KYT 2018: Bentonite investigations

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Bentonite!

Safety case

- Canister performance
- Microbiological effects
- Buffer and backfill performance
- Other coordinated projects?
- Other safety studies

Long-term safety of nuclear waste management
THEBES goals

Experimental research → Data for modelling → Creation & validation of numerical models → Implementation into numerical software → Case studies

feedback loop

Soft clay barriers: thermo – hydro – mechanical – chemical coupling
Outline

I. Introduction & overview
II. Research at Aalto
Bentonite

Highly compacted bricks, made of dry bentonite, used to construct a barrier preventing possible contamination.
Bentonite

Dry compacted bentonite bricks swell if wetted, hopefully leading to a self-healing and impermeable barrier.

© Villar, 2016
Bentonite behaviour is complex and to predict it reliably we need to understand the physical processes which leads to the observable macroscopic behaviour.
Bentonite behaviour is complex and to predict it reliably we need to understand the physical processes which leads to the observable macroscopic behaviour.
Bentonite - microstructure

Forces acting in bentonite:

**Macroscale:** forces from mechanical loading

**Meso:** capillary forces due to water menisci between aggregates

**Micro:** Forces within laminae of clay minerals (mainly montmorillonite) – inter-particle distance exceeds ~30-40 Å van der Waals attraction & electric repulsion on atomic level

inter-particle distance below ~10-20 Å – electric repulsion on atomic level

© Santamarina, 2001
Bentonite swelling

1. Number of Montmorillonite platelets in a pile decrease, spacing between them increase.

Interlaminar porosity increases.

Some swelling occurs.

More water in the smallest pores

© Villar, 2016

© Villar, 2016

formation of several particles

inside the saturated aggregates

particle size or thickness

initial particle

inter-layer space

inter-particle space

d₁ < d₂

high suction (> 50 MPa)
100 layers

low suction (< 7 MPa)
10 layers

Saiouri, Hicher & Tessier (2000)
Bentonite - microstructure

**MX 80 clay**

\[ \rho = 2 \text{ Mg/m}^3 \]

**SAMPLE AT HIGHER WATER CONTENT AND LOWER SUCTION HAS MORE WATER LOCATED IN VERY SMALL pores (< 35 nm)**
Bentonite swelling

2. Size of the aggregates changes. They become also more easy to break. Double porosity structure slowly disappears

Interlaminar porosity still increases.

More some swelling occurs.

© Delage et al. 2006
Bentonite swelling: montmorillonite water absorption

3. Amount of water between layers of montmorillonite changes

Additionally, the swelling is affected by the mesoscale – size of the aggregates changes and capillary forces make a difference

© Delage, 2015
© Sayiouri et al. 2000
Bentonite swelling

4. Swelling pressure is affected by the mechanical, thermal, conditions, as well as availability of water and water composition (e.g. salinity).

Similarly, the number of layers / volume change is different for different mechanical conditions: complex thermo-hydro-mechanical-chemical coupling

© Delage, 2015
Water transport

Due to complex microstructure, water transport is complex, mixture of transport via vapour and liquid.

Also highly temperature dependent

Necessary to predict swelling, as swelling depends on amount of water available.

Prediction in time is crucial, as material is affected by stress history
Temperature

Temperature affects forces between particles, both in microscale, as well as mesoscale.

Therefore the material properties are temperature dependent.

Thermal conductivity non-linear and coupled to water & mechanical properties

Prediction in time is crucial, as material is affected by stress history

© Tang et al., 2008

THEBES: KYT project investigating bentonite
Water salinity affects the hydraulic behaviour of bentonite, as well as mechanical properties. It also affects the swelling of bentonite aggregates and generally lowers the swelling pressure.
Salinity effects

Water in liquid phase transport salt, but water vapour not! In non-isothermal condition creation of high saline zones (zone reached wetted by liquid water which evaporates) likely. Effects on material being investigated.
Outline

I. Introduction & overview
II. Research at Aalto
   I. THMC modelling of bentonite / swelling clays
Thermo-hydro-mechanical FE framework

Taking into account well established laws of physics and thermodynamics

**mechanical**: amended BBM, models by della Vecchia et al. (2013, 2014, 2015), new models which take into account micro and macro structure of bentonite are in development

**hydraulic**: number of models for water retention, Philip & De Vries model for vapour transport, extended Darcy law for liquid water transport, Henry’s law for solubility of water, phase changes and heat effects are taken into account

**thermal**: heat flux in solid, water and gas phases, full energy balance / coupling

Some experiments on water retention behaviour of MX80 bentonite and its microstructure in saline solutions leading to inclusion of those into modelling (chemical coupling)
A study on how to couple thermo-hydro-mechanical behaviour of unsaturated soils: Physical equations, numerical implementation and examples

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1. Introduction

In some engineering applications the understanding of unsaturated soil behaviour becomes vitally important and necessary for an effective design. A pronounced example is the case of bentonite which is the material of choice for engineering barriers due to its very low permeability, effective resistance to chemicals and swelling behaviour upon wetting. For instance, bentonite is used as barriers for nuclear waste disposal sites where safety specifications are especially strict [1,2]. Ideally, barriers should be nearly impermeable, self-sealing (i.e. the influence of cracks and initial imperfections is eliminated) and possess properties such that the surrounding environment remains unaffected by radionuclide and chemical contamination. The design of the containment is governed by the behaviour of concrete materials for a very long time, typically tens of thousands of years. A suitable barrier material design requires prediction of complex behaviour under high temperature gradient, hydraulic processes and development of gas pressure. The development of numerical analysis methods requires prediction of the swelling and deformation properties obtained due to swelling upon wetting and high pressure state in the material. Nonetheless, the developed swelling pressure should not be too high, as that could adversely affect the containers for the nuclear material. Finally, the material is also affected by radioactivity and chemical reactions, though these factors are not included in this study.

A significant body of research has been devoted to the study of swelling mechanisms and its effect on the mechanical properties of bentonite. This paper presents a physical framework which can be employed to include chemical effects and radioactivity effects. The framework is general and suitable for unsaturated soils and geomaterials. It can also be used for porous materials, as each constitutive equation can be easily replaced by another formulation more suitable for a given application.

Experience gained in different scientific disciplines [3,5-8] suggests that the framework method is one of the best methods to numerically solve such a coupled system of equations. This study presents in details the coupled physical formulations, element discretization and implementation of the thermo-hydro-mechanical equations governing the behaviour of porous geomaterials. This paper also describes verification and validation against analytical solutions, well-established THM code (CODE_BRIGHT [11]) results, and experimental data. The numerical results are satisfactory from the point of view of checking theoretical solutions and approaching real physical behaviour.
Thermo-hydro-mechanical FE framework

Barcelona Basic Model (Alonso et al. 1990)
Thermo-hydro-mechanical FE framework

**mechanical:** BBM (Alonso et al. 1990)

<table>
<thead>
<tr>
<th>parameter</th>
<th>$\kappa$ (-)</th>
<th>$\kappa_s$ (-)</th>
<th>$k$ (-)</th>
<th>$G$ (MPa)</th>
<th>$\beta$ (MPa$^{-1}$)</th>
<th>$r$ (-)</th>
<th>$\lambda(0)$ (-)</th>
<th>$p^c$ (kPa)</th>
<th>$M$ (-)</th>
<th>$N(0)$ (-)</th>
<th>$p_0^*$ (kPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>value</td>
<td>0.02</td>
<td>0.117</td>
<td>0.08</td>
<td>10.1</td>
<td>0.05</td>
<td>0.20</td>
<td>0.5</td>
<td>41</td>
<td>0.5</td>
<td>6.36</td>
<td>variable</td>
</tr>
<tr>
<td>accuracy</td>
<td>+0.005</td>
<td>+0.10</td>
<td>+0.0</td>
<td>±0.5</td>
<td>+0.5</td>
<td>+0.2</td>
<td>+0.0</td>
<td>±30</td>
<td>+0.1</td>
<td>±0.5</td>
<td>–</td>
</tr>
</tbody>
</table>

**parameters established based on:**
- Villar (2005), Ciemat technical report, CIEMAT/DIAE/54540/5/04
- Dueck and Nilsson (2010), SKB Technical report, TR-10-32

Porté, Abed & Sołowski (in preparation)
Thermo-hydro-mechanical FE framework

**Mechanical:** amended BBM – enhanced for temperature effects

\[ p_{oT}^* = p_0^* + 2(\alpha_1 \Delta T + \alpha_3 \Delta T |\Delta T|) , \]

Gens (1995)

or

\[ p_{oT}^* = p_0^* \left( 1 - \gamma_T \log \left( \frac{T - T_{ref}}{T_0 - T_{ref}} \right) \right) \]


**Changes in elasticity:**

\[ \dot{\varepsilon}_e^T = \frac{(\alpha_o + \alpha_2 (T - T_0)) \dot{T}}{3} \]

\[ \kappa = \kappa_o (1 + \alpha_\kappa s) \]

**Salinity effects on mechanical behaviour:** in progress

Abed & Sołowski (2017)
Thermo-hydro-mechanical FE framework

**hydraulic**: number of models for water retention, Philip & De Vries model for vapour transport, extended Darcy law for liquid water transport, Henry’s law for solubility of air, phase changes and heat effects are taken into account. Also gas flow.

Advective liquid and gas flow (transport due to head difference):

\[
q^l = -K_l(\nabla h_w + 1)
\]

**Liquid phase**

\[
K_l = K_{sat} \left( \frac{S^l - S_{res}^l}{S_{sat}^l - S_{res}^l} \right)^3
\]

\[
k_{sat}^l = k_{ref}^l \frac{n^3}{(1 - n)^2} \left( \frac{1 - n_{ref}}{n_{ref}^3} \right)
\]

\[
K_{sat} = \frac{g \rho_w^l k_{sat}^l}{\mu_l}
\]

\[
\mu_l = (243.18 \times 10^{-7})10^{\frac{247.8}{140 - T}}
\]

\[
q^g = -K_g \left( \nabla h_g + \frac{\rho_g}{\rho_w^l} \right)
\]

**gas phase**

Abed & Sołowski (2017)
Thermo-hydro-mechanical FE framework

**hydraulic:** number of models for water retention, Philip & De Vries model for vapour transport, extended Darcy law for liquid water transport, Henry’s law for solubility of air, phase changes and heat effects are taken into account. Also gas flow.

Advective liquid and gas flow:

\[
q^g = -K_g \left( \nabla h_g + \frac{\rho^g}{\rho_w} \right)
\]

**gas phase**

\[
K^g = K_{dry}^g \left( \frac{S^g - S_{res}^g}{S_{dry}^g - S_{res}^g} \right)^3
\]

\[
K_{dry}^g = \frac{g \rho_w k_{dry}^g}{\mu_g}
\]

\[
\mu_g = 1.48 \times 10^{-6} \frac{\sqrt{T}}{1 + \frac{119}{T}}
\]

**Abed & Sołowski (2017)**

THEBES: KYT project investigating bentonite
Thermo-hydro-mechanical FE framework

Hydraulic: number of models for water retention, Philip & De Vries model for vapour transport, extended Darcy law for liquid water transport, Henry’s law for solubility of air, phase changes and heat effects are taken into account. Also gas flow.

Philip & De Vries: also non-advective flow of water vapour

\[
\begin{align*}
{j_w^g} &= j_{vw}^g + j_{vT}^g = -D_{vw} \nabla h_w + D_{vw} \nabla h_g - D_{vT} \nabla T \\
&\quad \text{moisture term} \quad \text{temperature term}
\end{align*}
\]

\[
D_{vw} = D_{atm} v_v \phi^g \tau \rho_w^g \frac{gM_w}{RT}
\]

\[
D_{vT} = f_{Tv} D_{atm} v_v \phi^g \tau \rho_w^g \left[ \frac{4974.0}{T^2} + \frac{gM_w \psi}{RT^2} \right]
\]

\[
D_{atm} = 2.2 \times 10^{-5} \left( \frac{P_{atm}}{P_g} \right) \left( \frac{T}{T_o} \right)^{1.75}
\]

Abed & Sołowski (2017)
Thermo-hydro-mechanical FE framework

**hydraulic:** number of models for water retention, Philip & De Vries model for vapour transport, extended Darcy law for liquid water transport, Henry’s law for solubility of air, phase changes and heat effects are taken into account. Also gas flow.

Henry’s law

\[ H = \frac{\rho_w^l \, RT}{H_c \, M_w} \]

\[ \frac{\partial H}{\partial t} = g \rho_w^l \beta_{wp} H \frac{\partial h_w}{\partial t} + \left( \frac{1}{T} - \beta_{wt} \right) H \frac{\partial T}{\partial t} \]

**Coupling:**

Formulation include mass balance for the phases and changes in density due to all the factors. Coupling due to saline concentration is being developed.

Abed & Sołowski (2017)
Thermo-hydro-mechanical FE framework

coupling: mass balance of solid, liquid and dry air

solid:

\[
\frac{\partial (\phi^s \rho^s)}{\partial t} + \nabla \cdot (\phi^s \rho^s \mathbf{v}^s) = 0,
\]

\[
\rho^s = \rho^{s_0} e^{\beta_{sp}(p - p^{ref}) - \beta_{st}(T - T_0)},
\]

\[
\frac{\partial \rho^s}{\partial t} = \frac{\partial \rho^s}{\partial p} \frac{\partial p}{\partial t} + \frac{\partial \rho^s}{\partial T} \frac{\partial T}{\partial t} = \beta_{sp} \rho^s \frac{\partial p}{\partial t} - \beta_{st} \rho^s \frac{\partial T}{\partial t}
\]

\[
\frac{\partial n}{\partial t} = (1 - n) \left( \frac{\partial \varepsilon_v}{\partial t} + \beta_{sp} \frac{\partial p}{\partial t} - \beta_{st} \frac{\partial T}{\partial t} \right)
\]

Abed & Sołowski (2017)
Thermo-hydro-mechanical FE framework

coupling: mass balance of solid, liquid and dry air

\[
\begin{align*}
\frac{\partial (\phi^l \rho^l \omega^l_w)}{\partial t} + \nabla \cdot (\phi^l \rho^l \omega^l_w \mathbf{v}^l_l) + \nabla \cdot j^l_w & \quad \text{water in liquid phase} \\
\frac{\partial (\phi^g \rho^g \omega^g_w)}{\partial t} + \nabla \cdot (\phi^g \rho^g \omega^g_w \mathbf{v}^g) + \nabla \cdot j^g_w & \quad \text{water in gas phase} \\
\end{align*}
\]

\[
\begin{bmatrix}
\begin{align*}
n(\rho^l_w - \rho^g_w) \frac{\partial S^l}{\partial T} - (1 - n)(S^l \rho^l_w + S^g \rho^g_w)\beta_{ST} - nS^l \beta_{WT} \rho^l_w
\end{align*}
\end{bmatrix}
\]

Abed & Sołowski (2017)
Thermo-hydro-mechanical FE framework

coupling: mass balance of solid, liquid and dry air

dry air:

\[
\frac{\partial (\phi^l \rho^l \omega_a^l)}{\partial t} + \nabla \cdot (\phi^l \rho^l \omega_a^l \mathbf{v}^l) + \nabla \cdot \mathbf{j}^l_a + \frac{\partial (\phi^g \rho^g \omega_a^g)}{\partial t} + \nabla \cdot (\phi^g \rho^g \omega_a^g \mathbf{v}^g) + \nabla \cdot \mathbf{j}^g_a + \nabla \cdot \mathbf{j}^d_a = 0
\]

dissolved dry air in liquid phase

dry air in soil voids

dry air in solid phase

\[
\begin{bmatrix}
\begin{align*}
n \rho_a [H - 1] \frac{\partial S^l}{\partial T} + n \rho_a S^l \frac{\partial H}{\partial T} - (1 - n) \rho_a [S^g + H S^l] \beta_{ST}
\end{align*}
\end{bmatrix}
\]
Thermo-hydro-mechanical FE framework

Thermal:

heat capacity:

$$\Phi_h = \phi^i \rho^i \omega_k^i E_{Tk}^i \quad E_{Tk}^i = c_k^i (T_k^i - T_{ko}^i)$$

$$\Phi_h = [(1 - n)\rho^s c_s + n(HS^l + S^g)\rho_a c_a + nS^l \rho_w^l c_w^l + nS^g \rho_w^g c_w^g] (T - T_o)$$

heat flux:

$$q_h = \begin{pmatrix} q_T \end{pmatrix}^{T} + \begin{pmatrix} \rho^i \omega_k^i E_{Tk}^i q^i \end{pmatrix}^{T} + \begin{pmatrix} E_{Tk}^i j_w^i \end{pmatrix}^{T}$$

$$q_h = -\lambda_T \nabla T + [(\rho_a c_a + \rho_w^g c_w^g) q^g + (\rho_w^l c_w^l + \rho_a c_a H) q^l] (T - T_o) + [c_w^g - c_a] j_w^g (T - T_o)$$

Abed & Sołowski (2017)
Thermo-hydro-mechanical FE framework

Energy balance: very complex

\[ \nabla \cdot q_h = -\lambda_T \nabla \cdot \nabla T + \left[ (\rho_a c_a + \rho_w^g c_w^g) \right] (T - T_o) \nabla \cdot q^g + \left[ (\rho_a c_a + \rho_w^g c_w^g) \right] q^g \cdot \nabla T \]
\[ + \left[ (\rho_w^l c_w^l + \rho_a c_a H) \right] (T - T_o) \nabla \cdot q^l + \left[ (\rho_w^l c_w^l + \rho_a c_a H) \right] q^l + \left[ c_w^g - c_a \right] j_w^g \cdot \nabla T \]
\[ + \left[ c_w^g - c_a \right] (T - T_o) \nabla \cdot j_w^g \]

\[ A = [-\rho^s c_s + HS^l \rho_a c_a + S^g \rho_a c_a + S^l \rho_w^l c_w^l + S^g \rho_w^g c_w^g] (T - T_o) \]

\[ B = [ (1 - n) \rho_s c_s ] (T - T_o) \]

\[ C = [ H \rho_a c_a - \rho_a c_a + \rho_w^l c_w^l - \rho_w^g c_w^g ] (T - T_o) \]

\[ D = n [ HS^l \rho_a c_a + S^g \rho_a c_a + S^l \rho_w^l c_w^l + S^g \rho_w^g c_w^g ] + (1 - n) \rho^s c_s \]

Abed & Sołowski (2017)
Thermo-hydro-mechanical FE simulations

![Graph showing the relationship between void ratio and isotropic net stress](image)

- **Alonso et al. (1990)**
- **Current BBM implementation in Numerrin**

**Abed et al. (2016)**

THEBES: KYT project investigating bentonite
Thermo-hydro-mechanical FE simulations

![Graph showing deviatoric stress vs. shear strain]

- Alonso et al. (1990)
- Current BBM implementation in Numerrin

Abed et al. (2016)
Thermo-hydro-mechanical FE simulations

Abed & Sołowski (2017)

Infiltration for 5 days

Close boundary

3.0 m

Groundwater table

Initial hydrostatic condition

Analytical solution by Srivastava et al. (1991)

Current implementation in Numerrin

Abed & Sołowski (2017)
Replication of data from Jyväskylä University

Abed et al. (2016)
Thermo-hydro-mechanical FE simulations

Infiltration test, Villar (2005)

Abed & Sołowski, (2017)
Thermo-hydro-mechanical FE simulations

Infiltration test, Villar (2005)

Abed & Sołowski, (2017)
Thermo-hydro-mechanical FE simulations

No perfect match between codes due to different water vapour transport models

Abed & Sołowski, (2017)
Thermo-hydro-mechanical FE simulations

non-isothermal infiltration

Abed & Sołowski, (2017)
Thermo-hydro-mechanical FE simulations

The effect of swelling on the water hydraulic conductivity

non-isothermal infiltration

Abed & Sołowski, (2017)
FE simulations: CIEMAT Mock-Up test

Example: Simulation of CIEMAT Mock-Up test for 2500 days (Martin et al. 2006)
The hydro-thermal coupling is based on the theory proposed by Philip & De Vries (1957).

Abed & Sołowski (2017)
FE simulations: CIEMAT Mock-Up test

Example: Simulation of CIEMAT Mock-Up test for 2500 days (Martin et al. 2006)
The hydro-thermal coupling is based on the theory proposed by Philip & De Vries (1957).

Abed & Sołowski (2017)
FE simulations: CIEMAT Mock-Up test

Example: Simulation of CIEMAT Mock-Up test for 2500 days (Martin et al. 2006)
The hydro-thermal coupling is based on the theory proposed by Philip & De Vries (1957).

Abed & Sołowski (2017)
FE simulations: CIEMAT Mock-Up test

Calculated relative humidity versus measurements

Relative humidity [%]

Time [days]

- RH1 (0.22, 1.0)
- RH2 (0.37, 1.0)
- RH3 (0.55, 1.0)
- RH4 (0.7, 1.0)
- Aalto Code

Abed & Sołowski (2017)
FE simulations: CIEMAT Mock-Up test

Calculated temperature versus measurements

Time [days]

Abed & Sołowski (2017)
FE simulations: CIEMAT Mock-Up test

Calculated swelling pressure versus measurements

Abed & Sołowski (2017)
FE simulations: CIEMAT Mock-Up test

Calculated water intake versus measurements

- Water intake measurements
- Aalto Code

Abed & Sołowski (2017)
FE simulations: CIEMAT Mock-Up test

Aalto Code prediction after a duration of 2500 days of the test
References:


Outline

I. Introduction & overview (15 min)

II. Research at Aalto
   I. THMC modelling of bentonite / swelling clays
   II. Investigation of effects of salinity on bentonite
Water retention behaviour of MX-80 bentonite

Aim: find out what is the influence of salinity on water retention behaviour of MX-80 bentonite

Lahtinen et al. 2016
Water retention behaviour of MX-80 bentonite

Aim: find out what is the influence of salinity on water retention behaviour of MX-80 bentonite.

Water retention curve of Mx-80

Yang & Sołowski (in preparation)
Water retention behaviour of MX-80 bentonite

Aim: find out what is the influence of salinity on water retention behaviour of MX-80 bentonite

Yang & Sołowski (in preparation)
Water retention behaviour of MX-80 bentonite

Aim: find out what is the influence of salinity on water retention behaviour of MX-80 bentonite

Yang & Sołowski (in preparation)
Water retention behaviour of MX-80 bentonite

Aim: find out what is the influence of salinity on water retention behaviour of MX-80 bentonite

Yang & Sołowski (in preparation)
Water retention behaviour of MX-80 bentonite

Microstructure characterization (note: issues in the test – higher pressure needed! – work in progress)
Water retention behaviour of MX-80 bentonite

Microstructure based model: Dieudonné et al. (2013)

PSD model after fitting on Boom clays experimental data (Dieudonné et al., 2013)

Porté, Abed & Sołowski (in preparation)
Water retention behaviour of MX-80 bentonite

Microstructure based model: Dieudonné et al. (2013)

Pore size distribution curve of Mx-80 bentonite (after Seiphoori et al., 2014)

Porté, Abed & Sołowski (in preparation)
Water retention behaviour of MX-80 bentonite

Microstructure based model: Dieudonné et al. (2013)

PSD test and calibrated model for Mx-80 bentonite which has a degree of saturation of 0.62.

Porté, Abed & Sołowski (in preparation)
Water retention behaviour of MX-80 bentonite

Microstructure based model: Dieudonné et al. (2013)

Calibrated water retention curve of Mx-80 compared with the tests used for the calibration process.

Porté, Abed & Sołowski (in preparation)
Water retention behaviour of MX-80 bentonite

Microstructure based model: Dieudonné et al. (2013)

Calibrated water retention curve of Mx-80 compared with the test made by the Aalto University with the WP4C instrument (after Yang and Sołowski, in preparation)

Porté, Abed & Sołowski (in preparation)
Water retention behaviour of MX-80 bentonite

• Dieudonné et al. 2013 is now available in the FE code now, so calculations will follow

• Constitutive models which incorporate micro- and macrostructure are being implemented (or are available already) in the FE code

• Salinity effects are being implemented

• Better microstructural investigations of salinity effects are thought of
Thank you !!!

Presentation will be uploaded and available at http://solowski.info and THEBES website
THEBES

THMC Behaviour of the Swelling Clay Barriers

Questions?