HYDRO-MECHANICAL MODELLING OF BENTONITE-BASED MATERIALS

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Motivations

In most concepts, bentonite-based materials will be used for sealing and backfilling of the excavated shafts, galleries and boreholes.

Bentonite is a natural material which primarily consists of montmorillonite (clay mineral).

Objectives:

- Limit water flow around the excavated galleries
- Delay the release of radionuclides to the biosphere
Motivations

Bentonite-based materials are used because of their:

1) Significant swelling upon hydration = swelling capacity

- **Swelling potential** = relative change of volume experienced upon wetting under unconfined conditions
  \[
  \frac{\Delta V}{V_0} = \frac{V - V_0}{V_0}
  \]

- **Swelling pressure** = pressure developed upon wetting under confined conditions
  \[S_p\]
Motivations

Bentonite-based materials are used because of their:

1) Significant swelling upon hydration = swelling capacity

2) Very low permeability (~ $10^{-20} - 10^{-21} m^2$ in saturated conditions)
Motivations

Bentonite-based materials are used because of their:

1) Significant swelling upon hydration = swelling capacity

2) Very low permeability ($\sim 10^{-20} - 10^{-21} \ m^2$ in saturated conditions)

3) Important radionuclides retardation capacities
Motivations

Objectives of the PhD: develop a hydromechanical model for the behaviour of compacted bentonite-based materials under *in situ* conditions.

- Buffer hydration
- Buffer swelling
- Desaturation of the host rock?
- Technological gap closure
- Swelling conditions evolve from *free swelling* to *constrained volume*.
- Host formation recompression

These processes are modelled using the finite element code **LAGAMINE**.
Outline of the presentation

Microstructure

Water retention behaviour

Mock-up test

Towards larger scales ...
Outline of the presentation

Microstructure

Water retention behaviour

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Towards larger scales ...
Microstructure of compacted bentonite

Compaction of bentonite creates a **double-porosity structure**.

Lloret et al. (2003)  
Wang et al. (2013)
Microstructure of compacted bentonite

Compaction of bentonite creates a double-porosity structure.

Lloret et al. (2003)
Microstructure of compacted bentonite

Clay aggregates are clusters of clay particles. It is at this scale that swelling occurs!

- Montmorillonite layers are electronegative
- The natural tendency is to ensure electroneutrality
- Hydrated cations and water molecules are attracted in the interlayer
Microstructure of compacted bentonite

Clay layers are sensitive to water.

- Hydration of bentonite-based materials yields important structural changes!

Seiphoori et al. (2014)
Microstructure of compacted bentonite

We want to **quantify** these processes to include information from the microstructure in constitutive models!

- Interpretation of a large number of pore-size distribution curves
- Micro-void ratio

\[
e_m = \frac{\text{volume of micropores}}{\text{volume of solids}}
\]

is **only a function of the water content**!
Outline of the presentation

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Towards larger scales ...
The water retention curve: \[ \text{amount of water stored} = f(\text{suction...}) \] (generally a unique relationship !)

- **Degree of saturation**
  \[ S_{rw} = \frac{\text{volume of water}}{\text{volume of voids}} \]

- **Water content**
  \[ w = \frac{\text{mass of water}}{\text{mass of solids}} \]

- **Water ratio**
  \[ e_w = \frac{\text{volume of water}}{\text{volume of solids}} \]
Experimental observations

\[ w = \frac{M_w}{M_S} \]

Gatabin et al. (2006), Wang et al. (2013)
Experimental observations

\[ \rho_d = 2.04 \text{ Mg/m}^3 \]

Confined conditions

Unconfined conditions

\[ S_r = \frac{V_w}{V_v} = \frac{e_w}{e} \]

A unique relationship cannot be defined!
Experimental observations

Competing effects of
- Water uptake
- Swelling

Need for a WR model capable of interpreting these data within a unified framework

\[ S_r = \frac{V_w}{V_v} = \frac{e_w}{e} \]
Water retention model

Equilibrium of suction is assumed between the structural levels

\[ e_w = S_r \cdot e = e_{wm} + e_{wM} \]

- **Intra-aggregate porosity**
- **Inter-layer porosity**
- **Adsorbed water**
- **Inter-aggregate porosity**

**“Capillary” water**

**“Van-Genuchten” model**

\[ e_{WM}(s, e, e_m) = (e - e_m) \left[ 1 + \left( \frac{s}{a} \right)^n \right]^{-m} \]

- Number of parameters:
  - Microstructure: 3 (2)
  - Microstructure WR model: 2
  - Macrostructure WR model: 3 (1)
Water retention model

« van Genuchten » model:  \( e_{WM}(s, e, e_m) = (e - e_m) \left[ 1 + \left( \frac{s}{a} \right)^n \right]^{-m} \)

- The water retention curve is density-dependent
- The effect of density is included in the parameter \( a \) (« air-entry » value)

\[
a = \frac{A}{e - e_m}
\]
Model validation

Hydration under **confined conditions** of bentonite compacted to **different dry densities**
Model validation

Hydration under **unconfined conditions** of high-density compacted bentonite
Model validation

Microstructure evolution under confined and unconfined conditions
The equations to solve are:

\[ e_w = e_w(s, e, e_m) \]

and

\[ e_m = e_m(e_w) \]

Suction \( s \) and void ratio \( e \) are given as input of the routine (pore pressure and total deformations).

A bisection method is used to solve the system of non-linear equations:

\[ e_w \in [0, e] \equiv S_r \in [0,1] \]

Severe convergence criterion required to achieve good convergence of large and strongly coupled problems BUT the time spent in to solve the model <<<<<< time required to solve the global problem.
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Towards larger scales ...
Infiltration test

Infiltration column test (Wang et al. 2013)

- H = 250 mm
- D = 50 mm

- Initial conditions:
  - w = 11%
  - $\rho_d = 1.67 \text{ Mg/m}^3$

- Hydration from bottom at $p_{atm}$

- Relative humidity (RH) monitoring
Multiphase flow model

Water in **liquid** and **vapour phases**

\[ f_w = \rho_w q_l + i^g_w \]

- **Liquid advection**: Generalized Darcy’s law:
  \[ k_{rw} = (S_r)^n \]
  \[ q_l = -\frac{k_{rw}K_w}{\mu_w}(\nabla u_w + \rho_w g) \]
  \[ n = \text{fitting parameter} \]
  \[ k_{rw} = 1.3 \times 10^{-20} \text{ m}^2 \]  
  (Gatabin et al. 2006)

- **Vapour diffusion**: Fick’s law

\[ i^g_w = -\phi(1 - S_r)\tau D^g_w \rho_g \nabla \left( \frac{\rho_v}{\rho_a} \right) \]

\[ \phi = 0.007 \]  
(estimated from effective gas diffusion coefficient)
Numerical results (uncoupled)

Uncoupled modelling (H)

\[ k_{rw} = (S_r)^{3.4} \]
Mechanical model

Barcelona Basic Model (Alonso et al. 1990)

\[
\begin{align*}
\delta \varepsilon & = \nu s + \varepsilon d s + \varepsilon p a t \\
q^2 + M^2 (p + p_s(s))(p - p_0(s)) &= 0
\end{align*}
\]

\[
d \varepsilon_v^e(p) = \frac{\kappa}{1 + e/p} dp
\]

\[
d \varepsilon_v^e(s) = \frac{\kappa_s}{1 + e s + p_{at}} ds
\]
Mechanical model

Barcelona Basic Model (Alonso et al. 1990)

Calibration on controlled-suction oedometer tests (Wang et al. 2013)
Numerical results (coupled)

Coupled modelling (HM)

\[ K_w = 1.3 \times 10^{-20} \text{ m}^2 \]
Numerical results (coupled)

Coupled modelling (HM)

\[ K_w = K_0 \frac{(1-\phi_M)^3}{(\phi_M)^2} \frac{(\phi_M)^2}{(1-\phi_M)^3} \text{ m}^2 \]

Experimental data
- RH1
- RH2
- RH3
- RH4

Model predictions
- RH1
- RH2
- RH3
- RH4

Relative humidity, RH: %

Time, t: hour
Numerical results (coupled)

- Modeled swelling pressure
- Measured swelling pressure
- Modeled injected water volume
- Measured injected water volume
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Conclusions

- Bentonite-based materials are characterized by a double-porosity structure. This structure evolves upon hydraulic and mechanical wetting.

- In this work, the microstructure is characterized by the volume of micropores.

- A water retention model (saturation – suction) is developed accounting for
  - The different water retention mechanisms
  - The evolution of the microstructure.

- This model is used to model the hydromechanical behaviour of bentonite under laboratory (and repository) conditions.
Perspectives

- For high-density compacted bentonite, the microstructure development upon hydration is limited by the volume constraints. In this case, mechanical stress may also affect the micropore volume.

- Non-equilibrium between the structural levels may further improve the modelling.
Thank you for your attention!

... Questions ? Comments ?