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Using COMSOL for the Transport Modelling of Some Special Cases in a Bentonite Buffer in a Final Repository for Spent Nuclear Fuel

Markus Olin, Veli-Matti Pulkkanen
Anniina Seppälä, Timo Saario, Aku Itälä,
Merja Tanhua-Tyrkkö & Matti Liukkonen

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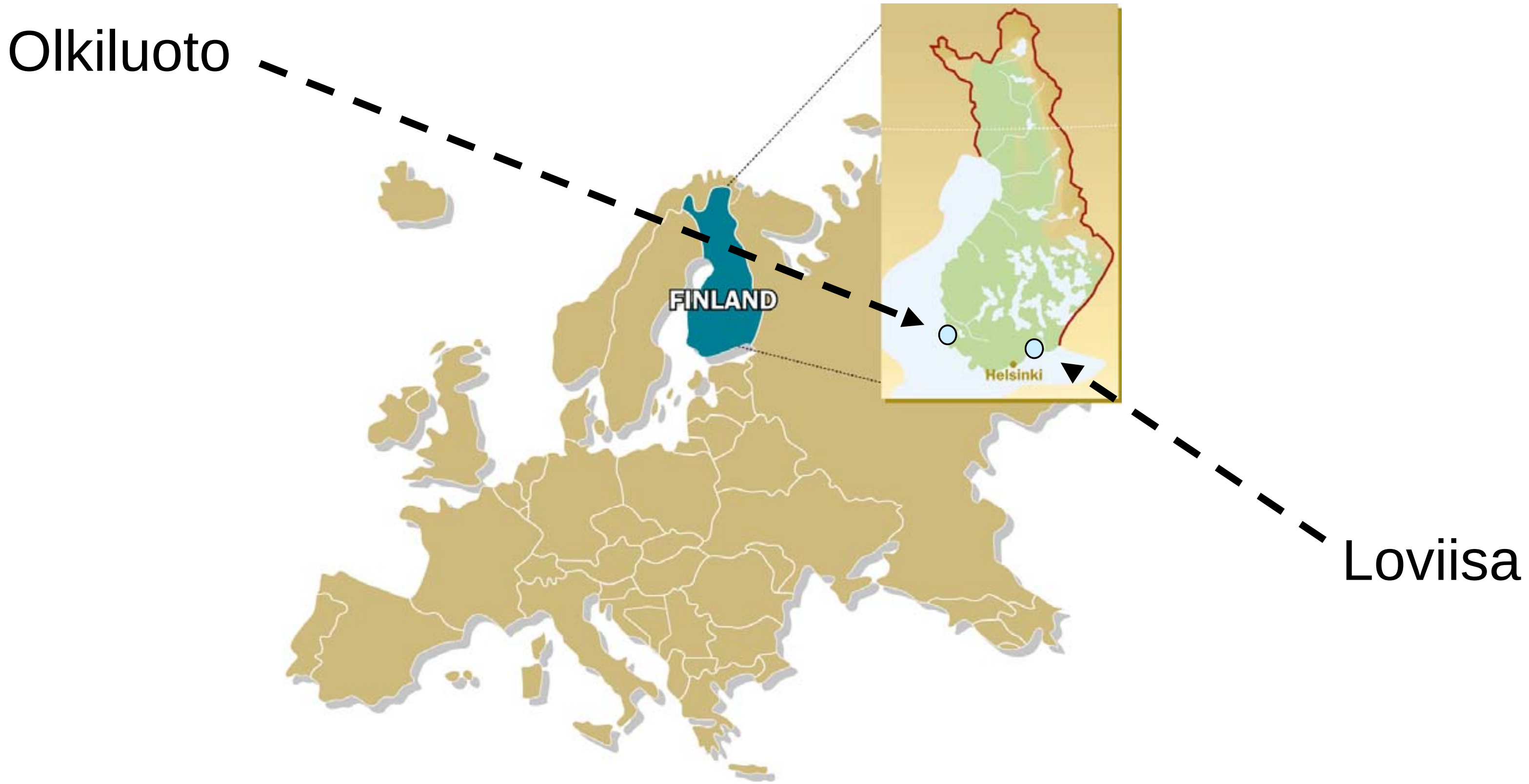
TOPICS

- Deep underground spent fuel repository – KBS-3
- Role of bentonite: density must be in narrow window
- Variable bentonite density
- Chemical equilibrium
- Equations
- Some cases and preliminary results
- Conclusions

Nuclear power plants in Finland, Olkiluoto and Loviisa

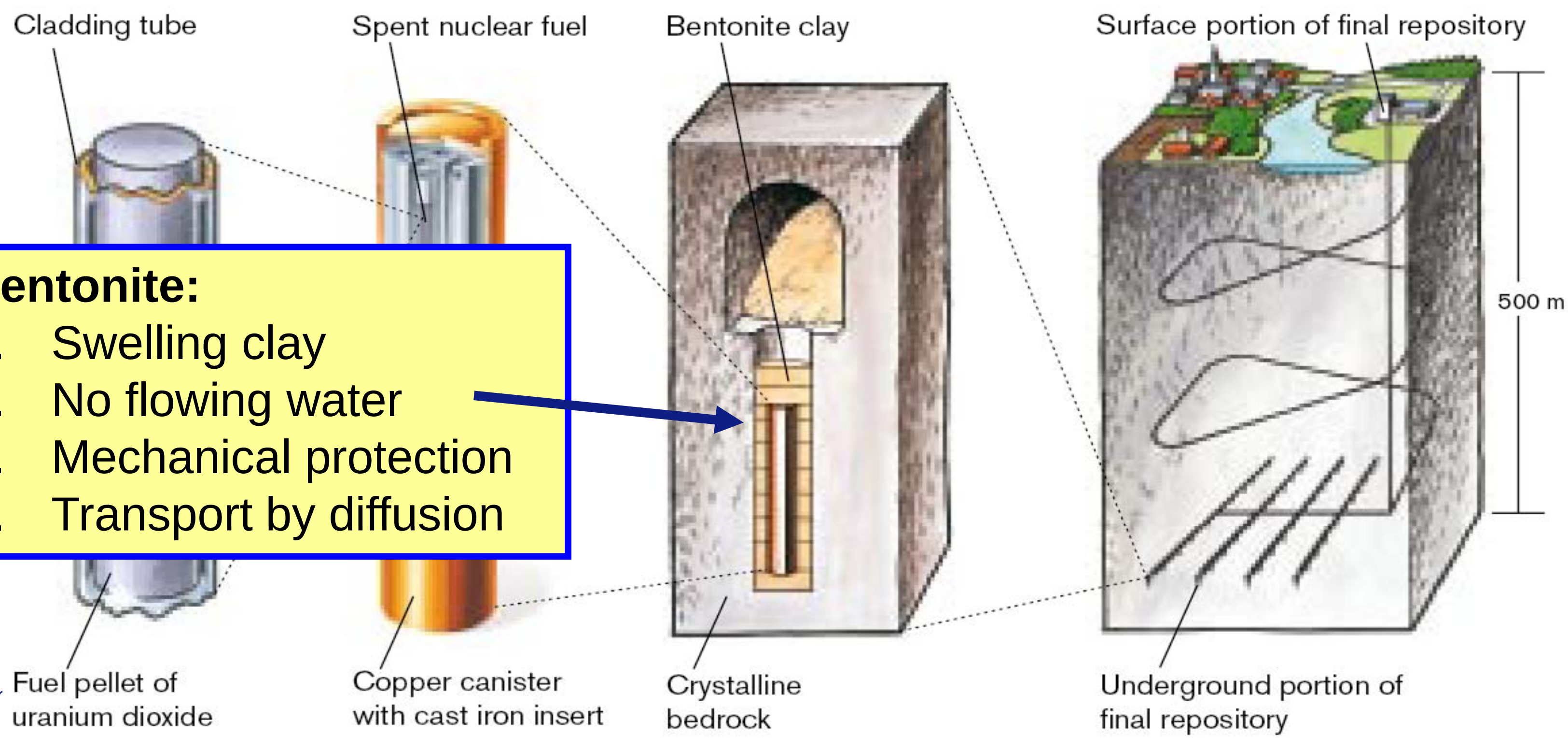


Source of the picture: Posiva, Finland

Density of bentonite in KBS-3V

- KBS-3V concept proposed to be used in Finland like in Sweden
- An essential part of the whole system is **bentonite buffer**
- Many beneficial properties demand enough high enough bentonite density
- Density may be changed by different erosion reactions
- During wetting the bentonite – pore water ratio is varying

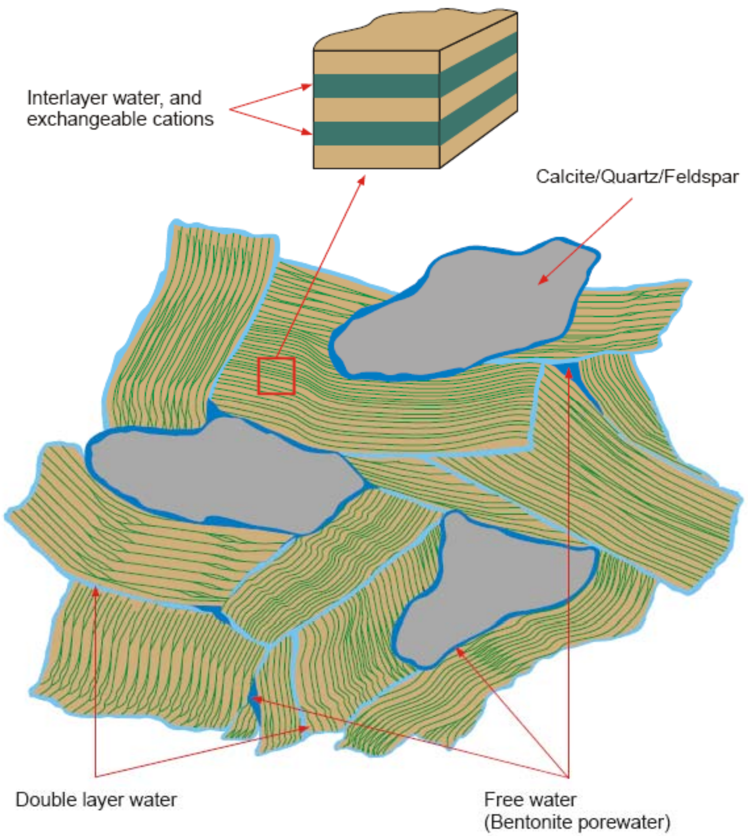
Source of the picture:
SKB, Sweden



Bentonite:
1. Swelling clay
2. No flowing water
3. Mechanical protection
4. Transport by diffusion

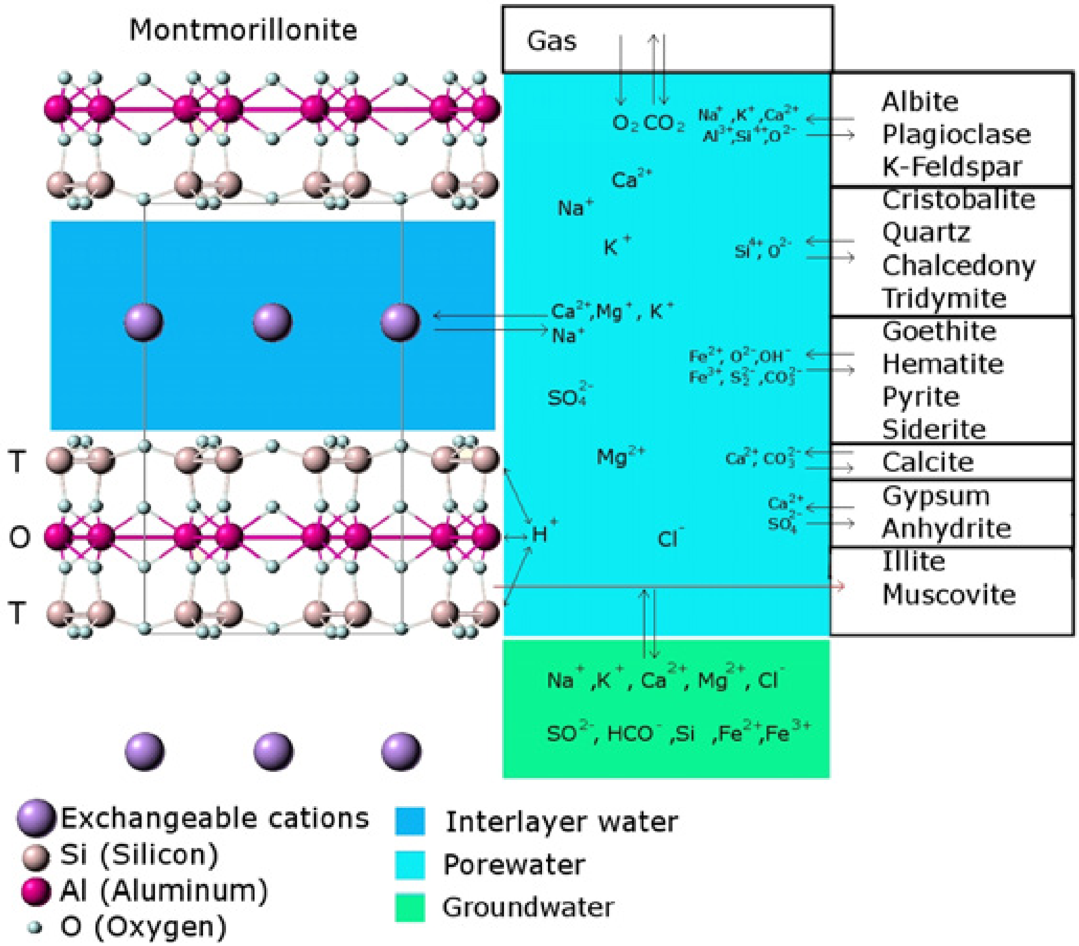
BENTONITE

- Bentonite is a swelling clay, which beneficial properties (for waste disposal) lie mainly on its main component **montmorillonite**
- Montmorillonite is a cation exchanger (Na, K, Ca, Mg):
  - e.g. one Ca ion can be taken out by putting to Na ions in
  - Charge of cations is compensated by negative layers very near each other
- Bentonite swells due water wanting to go between lamellae, where the salinity is higher, and due to forces between charged (but …) surfaces



CHEMICAL REACTIONS AT NANO-LEVEL

- Montmorillonite consists of very thin layers filled by cations and water molecules
- Bentonite includes many other minerals too
- Interaction with groundwater



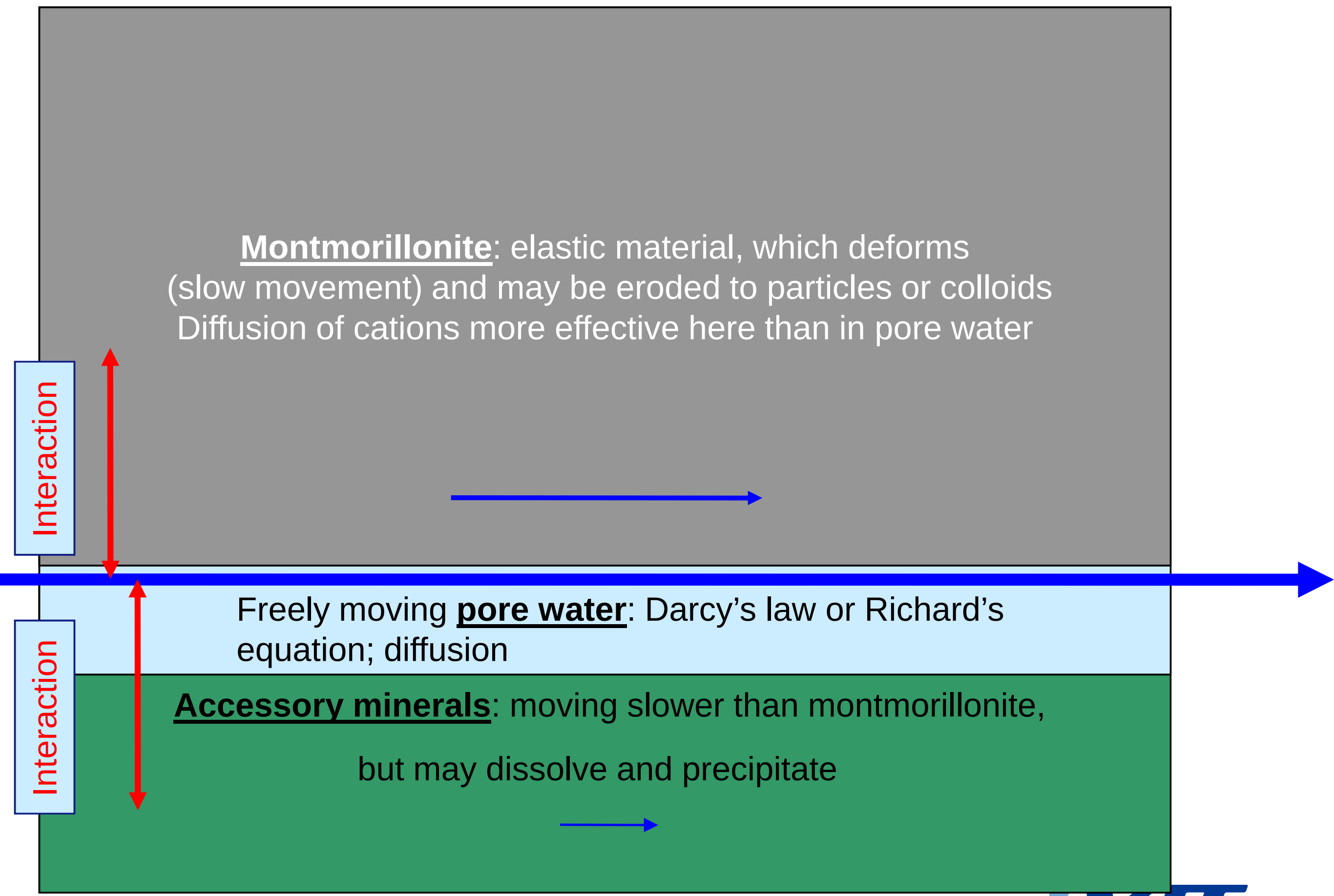
TRANSPORT MODELLING OF BENTONITE

1. Bentonite reacts with contacting water by cation exchange, surface reactions and mineral precipitation/dissolution
2. Mass transport in bentonite takes place by diffusion and in low density by advection
3. On the other hand bentonite swells during wetting and in closed space produces swelling pressure
4. During swelling bentonite deforms and the mass is re-distributed
5. In many cases all this takes place under temperature gradient

- Topics 5.1&2 = THC modelling (Thermo-Hydro-Chemical)
- Topics 5.2&3 = THM modelling (Thermo-Hydro-Mechanical)
- THC models are often developed by chemists and hydrologists
- THM models are quite often developed by physicists and mathematicians
- How to do all that by COMSOL?

CONCEPT

- All components are transporting: either directly or indirectly
- Time scales are very different for the important processes



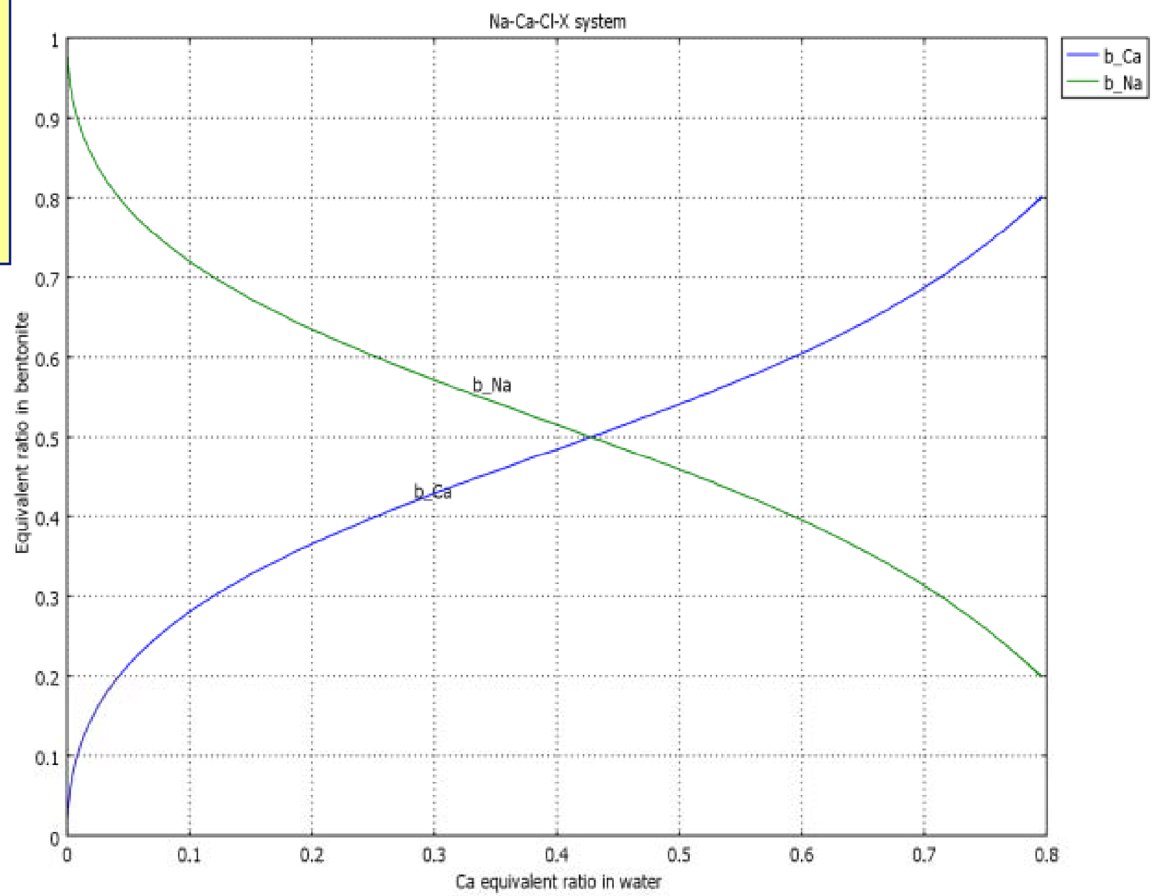
RESULTS I: Chemistry

$$\begin{cases} 2\mathrm{NaX}+\mathrm{Ca}^{2+}=\mathrm{CaX}_2+2\mathrm{Na}^+ & \lg K_{\mathrm{NaCa}}=-0.20 \\ K_{\mathrm{NaCa}}=\dfrac{\beta_{\mathrm{Ca}}\left[\mathrm{Na}^+\right]^2}{\beta_{\mathrm{Na}}^2\gamma_0^2\left[\mathrm{Ca}^+\right]} & K_{\mathrm{NaCa}}=0.62 \\ \mathrm{NaCl}(aq)=\mathrm{Na}^++\mathrm{Cl}^- & \lg K_{\mathrm{NaCl}}=0.78 \\ K_{\mathrm{NaCl}}=\dfrac{\gamma_0^2\left[\mathrm{Na}^+\right]\left[\mathrm{Cl}^-\right]}{\left[\mathrm{NaCl}(aq)\right]} & K_{\mathrm{NaCl}}=6.0 \\ \mathrm{CaCl}^+=\mathrm{Ca}^{2+}+\mathrm{Cl}^- & \lg K_{\mathrm{CaCl}}=0.79 \\ K_{\mathrm{CaCl}}=\dfrac{\gamma_0^4\left[\mathrm{Ca}^{2+}\right]\left[\mathrm{Cl}^-\right]}{\left[\mathrm{CaCl}^+\right]} & K_{\mathrm{CaCl}}=5.0 \end{cases}$$

$$\begin{cases} c_{\mathrm{Na}}=\left[\mathrm{Na}^+\right]+\left[\mathrm{NaCl}(aq)\right]+c_{\mathrm{NaX}} \\ c_{\mathrm{Ca}}=\left[\mathrm{Ca}^+\right]+\left[\mathrm{CaCl}^+\right]+c_{\mathrm{CaX2}} \\ c_{\mathrm{Cl}}=\left[\mathrm{Cl}^-\right]+\left[\mathrm{NaCl}(aq)\right]+\left[\mathrm{CaCl}^+\right] \\ \left[\mathrm{Na}^+\right]+2\left[\mathrm{Ca}^{2+}\right]+\left[\mathrm{CaCl}^+\right]=\left[\mathrm{Cl}^-\right] \end{cases}$$

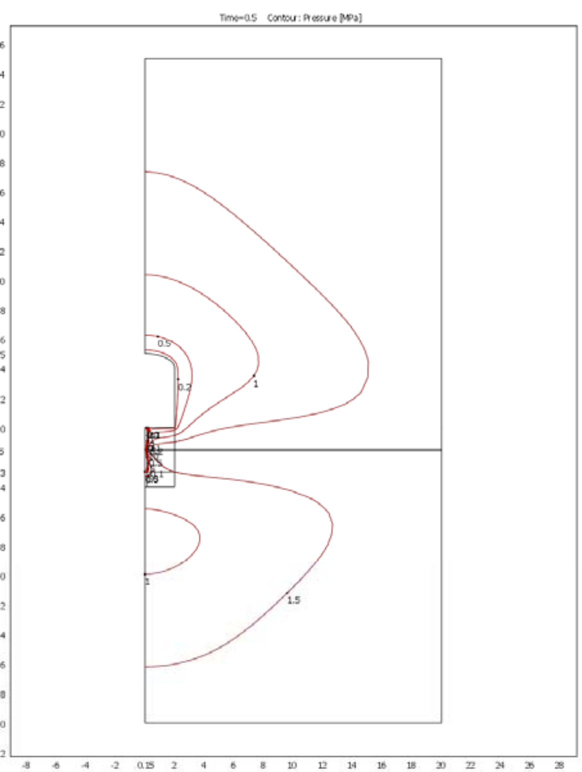
$$\begin{cases} \lg\gamma_0=-0.51\times\left(\dfrac{\sqrt{I}}{1+\sqrt{I}}-0.3I\right) \\ I=\dfrac{1}{2}\left(\left[\mathrm{Na}^+\right]+4\left[\mathrm{Ca}^{2+}\right]+\left[\mathrm{CaCl}^+\right]+\left[\mathrm{Cl}^-\right]\right) \end{cases}$$

- Na-Ca-Cl-X system calculated in CREL: sodium and calcium equivalent fractions vary non-linearly as a function of the calcium equivalent fraction in aqueous phase.



RESULTS II: Saturation of bentonite

- Below some results (pressure contours for whole system and near fracture, effective saturation) for saturation of bentonite
- Planning of an experimental system



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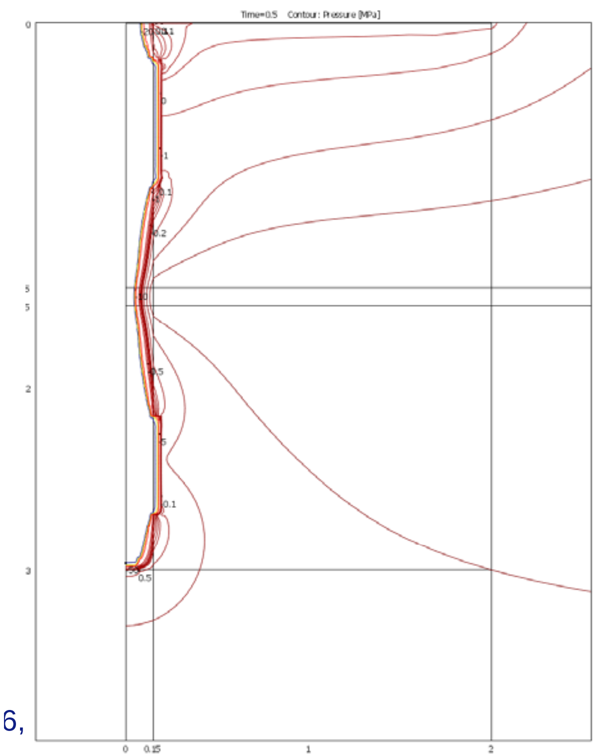

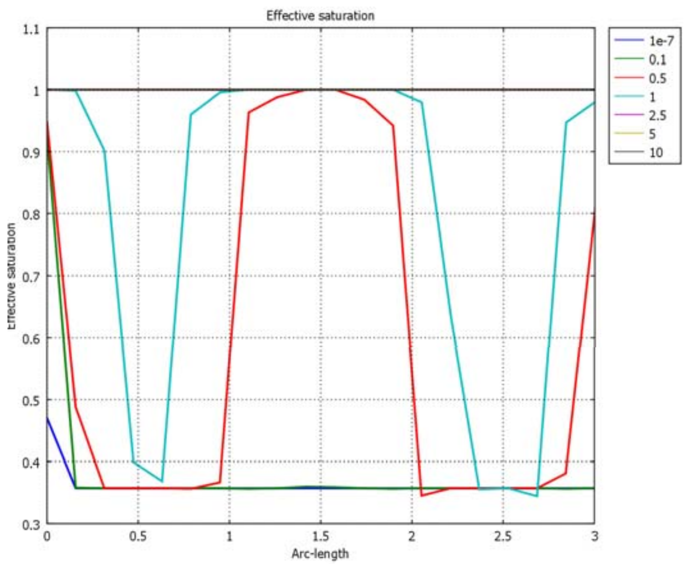

CONCLUSIONS

- COMSOL appeared to be a flexible tool in implementing our model of bentonite, when the bentonite-water ratio varies either due to different erosion processes or during wetting.
- Our first results have already shown how difficult it is to get accurate and stable solutions for variably saturated bentonite buffers.
- We are also working to add chemical reactionswith COMSOL Reaction Engineering Lab, into COMSOL transport modules.
- These reactions are essential in many nuclear waste related problems


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