

# **Modeling of HMC State of the Concrete Barrier Under Geological Repository Conditions**

In geological disposal system, passive safety does not rely on the geological environment only, but on engineered barriers also. Concrete is among the materials often considered for engineered barriers.

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### Abstract

In this study for modeling of concrete drying-wetting and mass transport under repository conditions (excavation phase, ventilation phase, post closure phase), COMSOL Multiphysics<sup>®</sup> flexibility to solve predefined and user defined partial differential equations was effectively employed.

The following hydro-mechanical-chemical (HMC) processes in the concrete were considered: advective water flow including relative permeability's and capillary pressure depending upon liquid

saturation; advective/dispersive and diffusive transport of dissolved CO<sub>2</sub> and in gaseous phase (respectively); aqueous complexation, advective/dispersive transport of dissolved species (solutes); dissolution/precipitation of minerals; poroelasticity and evolution of material stiffness due to chemical damage.

Numerical HMC model of concrete was implemented in COMSOL Multiphysics and coupled to PHREEQC via iCP interface developed by Amphos21 (Spain) [1].



## Methodology

Developed 2D numerical model considered the disposal tunnel of 9.7 m diameter at the depth of 520 m, the 0.5 thick concrete liner, surrounding excavation disturbed zone and part of clayey host rock (Figure 1). ½ of the

FIGURE 1. Left: Initial and boundary conditions for HM processes. Right: Porewater flow conditions (effective saturation) around the tunnel at 100 years after excavation

#### liner, EDZ and the host rock was modeled due to symmetry.

$$\begin{aligned} \mathsf{H}: \quad & \frac{\partial m_w}{\partial t} + \nabla(\rho_w \mathbf{q}_L) = Q; \qquad m_w = nS_e \rho_w; \qquad S_e = \frac{1}{(1 + (\alpha_{VG} S_M)^{n_{VG}})^{m_{VG}}}; \qquad \mathbf{q}_L = -\frac{k_w k_{rw}}{\mu_w} (\nabla P_L + \rho_w \mathbf{g}); \\ \mathsf{M}: \quad & E = E_0 (1 - d_c); \qquad d_c = d_{c,max} \left[ 1 - e^{(Ca^{solid} - Ca_0^{solid})} \right]; \\ \mathsf{C}: \quad & K = \frac{\prod_{products} a_p^{\nu_p}}{\prod_{reactants} a_r^{\nu_r}}; \qquad a_i = \gamma_i m_i; \qquad \text{extended Debye-Hückel} \quad \log \gamma_i = -\frac{Az_i^2 \sqrt{\mu}}{1 + Ba_i^0 \sqrt{\mu}} + b_i \mu \\ & \partial(\theta, c_i) = \partial(\theta, c_i) \end{aligned}$$

$$\frac{\partial(\theta_l c_i)}{\partial t} + \frac{\partial(\theta_g c_{i,g})}{\partial t} + \mathbf{q}_{\mathbf{L}} \cdot \nabla c_i = \nabla \cdot \left[ \left( D_{D,i} + D_{e,i} \right) \nabla c_i \right] + R_i$$

## Results

Modeling results showed that during ventilation phase the concrete and surrounding EDZ will become unsaturated (Figure 1). When the EDZ was re-saturated again (after ventilation is finished), the pH value at the concrete-EDZ interface did not return to the initial pH value of COx porewater (~7). Within certain distance from the liner-EDZ interface the higher pH values were observed in the EDZ (Figure 2). Within simulation time (10 000 years) no significant pH decrease in the concrete (to 11 and lower) was observed. Thus, it should not impose the chemical degradation of rebars in the concrete and the mechanical strength of the structure. Relating the mechanical properties of concrete (Young modulus) to calcium concentration in solid skeleton, the changes of elasticity modulus would be expected within limited extent (<20 cm) from the liner external boundary (Figure 3). Concrete material weakening in terms of decreasing Young modulus was observed within 5 cm from



liner-EDZ interface by the end of simulation (10 000 yr).

Analysis of these processes is a part of LEI activities in EC programme EURAD Work package MAGIC [2].



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### REFERENCES

1. Nardi, A.; Idiart, A.; Trinchero, P.; de Vries, L. M.; Molinero, J. (2014). Interface COMSOL-PHREEQC (iCP), an efficient numerical framework for the solution of coupled Multiphysics and geochemistry. Computers & Geosciences. 69, 10–21. <u>http://dx.doi.org/10.1016/j.cageo.2014.04.011</u> 2. Ibrahim L., Gonzales S., Lacarriere L., Vilarrasa V., Narkuniene A., Poskas P., Sellier A. (2024): Title. Final version as of 28.05.2024 of deliverable D16.9 of the HORIZON 2020 project EURAD. EC Grant agreement no: 847593





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