Presented at the COMSOL Conference 2008 Hannover

Thermo-Hydro-Mechanical-Chemical (THMC) Modelling of the Bentonite Barrier in Final Disposal of High Level Nuclear Waste

> Merja Tanhua-Tyrkkö, Markus Olin, Veli-Matti Pulkkanen, Aku Itälä, Kari Rasilainen, Anniina Seppälä & Matti Liukkonen

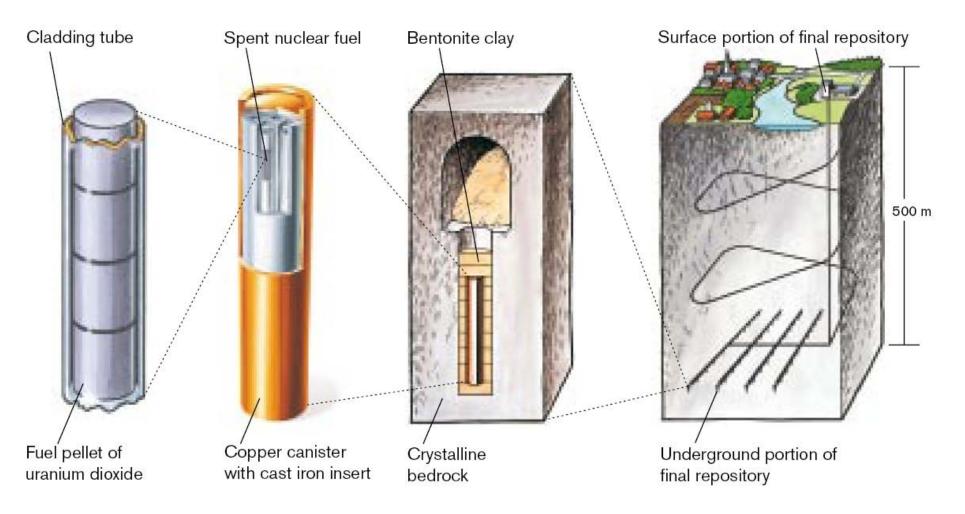


Contents

- KBS-3V concept for spent fuel disposal
- Relevant phenomena and processes
- Equations used
- Modelling tools applied
 - COMSOL
 - EQ3/6, PetraSim and GoldSim
- Cases to be studied
- Preliminary results
- Conclusions
- Future prospects



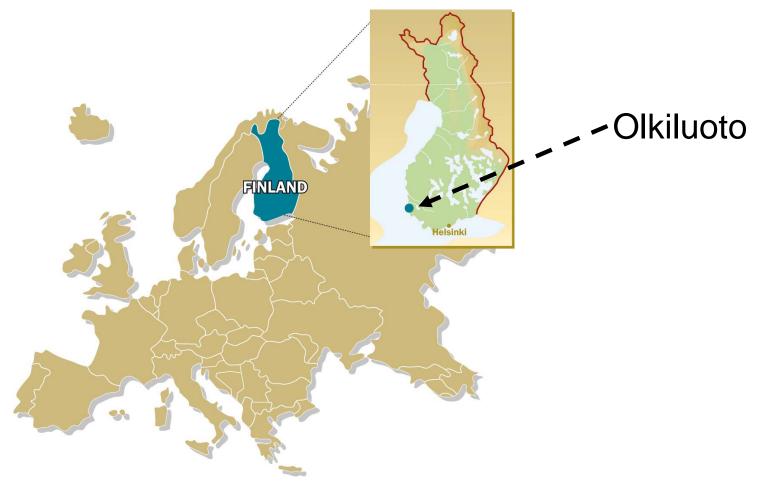
KBS-3V concept for spent fuel disposal



Source of the picture: SKB, Sweden



The planned site for spent fuel disposal in Finland, Olkiluoto



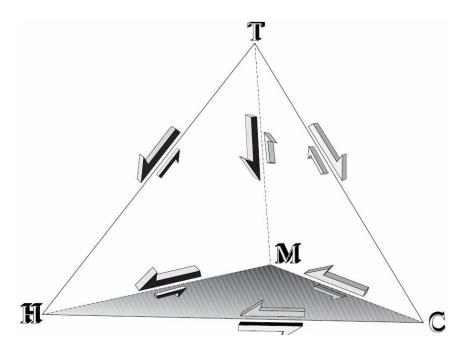
Source of the picture: Posiva, Finland



Relevant phenomena and processes

Main functions of bentonite buffer:

- to minimize hydraulic conductivity near waste canisters (hydraulic processes (H))
- to maintain beneficial chemical environment (chemical (C) and thermal (T) processes)
- to delay or limit release of radionuclides (CH) and
- to limit stresses acting on the canister (mechanical processes (M))



Schematic view of couplings between the THMC processes.



Equations used

- Darcy's law fluid flow, fully saturated porous media
- Richard's equation fluid flow, partially saturated porous media
- Heat equation
- Fick's law Solute transport
- Theory of elasticity
- Chemical reactions
 - Equilibrium
 - Kinetics
 - Surface reactions

$$\alpha_{i} \frac{\partial c_{i}}{\partial t} = \nabla \cdot (D_{a} \nabla c_{i}) - \nabla \cdot (-\mathbf{u}c_{i}) + R_{i}$$

Diffusion Advection Reaction



Modelling tools applied

- COMSOL (main tool)
 - General tool for solving partial differential equations
 - Limited chemistry
- EQ3/6
 - Chemical reactions
 - Limited transport
- PetraSim
 - Coupled THC modelling
 - Limited chemistry support
- GoldSim
 - Radionuclide transport modelling



7

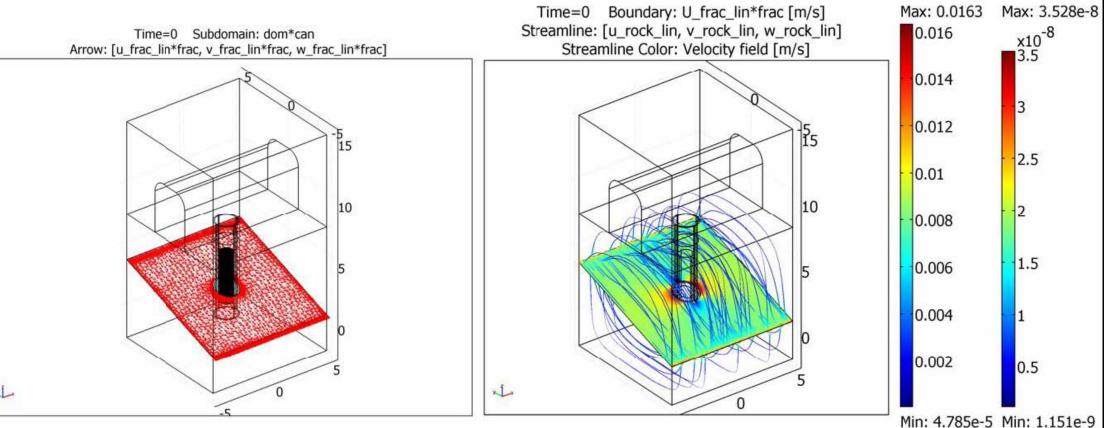
Cases to be studied

- 3D model
 - whole buffer volume and surrounding rock, including various fractures cutting the deposition whole; scale 10x10x8 m³
 - bentonite buffer and fracture cutting it, either cylindrical or bit simpler rectangular; scale 2x1x0.5 m³
- 2D model for diffusion or heat transport calculations between fracture and buffer, combined possibly with chemical reactions; scale 0.5x0.5 m²
- 1D model for transport between the fracture and buffer in very complicated chemical reaction combined with variably saturated bentonite buffer



Preliminary results - 3D model of the disposal site.

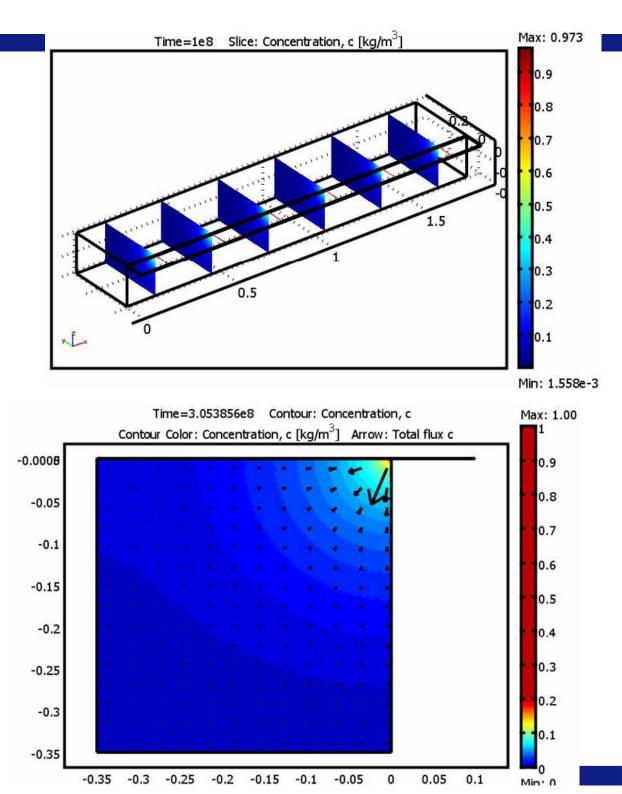
- Velocities by Darcy's law. The velocity field is shown by arrows in the left figure and by streamlines in the right figure.
- Dimensions:
 - copper canister: radius = 0.53 m, height 4.8 m
 - bentonite: thickness = 0.35 m, height = 1+4.8+1 m
 - rock block: 10m x 10m x 8m.
 - The tunnel section is not yet in use, but gives a rough idea of the scale.



VTT TECHNICAL RESEARCH CENTRE OF FINLAND

Preliminary results

- Simplest possible 3D-geometry: Bentonite around the canister is "straightened" to a rectangular slab and the fracture is in front of the bentonite. Water flows along the fracture and diffusion is in horizontal (towards canister) and vertical directions
- Simple 2D-geometry, which enables the use of very thin fracture, but lacks groundwater flow. Diffusion in two directions: horizontally, where on the left side of the figure is the canister, and vertically, where there are possibly several meters of bentonite.



Conclusions

- Some challenging issues:
 - Couplings between THMC-phenomena
 - Geometry: fracture, bentonite
 - Meshes
- COMSOL
 - appears to suite quite well for transport studies
 - BUT Modelling of chemical equilibrium seems to be clumsy



Future prospects

- Further modelling is needed to predict the evolution of nuclear waste repository
- Parellel use of our modelling toolbox
- Long-term goal is integrated THMC model



