THMC Modeling for Clay-based Barrier Materials

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Outline

- Modeling THMC Alterations in EBS bentonite under Higher (>100 ^{o}C) Temperature
- A dual structure constitutive model for simulating the mechanical behavior of expansive soils

Modeling THMC Alterations under Higher (>100 ^{o}C) Temperature:

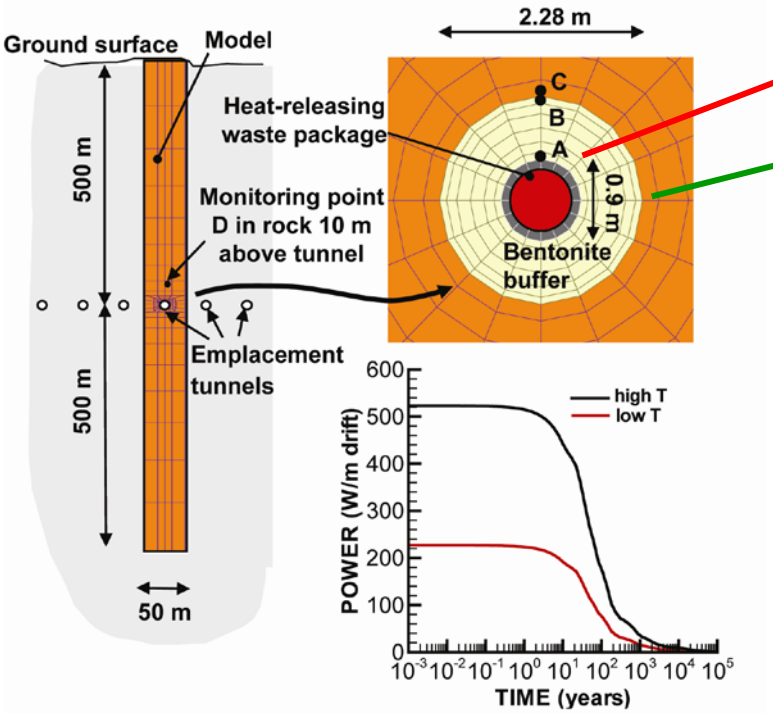
Motivation and approach

The first step to answer whether we can use a thermal limit >100 ^{o}C for clay repository with bentonite EBS?

- Among disposal concepts all over the world, despite their differences in some details, a thermal constrain of 100 ^{o}C is uniformly used for EBS bentonite, and major concerns are chemical alteration (illitization), water boiling, canister corrosion.
- Although illitization is extensively evidenced from geological system, laboratory experiment, field test and modeling studies show no conclusive evidence that illitization will occur and swelling capacity will be lower in bentonite.
- THMC model is used to evaluate whether illitization will be enhanced at higher temperature and the resulting hydraulic and mechanical consequence, with the following modeling strategy:
  - ✓ *Finding out the mechanisms of illitization and major controlling factors through literature review*
  - ✓ *Testing our illitization model and reaction rate with field data*
  - ✓ *Developing coupled THMC model to evaluate illitization and the hydraulic and mechanical consequence of > 100 ^{o}C heating.*

Modeling THMC Alterations under Higher (>100 ºC) Temperature:

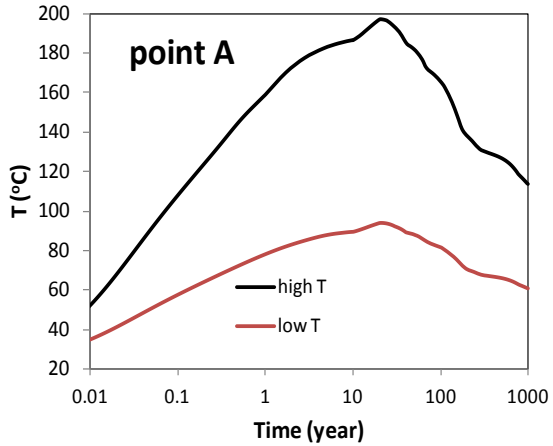
Modeling scenario



EBS Bentonite: Kunigel-V1

Clay formation : Opalinus Clay

Two cases for comparison: a "high T" case and a '"low T" case



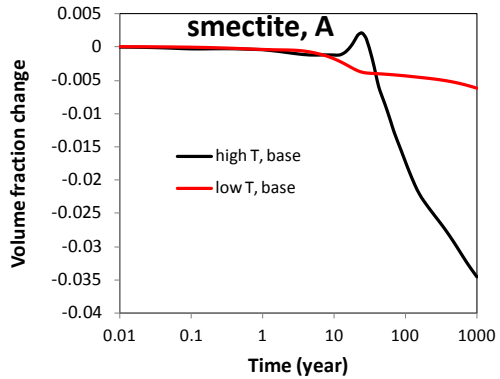
- *Illitization can be modeled as smectite dissolution and neo-formation of illite*
- *The reaction rate from 4.5e-14 to 2.4e-13 mol/g/s calibrated against data from Kinnekulle bentonite, Sweden (Push&Madsen, 1995)*
- *Linear elastic swelling model is used to model the effect of chemical changes:*

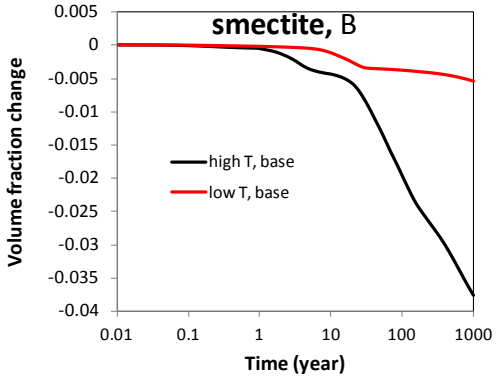
$$d\sigma_s = 3K\beta_{sw} ds_l - A_n dC + A_{sc} dm_s$$

Modeling THMC Alterations under Higher (>100 ºC) Temperature:

illitization (smectite dissolution and illite precipitation)

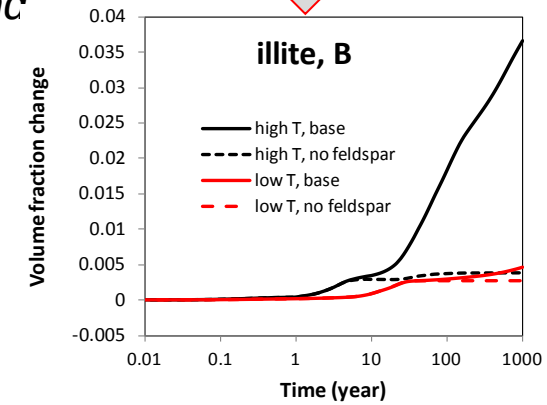
- *Smectite volume fraction in EBS bentonite decreases by 0.035, or 11% of the initial amount (0.314) for "high T" case (VS 1.5% for "low T" case) after 1000 years*



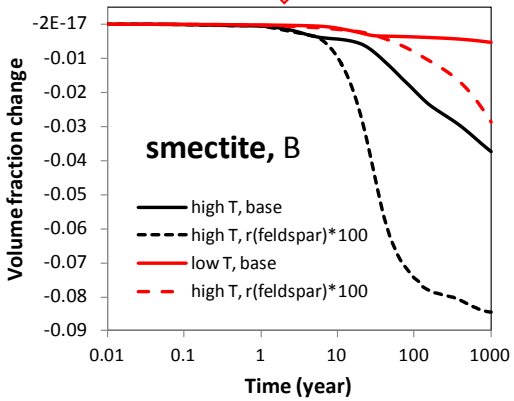


- *The quantity of illitization is affected by many chemical factors and subsequently varies a great deal. The most important chemical factors are the concentration of K and dissolution rate of K-feldspar; less important are the concentration of Na and quartz precipitation rate.*

Model without K-feldspar dissolution

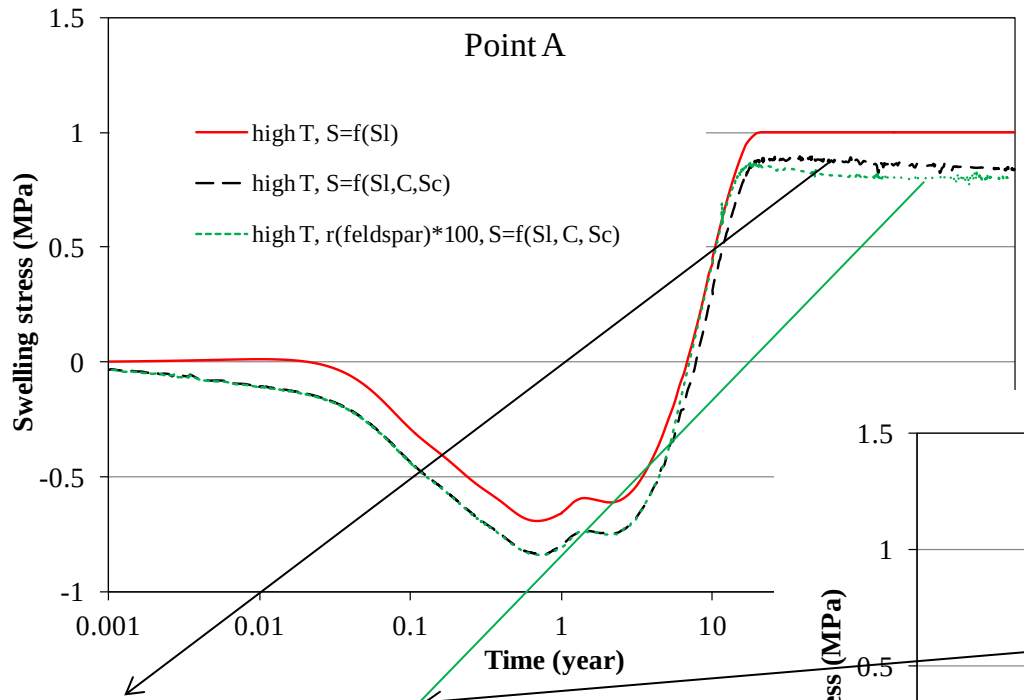


Model with K-feldspar dissolution rate two orders of magnitude higher



Modeling THMC Alterations under Higher (>100 ºC) Temperature:

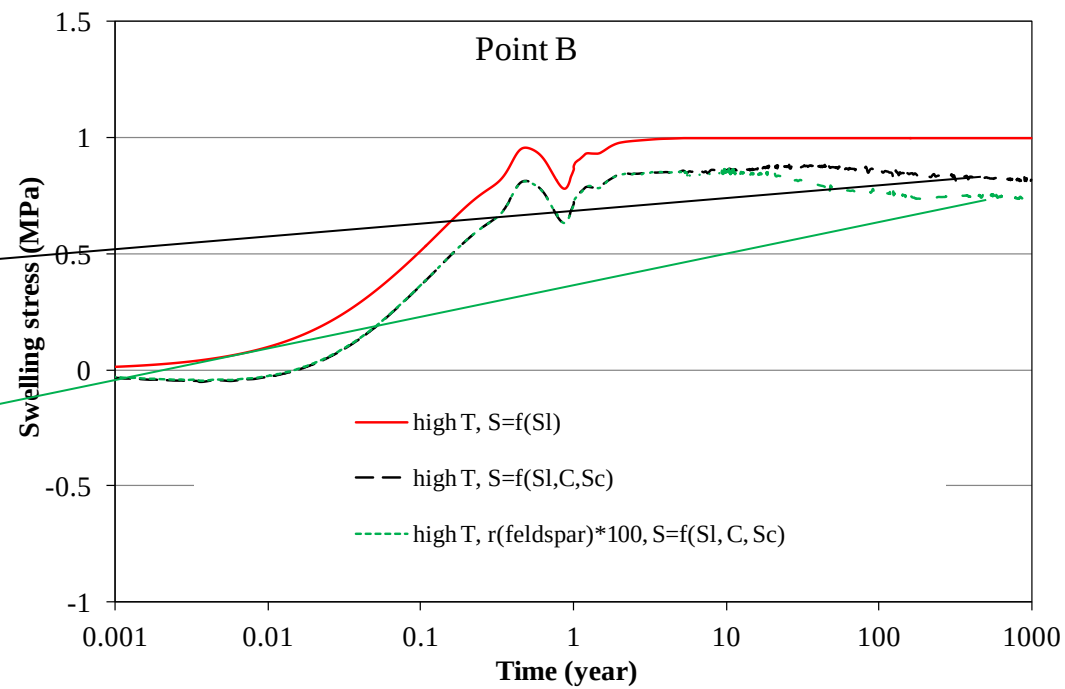
Model Results: Chemical effect on swelling stress



*The swell stress reduction for the case with the maximum smectite dissolution in EBS bentonite, the "high T" case with higher K-feldspar dissolution rate "r(feldspar)*100".*

"high T" base case: 16-18% reduction in swelling stress

*"high T" "r(feldspar)*100" case: 20-26% reduction in swelling stress*



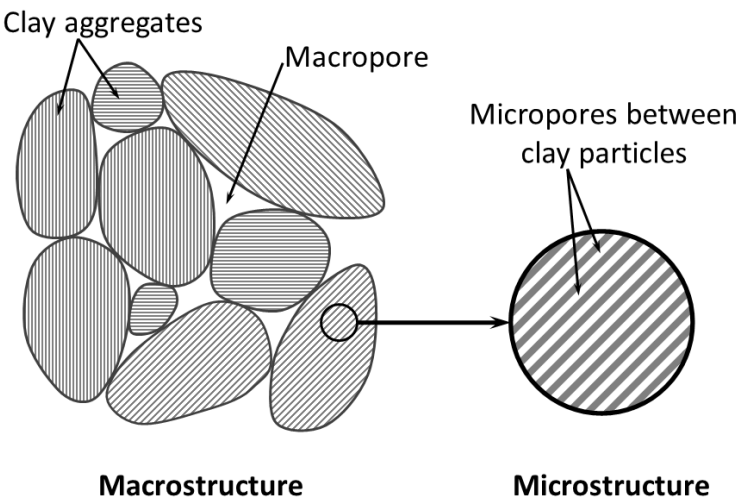
Modeling THMC Alterations under Higher (>100 ^{o}C) Temperature:

Summary and Future Work

- *In general, illitization in the bentonite is enhanced at a higher temperature. However, the quantity of illitization is affected by many chemical factors and subsequently varies a great deal.*
- *The most important chemical factors are the concentration of K and dissolution rate of K-feldspar; less important are the concentration of Na and quartz precipitation rate.*
- *The decrease in smectite volume fraction in bentonite ranges from 0.004 to a maximum of 0.085, or up to about 27% of the initial volume fraction of smectite.*
- *Chemical changes including the changes in pore water ion concentration and smectite volume fraction lead to a reduction in swelling stress up to 16-18% for the base case. However, more dissolution of smectite under some chemical conditions and the variation of the key parameters could result in further reduction of swelling and total stress*
- *In the future, the effect of the hydrogeological parameters (processes) on illitization need to be evaluated.*
- *Illitization and the changes in swelling stress needs to be incorporated in the large 3D models and PA models to assess their effect on the performance of repository*

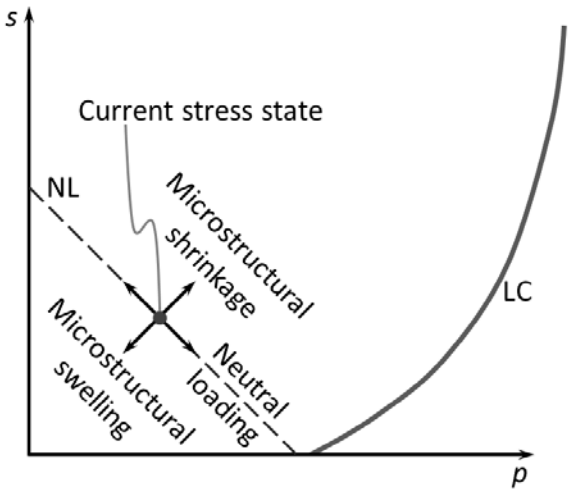
Dual Structure Constitutive Model: Background

Motivation



We need a constitutive model considering two pore levels:
- Microstructure accounts for active clay minerals
- Macrostructure is related to major structural rearrangement

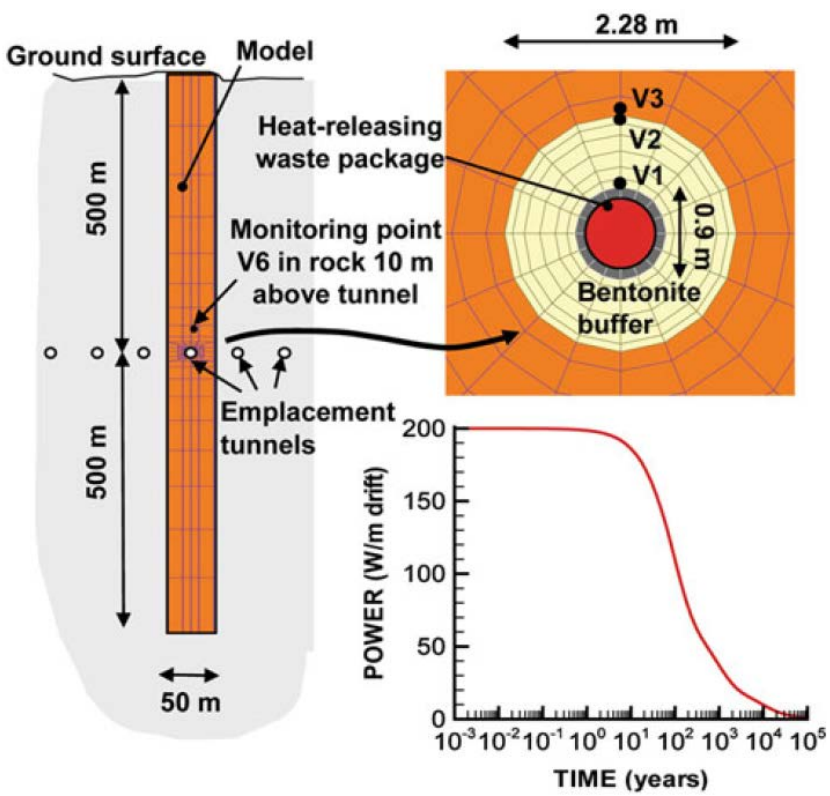
Methodology



- *Macrostruture can be modeled with an elasto-plastic constitutive model for unsaturated soils (e.g. BBM)*
- *Microstructure behaves elastically and is fully saturated, so the effective stress principle applies*
- *Microstructural strain induce plastic strain of the macrostructure, leading to plastic strain accumulation upon suction cycles*

Dual Structure Constitutive Model: Current Status

Application of double-structure THM models to a generic repository emplacement tunnel



We compare the behavior of the bentonite buffer using either the BBM or the dual structure model

Permeability variation

Dual structure model

$$\mathbf{k} = k_{0M} \exp\left[b\left(\phi_M - \phi_0\right)\right]\mathbf{I}$$

BBM

$$\mathbf{k} = k_0 \exp\left[b\left(\phi - \phi_0\right)\right]\mathbf{I}$$

$$\mathbf{k}_0 = 2 \cdot 10^{-21}\,\mathrm{m}^2$$

Dual Structure Constitutive Model: Current Status

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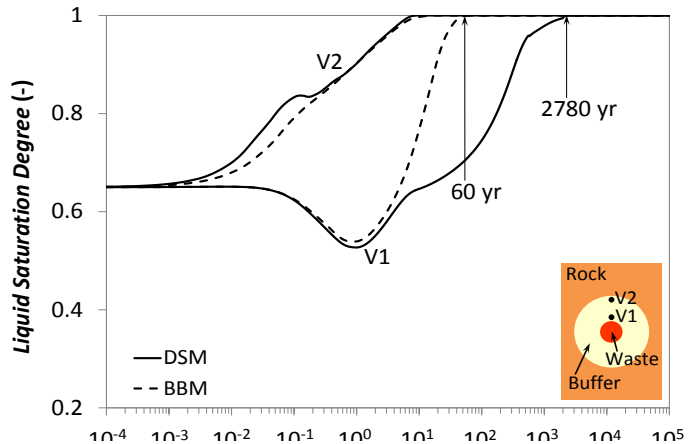
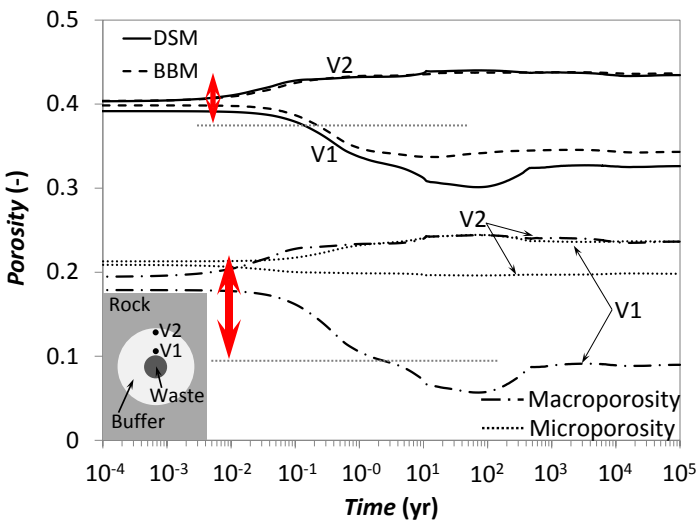
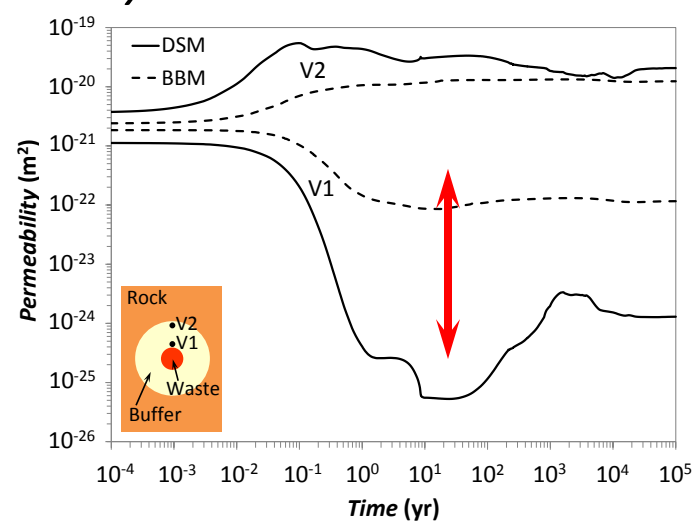


The dual structure model (DSM) predicts a delay in the saturation of the buffer because water can only flow through the macropores. The macropores reduction is larger than the total porosity reduction predicted with the BBM close to the waste, leading to a larger permeability reduction





Dual Structure Constitutive Model: Ongoing Work

Developing more rigorous approach to link chemistry to mechanics through the micro-structure strain.

$$\mathrm{d}\varepsilon_{vm}^{e} = \frac{f_s}{K_m}\mathrm{d}\hat{p} \qquad K_m = \frac{e^{-\alpha_m \hat{p}}}{\beta_m} \qquad \hat{p} = p + s_m \qquad s_m = s + s_o$$

The effect of ionic strength is accounted through osmotic suction

$$s_o = -10^{-6}\frac{RT}{V_w}\ln(a_w)$$

The effect of exchangeable cations is accounted through β_m

$$\beta_m = \sum_i \beta_m^i x_i$$

The effect of the amount of smectite is accounted through the mass fraction of smectite f_s

Dual Structure Constitutive Model: Summary and Future Work

- Dual structure constitutive model for expansive clay has been implemented in TOUGH-FLAC3D and tested with published data.
- Dual structure models has been applied to evaluate the THM behavior in EBS bentonite for a generic repository emplacement tunnel
- In the future dual structure THMC models will be applied for mechanistic modeling of long-term buffer in EBS and clay rock under higher than 100 ^{o}C.
- In the future MC coupling relation to describe effects of cementation on mechanical properties of bentonite (transition from plastic to brittle) will be developed.