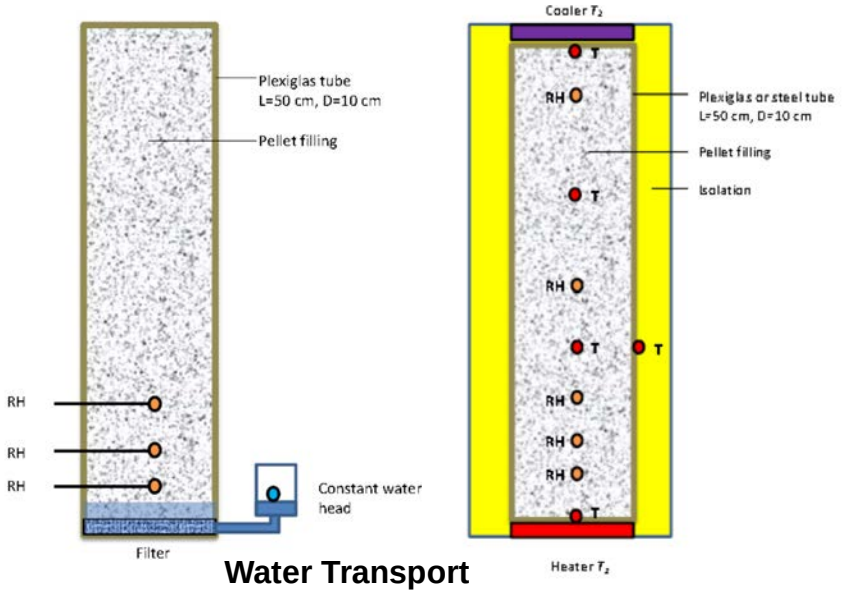
New THM Tasks

- Febex in situ test (A.Gens) – <u>Data not available until 2017</u>
- Water transport in pellet-filled slots (L. Börgesson)
- Gas transport in bentonite (P. Marschall)

Source: Meeting notes from A. Gens



FEBEX in situ test



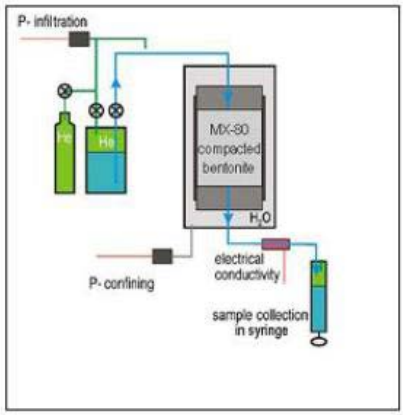
Water Transport In Pellet-Filled Slots

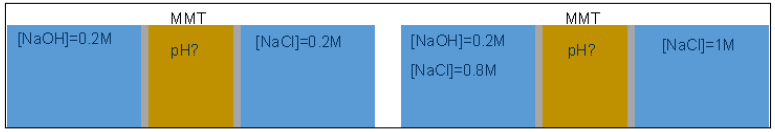
SKB TF: Proposed New Tasks: HM-C

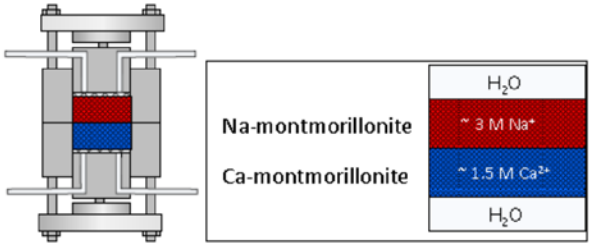
Newly Proposed "C" Tasks

- Multi-component transport
- pH inside clay under alkaline conditions
- HM-C squeezing experiment
- Micro-ABM test
- Uphill diffusion

Mainly HM-C issues!!!

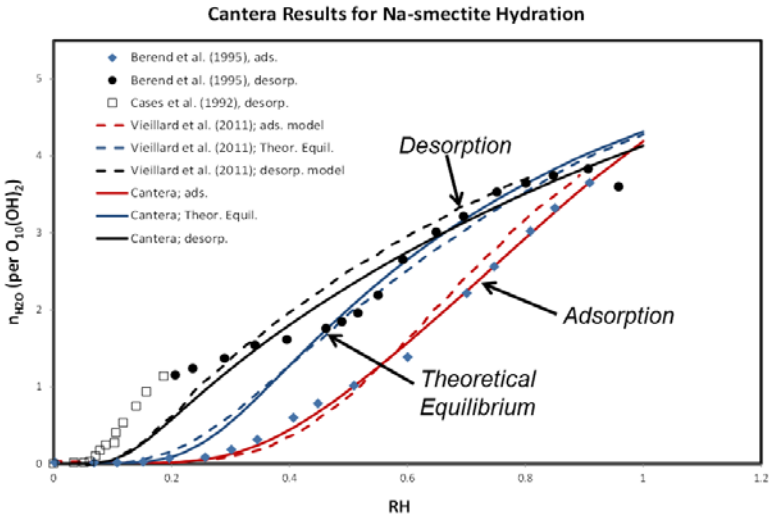


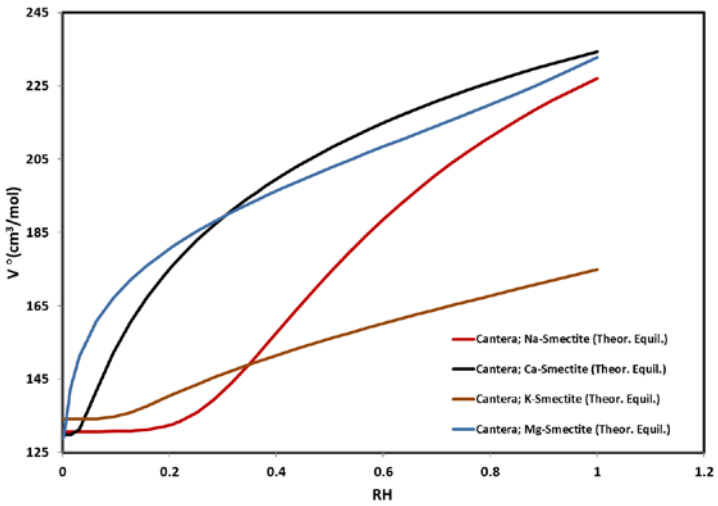




Source: Meeting notes from A. Gens

Clay Hydration Thermodynamic Model





- Fitting H_2O adsorption data for various smectite clay compositions
- Use thermodynamic model to predict changes in mineral volume with RH

$$Smectite\ (dehyd.) + nH_2O = Smectite\ (hyd., nH_2O)$$

$$H^{EX} = X_{smect.\ hyd.} X_{smect.\ dehyd.} (W_{H1} + W_{H2} X_{smect.\ dehyd.})$$

$$S^{EX} = X_{smect.\ hyd.} X_{smect.\ dehyd.} (W_{S1} + W_{S2} X_{smect.\ dehyd.})$$

$$G^{EX} = H^{EX} - TS^{EX}$$

Margules parameterization – hydrated & dehydrated clay end-members

SKB-Task Force
Engineered Barrier System (EBS)
BRIE Experiment

Bentonite Rock Interaction Experiment (BRIE) Characterization of rock and installation, hydration and dismantling of bentonite parcels

Goals:

- **An increased scientific understanding of the exchange of water across the bentonite-rock interface**
- **Improve predictions of the wetting of the bentonite buffer**
- **Improve characterization methods of the deposition holes**

Bentonite Parcels

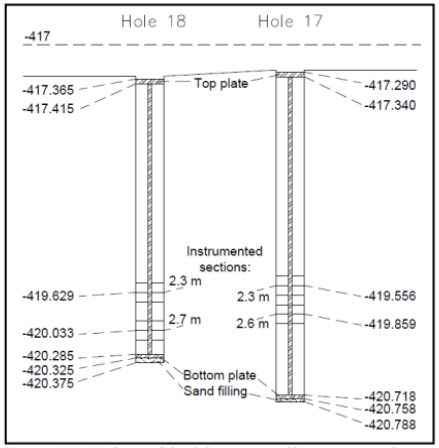
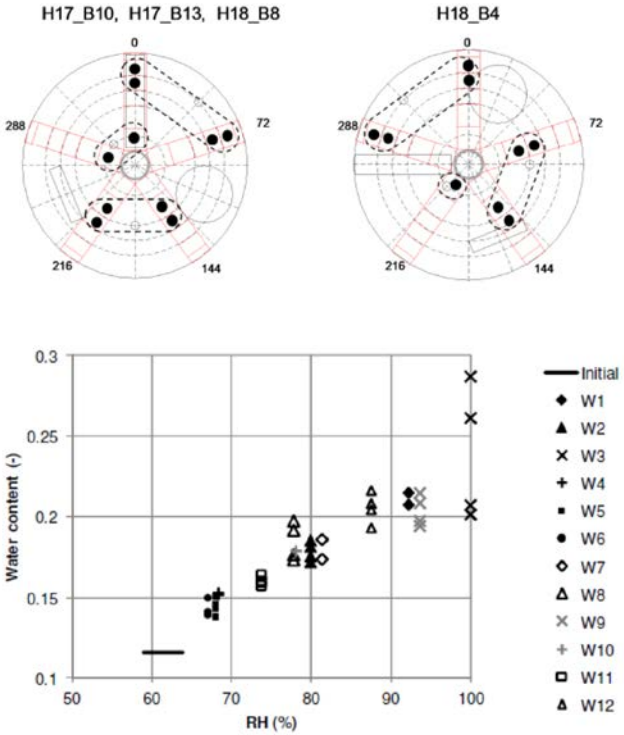


Figure 6-11. Outline and final dimensions of bentonite parcels.



Source: SKB TF BRIE Report Characterization
Bentonite Parcels R-14-11 DRAFT (2014, 2016)

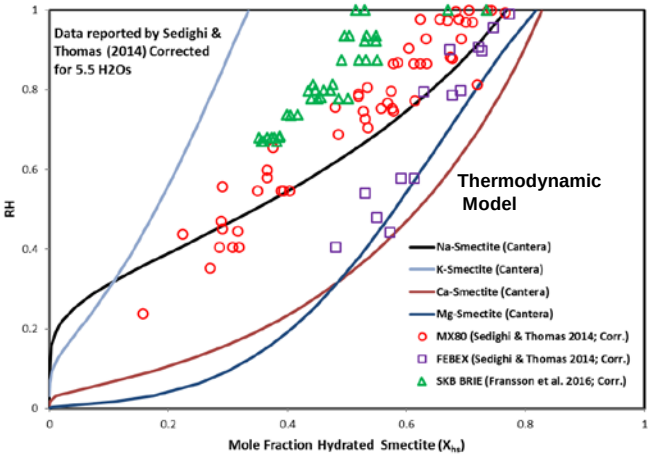
Clay Hydration Modeling and Micro-Porosity Evolution: Model Comparison with BRIE Water Retention Data

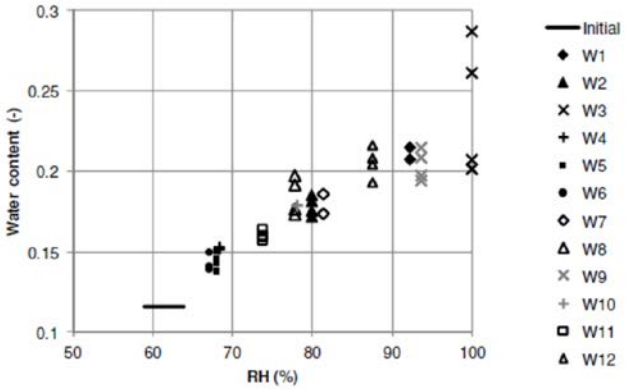
- **Relationships between swelling clay micro-porosity and clay hydration (Sedighi and Thomas 2014)**
- **Data retrieval from URL and laboratory experiments**
  - **FEBEX**
  - **Bentonite H_2O retention (SKB TF BRIE)**
- **Trend for Na- and Ca-bearing consistent with thermodynamic model predictions for clay hydration**

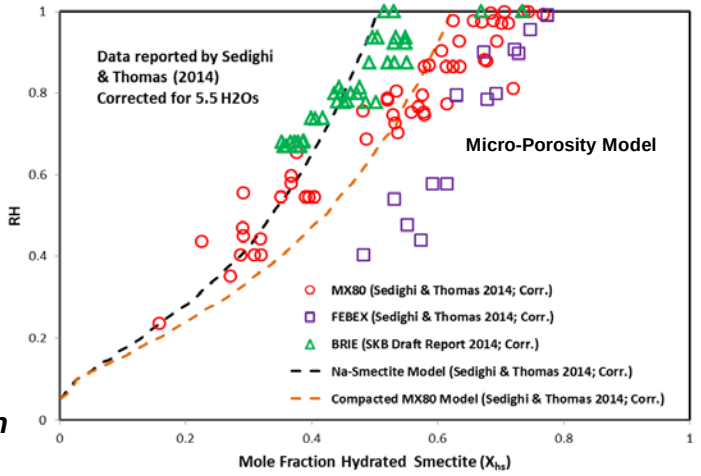
Sedighi and Thomas (2014)

$$n_{micro} = X_{hs} \frac{n_c \upsilon_{il}}{Fw_{sm}} \rho_{dry}^{sm}$$

n_{micro} = Clay micro-porosity = θ_{wc}^{il} = water content
X_{hs} = Mole fraction of hydrated smectit
Fw_{sm} = Formula weight of anhydrous smectite
n_c = Number of H2Os in the interlayer
υ_{il} = Molar volume of H2O (interlayer)
ρ_{dry}^{sm} = Clay dry density







Source: SKB TF BRIE Report Characterization
Bentonite Parcels R-14-11 DRAFT (2014, 2016)

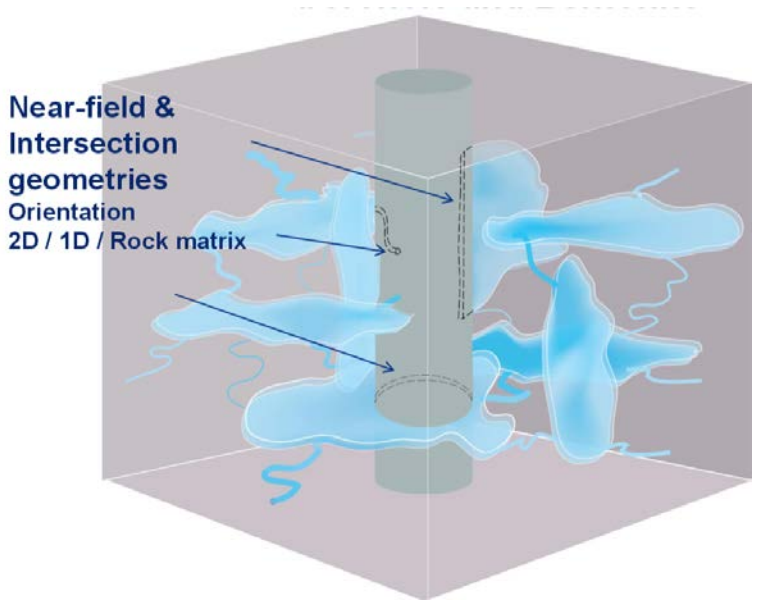
SKB-Task Force
Engineered Barrier System (EBS)

- THC – Future direction – C Issues and Coupled Processes – i.e., HM-C
  - *Experiments discriminating among concepts (e.g., diffusive transport)*
  - *Interlayer chemistry*
  - *HM-C coupling*
  - *Soluble accessory phases that influence bentonite pore water composition*
  - *Additional issues?*
- THC – DOE-LBL participation
  - *Benchmarking*
  - *HM-C coupling*
  - *Soluble accessory phases that influence bentonite pore water composition*
- THC – DOE-SNL participation
  - *Benchmarking*
  - *Interlayer chemistry*
  - *HM-C coupling*
  - *Soluble accessory phases that influence bentonite pore water composition*
  - *Additional issues: Temperature effects?*

BACKUP SLIDES

SKB-Task Force
Engineered Barrier System (EBS)

- THM – Task 8 in *GWFTS*
  - *The Bentonite Rock Interaction Experiment (BRIE) at Äspö HRL*



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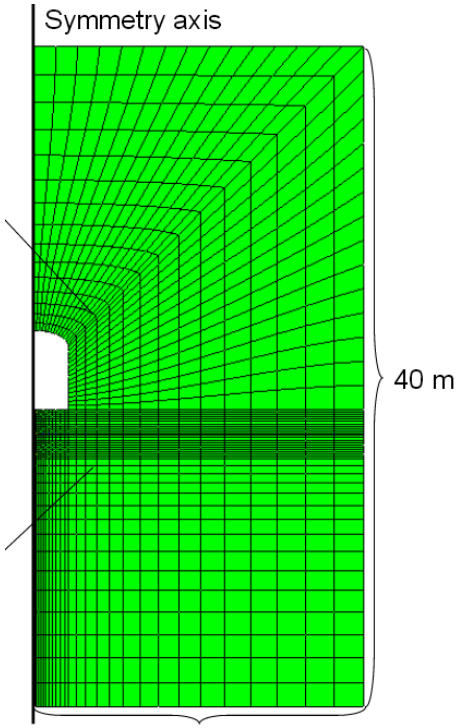
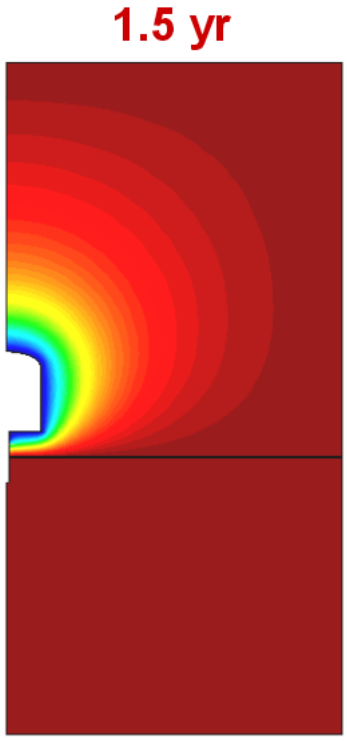




SKB-Task Force

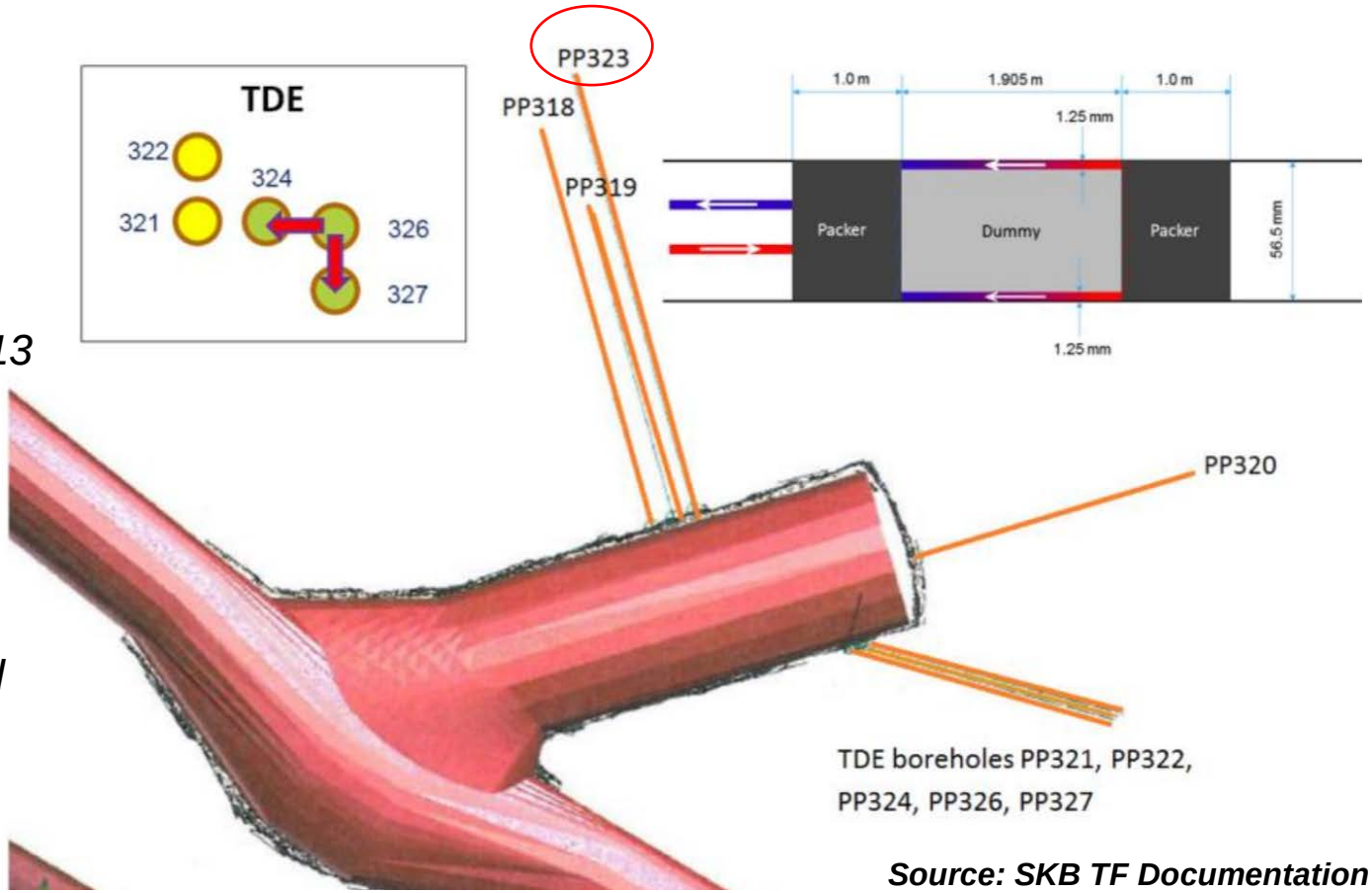
Modeling of Groundwater Flow and Transport of Solutes (GWFTS)

Task 9A – Water Phase Diffusion Experiment (WPDE)

WPDE-1: HTO, Na-22, Cl-36, I-125, tracer injection on March 2012

WPDE-2: HTO, Na-22, Cl-36, Sr-125, Ba-133 injection on January 2013

Predictive modeling results will be presented on October 2015 in Kalmar, Sweden



Source: SKB TF Documentation

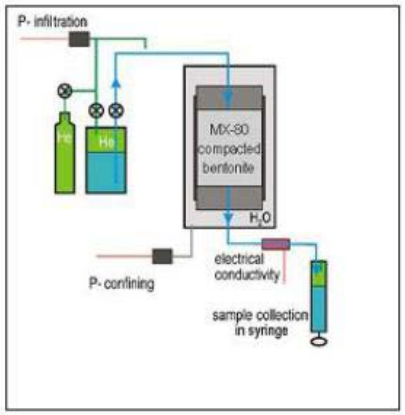
Used Fuel Disposition

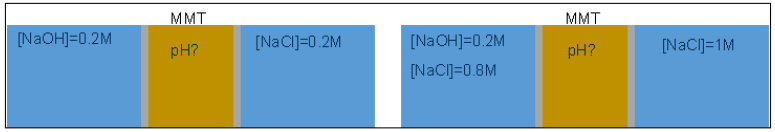
SKB TF: Proposed New Tasks: HM-C

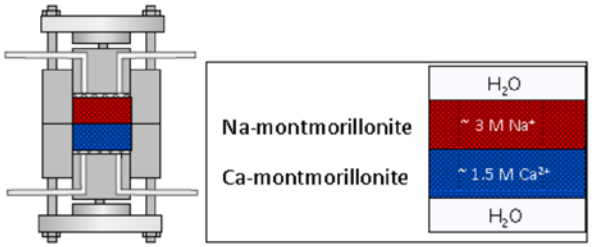
Newly Proposed "C" Tasks

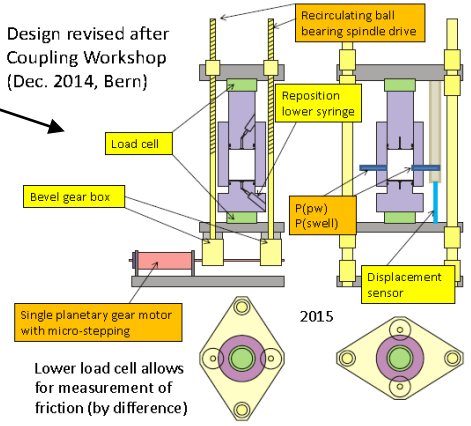
- Multi-component transport PV Control
- pH inside clay under alkaline conditions
- HM-C squeezing experiment
- Micro-ABM test
- Uphill diffusion

Mainly HM-C issues!!!









SKB-Task Force

Engineered Barrier System (EBS)

- THC - *The main focus of the "C" section was:*

  - *"To develop and test alternate porosity concepts that explain fundamental properties like ion and water transport and swelling pressure"*
  - *"To assemble experimental data sets (literature and/or own experiments) that allow testing of alternate concepts and assess so their relative merits"*
  - *"To gain insight at the molecular scale of physico-chemical processes within smectite interlayers (e.g., via MD simulations)"*
  - *"To further develop numerical tools that allow for a general implementation of these chemical aspects into a THM framework"*

Source: SKB TF Communication
"Chemistry issues"
Dr. Urs Mäder, University of Bern