# Numerical simulation of THM coupled behavior in the highlevel radioactive waste disposal using OGS-FLAC

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ABSTRACT: Geological disposal of high-level radioactive waste (HLW) is considered the most feasible way to isolate waste from the sphere of human life. It is essential to predict the coupled thermo-hydro-mechanical-chemical (THMC) effect on the disposal system under the deep depth condition to secure the safety of the disposal system. Especially numerical simulation is an effective method for evaluating long-term behavior. We performed a series of numerical simulations to model the THM coupled behavior of the Full-scale Emplacement (FE) experiment as a part of Task C in the DECOVALEX-2023 project. We compared the numerical simulation results using OGS-FLAC to the field data, including pore pressure, relative humidity, temperature, displacement, and stress at the bentonite and host rock, considering the ventilation process. The capillary pressure was the dominant factor in the flow of the buffer system, and we observed thermal-induced pressurization in the far-field host rock.

Keywords: THM coupled behavior, FE experiment, DECOVALEX, OGS-FLAC.

# 1 INTRODUCTION

High-level radioactive waste has high toxicity and a long half-life of up to thousands of millions of years. Therefore, it is crucial to isolate the HLW waste from the biosphere securely, and geological disposal is considered the most feasible way.

The geological disposal system consists of the engineered barrier system (EBS), including a canister and bentonite, and the natural barrier system (NBS), the host rock. EBS and NBS have a role in delaying the possible nuclide migration from the waste. Hence it is essential to comprehend the thermo-hydro-mechanical-chemical (THMC) coupled interactions induced by the disposal system components to maintain the barrier system performance for a long period.

Various studies have been performed to investigate the coupled behavior, and numerical simulation has the advantage of cost-effectiveness and long-term behavior prediction of the disposal system.

DECOVALEX is one of the most famous international cooperative projects to develop numerical methods and models validating with test results to predict THMC interactions in the disposal system. DECOVALEX-2023 consists of 7 tasks, and among them, Task C aims to model the Full-scale Emplacement (FE) experiment at Mont-Terri underground research laboratory (URL) to develop numerical methods for THM coupled interaction.

In the FE experiment, after five years of ventilation process, three heaters were emplaced in the tunnel horizontally based on the Nagra concept (Nagra 2019). Heating from three heaters was applied for five years, and the temperature, relative humidity, pressure, displacement and gas composition were measured in the bentonite and the host rock around the tunnel. Hence, Task C participating groups aim to enhance the knowledge about the coupled behavior in the disposal system and compare the simulation results to the field data for validation. Additionally, we conduct a brief sensitivity analysis to investigate the effect of input parameters and present some of the simulation results in progress.

#### 2 NUMERICAL CODE AND MODEL

In this study, we used OGS-FLAC, a self-developed numerical simulator combining OpenGeoSys and FLAC3D, to simulate the complex THM coupled behavior in the disposal system (Park et al. 2019 and Kim et al. 2021). OpenGeoSys analyze TH coupled interaction based on the Galerkin Finite Element Method, and FLAC3D simulates mechanical behavior using the Finite Difference Method through a sequential coupling method. In the OGS-FLAC, OpenGeoSys acts as a master and decides the time step; hence, OGS-FLAC takes both strengths in the two numerical codes.

For the grid generation, we used GMSH and python code for mesh conversion between OpenGeoSys and FLAC3D. Considering the boundary effect, we generated a three-dimensional geometry of  $(100 \times 60 \times 100)$  m for the simulation. The numerical model comprises about 72000 prism meshes.

The tunnel diameter was 2.54 m, and three heaters having a diameter of 1.05 m were emplaced along the tunnel at intervals of 3.0 m. Bentonite blocks supported the heaters, and granular bentonite filled the rest of the tunnel.

Based on the provided data, we applied the boundary conditions and input parameters for the simulation. Additionally, we modeled the ventilation process to simulate the initial groundwater pressure conditions. After the ventilation process, the heating hysteresis was also referred from the experimental schedule with step-by-step increasing heating power with a maximum of 1350 W for five years.

The initial saturation of the bentonite block and granular bentonite was 0.64 and 0.18. The maximum and minimum principal stresses were 6.5 MPa and 2.5 MPa in the vertical and horizontal directions, respectively, and we assumed that there was no heat and fluid flow along with the fixed boundary condition. The host rock, Opalinus clay, has anisotropy at an angle of 34° to the horizontal direction, and the initial temperature of the entire model was assumed to be 16.5°C.

#### 3 RESULTS

#### 3.1 Sensitivity analysis

As a preliminary study, we conducted a brief sensitivity analysis for thermal conductivity and pore compressibility of bentonite and host rock. As shown in Figure 1, when thermal conductivity decreased, the temperature measured at the interface between the heater and bentonite increased. As the thermal conductivity decreases, heat cannot transfer to the host rock, and due to the blocking effect, the temperature at the heater increases.



Figure 1. Temperature at the heater surface depending on the thermal conductivity variation of the host rock: 2.4 and 1.3 W/m·K (parallel and perpendicular direction to the anisotropic plane) (left) and 2.15 and 1.19 W/m·K (parallel and perpendicular direction to the anisotropic plane).

Figure 2 shows the relative humidity and temperature results at the bentonite depending on the bentonite compressibility. Pore compressibility is related to the storage term affecting the flow, and increasing pore compressibility means a larger storage capacity, which means a slow flow rate. Therefore, relative humidity increased sharply with decreasing pore compressibility, and hence the temperature decreased due to the saturation-dependent thermal conductivity. Based on this sensitivity analysis, we set the input parameters for the following numerical simulation.



Figure 2. Relative humidity(up) and temperature(down) results depending on pore compressibility: bentonite compressibility 0.0 Pa<sup>-1</sup> (left), 5e-9 Pa<sup>-1</sup> (middle), 2e-8 Pa<sup>-1</sup> (right).

# 3.2 Simulation results

We monitored the temperature, water pressure, and relative humidity at the bentonite and host rock. Figure 3 shows the temperature and relative humidity at the bentonite, and Figure 4 shows the temperature and pressure at the host rock. In the two figures, the solid lines indicate the simulation results at each monitoring point, and the dots mean the field data.

Simulation results agreed well with the relative humidity, temperature, and pressure evolution field data. At the initial stage, the temperature increased sharply following the heater power generation. Relative humidity also increased initially and decreased rapidly due to the temperature increase. Groundwater inflow to the bentonite from the host rock occurred slowly, as shown in the relative humidity increase after a rapid decrease. The slow resaturation might occur due to several

causing factors, including the bentonite's high air entry pressure value, low permeability, and low compressibility of the host rock.

At the host rock, the temperature evolution matched well with the field data, and the well-matched initial pressure to the field data shows the effect of the ventilation process. At the near-field of the canister, the pressure decreased as time continued (blue line), and this means the capillary effect of the bentonite was the dominant factor for the flow. While as the distance increases, thermal pressurization becomes more dominant (red line). We will investigate the displacement and stress results in further study.



Figure 3. Temperature at the heater surface depending on the thermal conductivity variation of the host rock: 2.4 and 1.3 W/m·K (parallel and perpendicular direction to the anisotropic plane) (left) and 2.15 and 1.19 W/m·K (parallel and perpendicular direction to the anisotropic plane).



Figure 4. Temperature at the heater surface depending on the thermal conductivity variation of the host rock: 2.4 and 1.3 W/m·K (parallel and perpendicular direction to the anisotropic plane) (left) and 2.15 and 1.19 W/m·K (parallel and perpendicular direction to the anisotropic plane).

#### 4 CONCLUSIONS

We performed a THM coupled simulation considering multiphase flow for a disposal system using OGS-FLAC as a part of Task C in the DECOVALEX project. We modeled a three-dimensional model considering the boundary effect and performed a sensitivity analysis to investigate the effect of input parameters.

Based on the results, we verified the influence of thermal conductivity and pore compressibility on the temperature and flow. We confirmed that the temperature and flow were closely related and interacted. We also set the input parameters and performed a series of numerical simulations to model the FE experiment. The simulation results matched well with the field data, and we investigated each measured parameter depending on time. The dominant mechanism of the pressure evolution at the host rock differed depending on the distance from the canister, and the capillary effect of the bentonite might induce this phenomenon. Further analysis will be continued considering mechanical aspects.

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