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Numerical Implementation of a Multivariable Thermomechanical Model for Unsaturated Bentonite

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Background

- Bentonite clay is planned to be used as a part of the spent nuclear fuel disposal concept in Finland
- Models for and experiments of bentonite are needed to assess the safety of disposal system
- Geological disposal environment is somewhat complex: many phenomena has to be included into the models

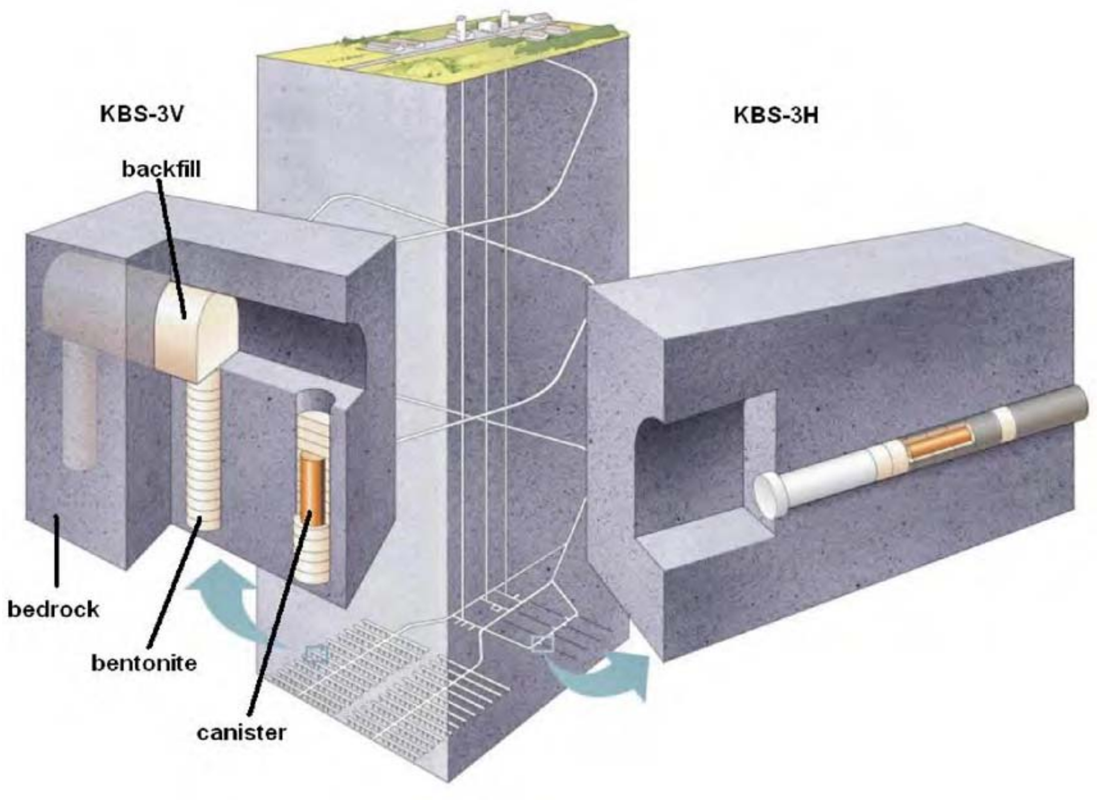
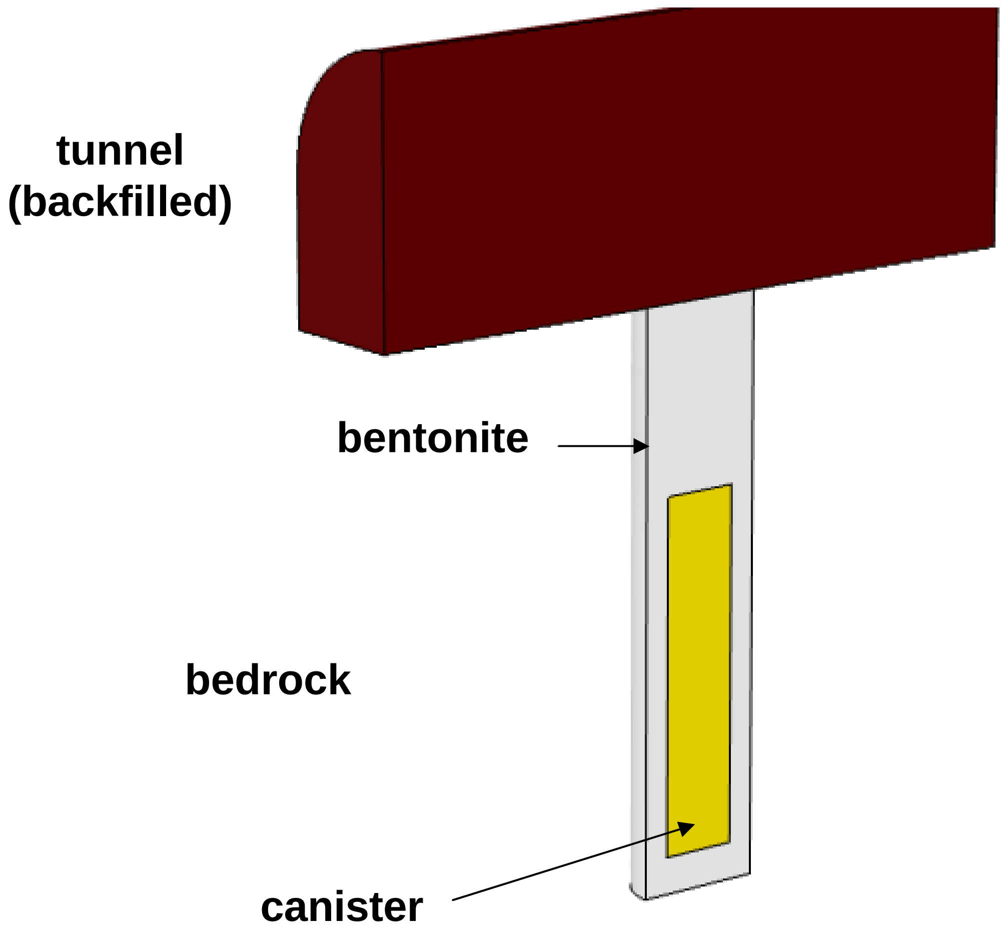


Figure by Posiva Oy (www.posiva.fi)

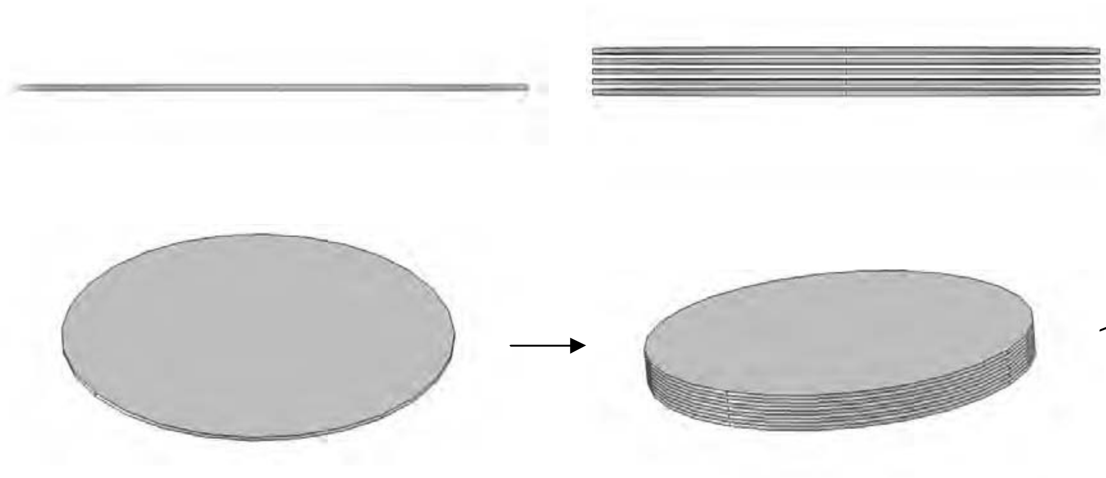
Background (2)



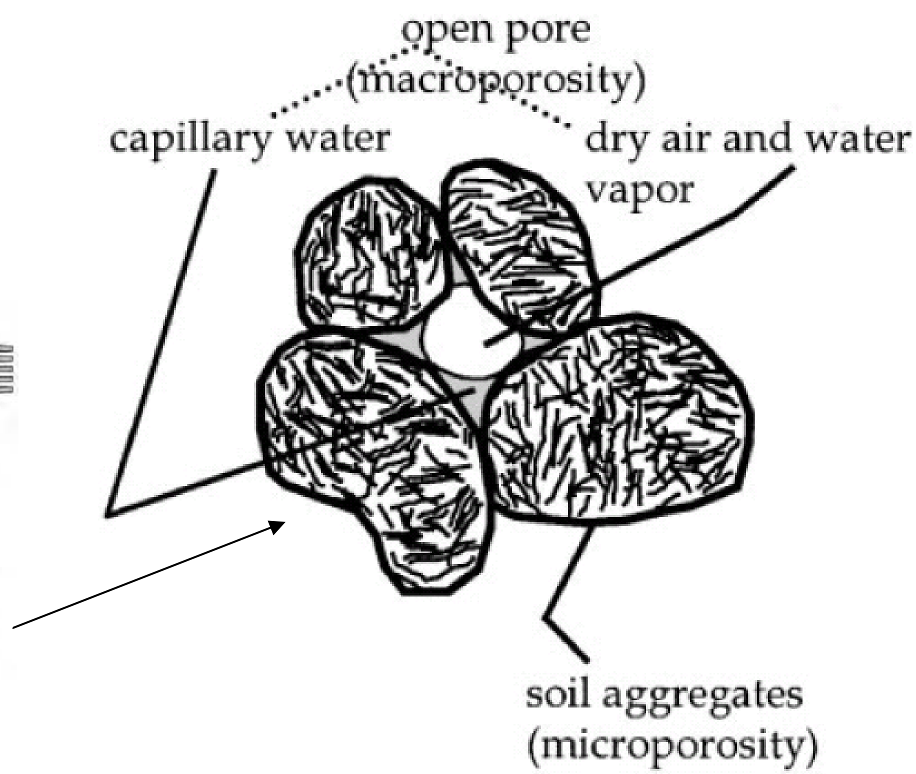
- initially disposal canister is hot (maybe 80-90°C)
- water comes to bentonite unevenly from fractures in bedrock
- almost all boundaries of bentonite are fixed
- tunnel is backfilled with some clay mixture

The structure of bentonite and the constituents in Jussila's model

- solid skeleton
- liquid water
- water vapor
- air



platelet **stack**



Picture by V.Navarro & E.E.Alonso (Modelling swelling clays for disposal barriers, Computers and Geotechics, 27 (2010) p.19-43)

Jussila's model: phenomena

- deformation of the solid skeleton
- movement of liquid water, water vapor and air
- evaparotation of water
- adsorption of water
- the effect of pore water pressure on the deformation of the solid
- heat transfer

all the phenomena are coupled

Energy approach

- the mathematical model has been built such that only free energies of the contituents and a dissipation function have to be defined
- the final constitutive laws can be obtained from the defined free energies and dissipation function
- principle:

dissipation defined by Clausius-Duhem inequality = dissipation defined by principle of maximum entropy production

general contitutive relations

Energy approach (2)

general contitutive relations

+

free energies & dissipation function
(& some equation manipulations and simplifications)

=

final constitutive equations

Free energies and dissipation function

- the chosen free energies cover the free energies of each constituent and the following interactions:
  - mixing of the gaseous constituents
  - adsorption between the liquid and solid constituents
  - swelling between the liquid and solid constituents

- the dissipation function covers the following dissipative processes
  - heat transfer
  - movement of liquid and gaseous phases
  - relative movement of water vapor and air

Final equations(1): balance laws & other equations

- volume fraction restriction $\xi_s + \xi_l + \xi_v + \xi_a = 1$
- continuity of
  - solid mass $\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \mathbf{U}_s) = 0$
  - liquid water $\frac{\partial \rho_l}{\partial t} + \nabla \cdot (\rho_l \mathbf{U}_l) = \theta_l$
  - water vapor $\frac{\partial \rho_v}{\partial t} + \nabla \cdot (\rho_v \mathbf{U}_v) = -\theta_l$
  - air $\frac{\partial \rho_a}{\partial t} + \nabla \cdot (\rho_a \mathbf{U}_a) = 0$

constraints:

$\xi_k \geq 0$ for k=s,l,v,a

- momentum balance $-\nabla \cdot \boldsymbol{\sigma} - \rho_s \mathbf{g} = 0$
- energy balance $(\rho c)_{\text{eff}} \frac{\partial T}{\partial t} - (e_v - e_l)\theta_l - \nabla \cdot (\lambda \nabla T) = 0$
- Clausius-Clapeyron equation

$$\ln \frac{\zeta \hat{B}}{(\zeta \hat{B})_0} = \frac{M_v}{RT}\left[L \frac{T - T_0}{T_0} + (c_v^p - c_l^p) T \ln \frac{T}{T_0} + \frac{\hat{B} - \hat{B}_0}{\tilde{\rho}_l} \right] + \frac{\partial(\xi_l f)}{\partial \xi_l} + \frac{M_v}{\tilde{\rho}_l RT}\left[\xi_s \frac{\partial f_\Pi}{\partial \xi_l} \hat{B}_0 \operatorname{tr}\epsilon + \frac{1}{2} \xi_s \frac{\partial K}{\partial \xi_l} (\operatorname{tr}\epsilon)^2 \right]$$

Final equations(2): constitutive laws

- gaseous phase state equations

$$\hat{B} = \tilde{\rho}_\mathrm{k} \frac{RT}{M_\mathrm{k}} \text{ for } k \in \{\mathrm{a},\mathrm{v}\}$$

- flux of
  - liquid water

$$\rho_\mathrm{l} \mathbf{U}_\mathrm{l} = -\tilde{\rho}_\mathrm{l} \frac{k_\mathrm{l}}{\mu_\mathrm{l}} \Bigg[\nabla\hat{B} - \tilde{\rho}_\mathrm{l}\mathbf{g} + \tilde{\rho}_\mathrm{l} \frac{RT}{M_\mathrm{v}} \nabla \left(\frac{\partial(\xi_\mathrm{l} f)}{\partial \xi_\mathrm{l}} \right) +$$

$$\rho_\mathrm{l} \frac{R}{M_\mathrm{v}} \frac{\partial f}{\partial \xi_\mathrm{l}} \nabla T + \xi_\mathrm{s} \frac{\partial f_\Pi}{\partial \xi_\mathrm{l}} \hat{B}_0 \nabla(\mathrm{tr}\boldsymbol{\epsilon}) + \hat{B}_0 \mathrm{tr}\boldsymbol{\epsilon} \nabla \left(\xi_\mathrm{s} \frac{\partial f_\Pi}{\partial \xi_\mathrm{l}} \right) \Bigg] + \rho_\mathrm{l} \mathbf{U}_\mathrm{s}$$

  - water vapor

$$\rho_\mathrm{v} \mathbf{U}_\mathrm{v} = -\tilde{\rho}_\mathrm{v} (\xi_\mathrm{v} + \xi_\mathrm{a}) D \nabla\zeta - \zeta\tilde{\rho}_\mathrm{v} \frac{k_g}{\mu_g} \nabla\hat{B} + \rho_\mathrm{v} \mathbf{U}_\mathrm{s}$$

  - air

$$\rho_\mathrm{a} \mathbf{U}_\mathrm{a} = -\tilde{\rho}_\mathrm{a} (\xi_\mathrm{v} + \xi_\mathrm{a}) D \nabla\zeta - (1-\zeta)\tilde{\rho}_\mathrm{a} \frac{k_g}{\mu_g} \nabla\hat{B} + \rho_\mathrm{a} \mathbf{U}_\mathrm{s}$$

- stress-strain relation

$$\sigma = 2\xi_\mathrm{s} G \epsilon^D - (\hat{B} - \xi_\mathrm{s} K \mathrm{tr}\epsilon - \xi_\mathrm{s} f_\Pi \hat{B}_0) \mathbf{I}$$

- heat flux

$$\mathbf{q} = -\lambda \nabla T$$

- evaporation energy

$$e_\mathrm{v} - e_\mathrm{l} = l_0 + (c_\mathrm{v}^p - c_\mathrm{l}^p)(T - T_0) - RT / M_\mathrm{v}$$

Final equations(3): material parameters

- adsorption function

$$f = \begin{cases} a_1 \left(\frac{\xi_s}{\xi_l} - \left(\frac{\xi_s}{\xi_l} \right)_0 \right)^{a_2} & \text{for } \frac{\xi_s}{\xi_l} \le \left(\frac{\xi_s}{\xi_l} \right)_0 \\ 0 & \text{for } \frac{\xi_s}{\xi_l} > \left(\frac{\xi_s}{\xi_l} \right)_0 \end{cases}$$

- swelling function

$$f_\Pi = a_3 \left(\frac{\xi_\text{s}}{xi_\text{l}} \right)^2 + a_4 \left(\frac{\xi_\text{s}}{xi_\text{l}} \right) + a5$$

- mechanical parameters

$$K = K_\text{init} \left(\frac{\xi_\text{s} / \xi_\text{l}}{(\xi_\text{s} / \xi_\text{l})_\text{init}} \right)^b \qquad E = 3(1-2\nu)K \qquad G = E / (2(1+\nu))$$

- permeabilities

$$k_j = k_{j,\text{rel}} k_\text{sat} \qquad k_\text{l,rel} = \xi^n \qquad k_\text{g,rel} \approx \text{constant}$$

- viscosities

$$\mu_\text{l} = 2.1 \cdot 10^{-6} \frac{\text{kg}}{\text{sm}} e^{\frac{1808.5\text{ K}}{T}} \qquad \mu_g = 1.48 \cdot 10^{-6} \frac{\text{kg}}{\text{sm}} \frac{\sqrt{T / 1\text{K}}}{1 + (119.4\text{K}) / T}$$

- diffusion coefficient

$$D = D_\text{ref} \left(\frac{T}{T_\text{ref}} \right)^\alpha$$

- heat related parameters

$$\lambda = \lambda_\text{sat} + (\lambda_\text{dry} - \lambda_\text{sat}) / (1 + e^{(\chi - \chi')/dx})$$

$$(\rho c)_\text{eff} \approx \rho_\text{l} c_\text{l}^v + \rho_\text{dry} c_\text{s}^v$$

$$c_\text{s}^v = 1.38 \frac{\text{J}}{\text{kgK}^2} (T - 273.15\text{K}) + 732.5 \frac{\text{J}}{\text{kgK}}$$

Use of COMSOL Multiphysics

- Structural mechanics module for momentum balance equation
  - modified bulk and shear moduli + use of weak contribution
- General Form PDEs for rest of the equations
- Solution strategy:
  1. solve energy equation, Clausius-Clapeyron equation, liquid, vapor and air mass balances as fully coupled problem
  2. solve momentum and mass balance equations
- Solvers:
  - time dependent solver: implicit Euler (1st order BDF)
  - nonlinear solver: Newton with high number of iterations
  - linear solver: MUMPS

Current status

- The implementation of the model is on test stage
- The progress is somewhat slow because the development of the model is an extra project currently
- We have come to a conclucion that the conceptual and the mathematical model require some modifications and extensions to describe the behaviour of bentonite in the parameter scale that we want
  - Therefore, we have to do some theoretical work before we continue the implementation
  - by theoretical work, we mean inclusion of some micro-scale phenomena