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***M4 Summary of EBS International***
***SAND#:***

# 1 DECOVALEX 2023, Task C: TH Simulations of a Full-Scale Heater Emplacement in Opalinus Clay

## 1.1 Introduction

Thermal-Hydrologic-Mechanical (THM) modeling of DECOVALEX 2023, Task C has continued. In FY2022 the simulations have progressed to Step 1, which is on 3-D modeling of the full-scale emplacement experiment at the Mont Terri Underground Rock Laboratory (Nagra, 2019). This report summarizes progress in Thermal-Hydrologic (TH) modeling of Step 1. THM modeling will be documented in future reports.

## 1.2 Model Development of Task C, Step 1

Step 1 continues from Step 0, which was on benchmarking of models using a 2-D geometry. Step 1 builds on the model that was built in Step 0. A description of Step 1 and the modeling sequence, given by DECOVALEX 2023 Task C, is described below.

**Step 1 – Heating phase**: Modeling the change in pore pressure in the Opalinus Clay as a result of heating in the FE experiment. This will require 3D THM simulations with representation of partially saturated conditions.

> **Step 1a: Prediction** – the teams will not be given data from the experiment but will be given information on material properties. A limited number of output data points are requested.
>
> **Step 1b: Analysis** – the teams will be given a large amount of data and asked to compare this to their model results. Thinking about ways to handle the large amount of data is part of this step.
>
> **Step 1c: Calibration** – the teams will be asked to calibrate their model based on the data available.

### 1.2.1 Step 1 Model Geometry

For Step 1 modeling a simplified 3-D geometry is used as shown in Figure 1, with the experiment tunnel represented as a cylinder, and heaters placed in the tunnel with the center-line of the heater aligned to the center-line of the tunnel. The cross-sectional geometry through the tunnel is the same as in Step 0 (Figure 2). The Opalinus Clay is bedded and has anisotropic THM properties in directions parallel and perpendicular to bedding. The bedding dips at 34˚ from the horizontal as shown in Figure 2. Dimensions of the materials in Figure 1 are given in Table 1. A 50 m x 50 m x domain outer boundary was selected.

Table 1. Details of the geometry for the 3-D model (Task C Specifications).

| **Description** | **Value** | **Reference** |
|---|---|---|
| Diameter of FE tunnel (Dt) | 2.48 m | Nagra, 2019 |
| Heater diameter (Dh) | 1.05 m | Nagra, 2019 |
| Pedestal width at base (Wp) | 0.8 m | Nagra, 2019 |
| Length of sealing section (Ls) | 12.5 m | NAB 18-39 |
| Length of heaters (Lh) | 4.6 m | NTB 15-02 |
| Length of gap 1 (Lg1) | 3 m | NTB 15-02 |
| Length of gap 2 (Lg2) | 3 m | NTB 15-02 |
| Length of gap 3 (Lg3) | 3 m | NTB 15-02 |
| Length of plug (Lp) | 5 m | NTB 15-02 |
| Length of access section (La) | 9 m | NAB 18-39 |

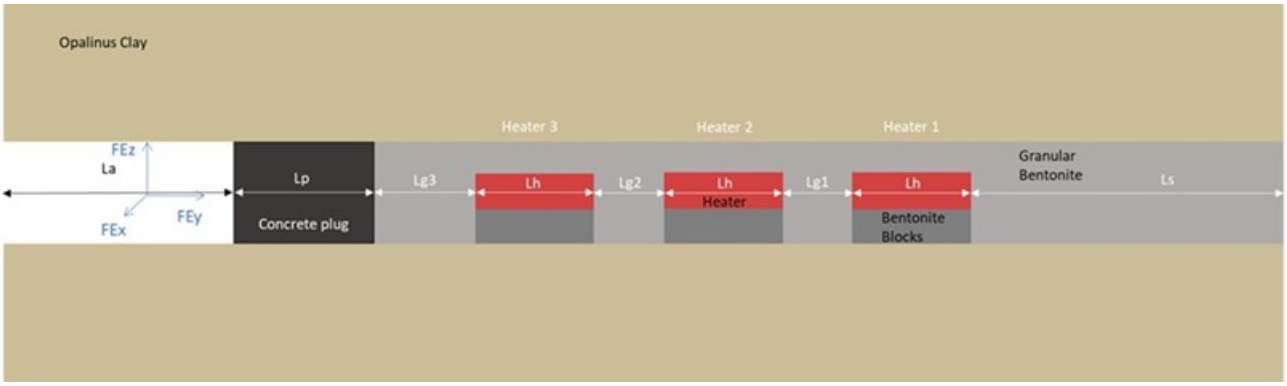


Figure 1. Model geometry for Step 1 (Task C Specifications).

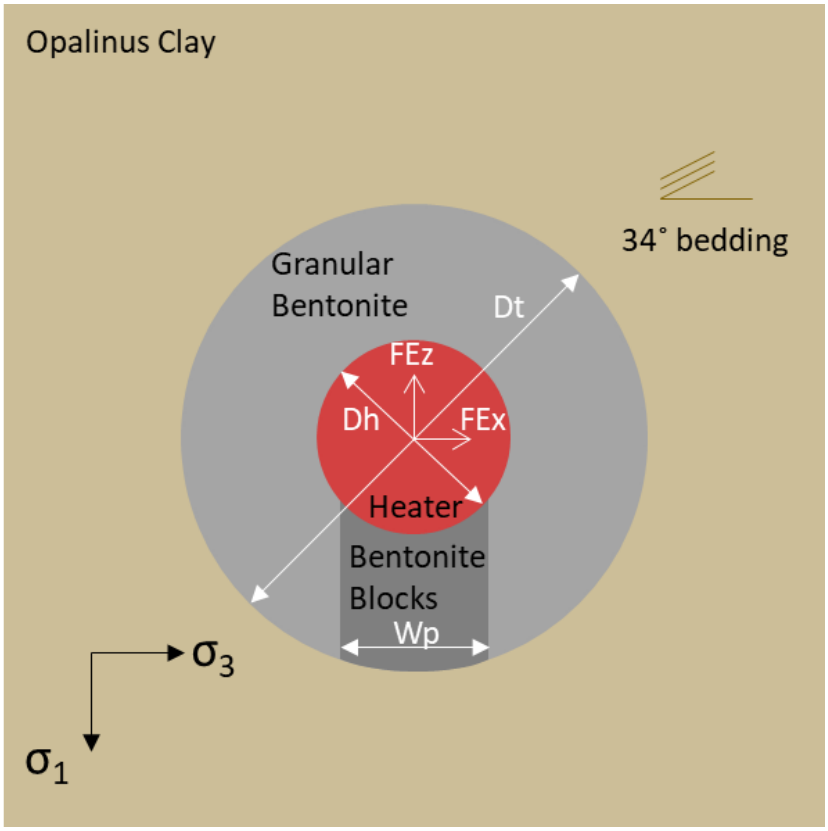


Figure 2. Model geometry for Step 0 (Task C Specifications).

## 1.3 Step 1 Modeling

Preliminary TH modeling of Step 1 for the full-scale heater test have been conducted. For the simulation properties developed in Step 0 were used. For Step 1 TH simulations the numerical code PFLOTRAN (Hammond et al., 2014) was used. Simulations were run for 5 years from the start of heating.

### 1.3.1 Material Properties

DECOVALEX, Task C provided material properties to be used for the simulations are given in Table 2.

Table 2. Material parameters for Step 1 (Task C Specifications)

| Input parameters | | Symbol | Unit | OPA [1] | GBM [3] | Bentonite blocks [4] | Concrete | Source |
|---|---|---|---|---|---|---|---|---|
| Thermal parameters | Dry thermal conductivity parallel and perpendicular to bedding | $\lambda_{dry,\parallel}$ | *W/mK* | 2.4 | 0.35 | 0.26 | 0.1 | |
| | | $\lambda_{dry,\perp}$ | *W/mK* | 1.3 | | | | |
| | Saturated thermal conductivity parallel and perpendicular to bedding | $\lambda_{sat,\parallel}$ | *W/mK* | 2.4 | 1.2 | 0.96 | 0.3 | |
| | | $\lambda_{sat,\perp}$ | *W/mK* | 1.3 | | | | |
| | Solid specific heat capacity | $c_s$ | J/kgK | 995 | 800 | 800 | 750 | |
| Hydraulic parameters | Dry Bulk Density | $\rho_{bulk}$ | *kg/m* $^3$ | 2340 | 1490 | 1690 | 1725 | NTB 15-02 |
| | Porosity | $\phi$ | - | 0.13 | 0.331 | 0.331 | 0.25 | |
| | Intrinsic permeability | $k_{i,\parallel}$ | *m* $^2$ | 5.0E-20 | 3.5E-20 | 1.0E-22 | 1.0E-19 | |
| | | $k_{i,\perp}$ | | 1.0E-20 | | | | |
| | Van Genuchten Entry Pressure | $p_e$ | *MPa* | 20.0 | 28.6 | 30 | 1 | |
| | van Genuchten n | n | - | 2.5 | 2.0 | 1.67 | 1.49 | |
| | van Genuchten maximum water saturation | $s_{max}$ | - | 1.0 | 1.0 | 1.0 | 1 | |
| | van Genuchten residual water saturation | $s_r$ | - | 0.0 | 0.0 | 0.0 | 0.01 | |
| | Pore compressibility | $c_{pore}$ | *1/Pa* | 8.66E-10 | 1.05E-07 | 1.13E-07 | 1.40E-10 | calculated from E, ν |
| Mechanical parameters | Young's modulus | $E_\parallel$ | *MPa* | 8000 | 18 | 24 | 20000 | |
| | | $E_\perp$ | | 4000 | | | | |
| | Shear modulus | $G_\perp$ | *MPa* | 3500 | - | - | - | |
| | Poisson ratio | $\nu_\parallel$ | - | 0.35 | 0.35 | 0.2 | 0.15 | |
| | | $\nu_\perp$ | | 0.25 | | | | |
| | Linear thermal expansion | $\alpha_T$ | *1/K* | 1.5E-05 | 3.0E-06 | 3.0E-06 | 1.5E-05 | |
| | Biot coefficient | $\alpha$ | - | 1 | 1 | 1 | 1 | |
| Fluid parameters | Reference water density | $\rho_{fluid\_ref}$ | *kg/m* $^3$ | 1000 | | | | |
| | Fluid compressibility | $c_{fluid}$ | *1/Pa* | 4.65E-10 | | | | |
| | Linear thermal expansion water | $\alpha_w$ | *Pa s* | 4.00E-04 | | | | |
| | Vapour diffusivity (vapour in air) | D_v | *m* $^2$*/s* | 2.42E-05 | | | | |

### 1.3.2 Simulation model setup

Model geometry and meshing were developed for Step 1 PFLOTRAN simulations as shown in Figure 3. The domain size is 50 m x 50 m x 50 m x 50 m, and the mesh has 1,038,463 grid blocks. Figure 4 shows representation of the experimental tunnel. Heating schedule for the three heaters is shown in Table 3. Based on the specified material properties (Table 2) and other Task C specifications, the following initial and boundary conditions were used.

- Initial condition:
    - T = 15 °C everywhere
    - Pore water pressure 2 MPa. Hydrostatic pressure assumed at Opalinus Clay.
    - Bentonite blocks initial condition:
        - Initial water content 18 % (Nagra, 2019). Calculated liquid saturation = 0.919
    - Granular bentonite initial condition:
        - Initial water content 5 % (Nagra, 2019). Calculated liquid saturation = 0.227
    - Initial water saturation at Opalinus Clay = 1
    - Initial concrete liquid saturation = 0.1
- Diffusion Coefficient:

- Liquid phase: 2.0 x $10^{-9}$ $m^2/s$
- Gas phase: 2.0 x $10^{-5}$ $m^2/s$

- Boundary Condition:
  - No heat flow, no water flow, no vapour flow, no displacement on outer boundaries.
  - Heater power schedule is given in Table 3.
  - Column outer boundary at 2.0 MPa and 15 °C
  - Heater boundary no water flow, no displacement.
- Opalinus Clay:
  - Anisotropy in permeability and thermal conductivity applied

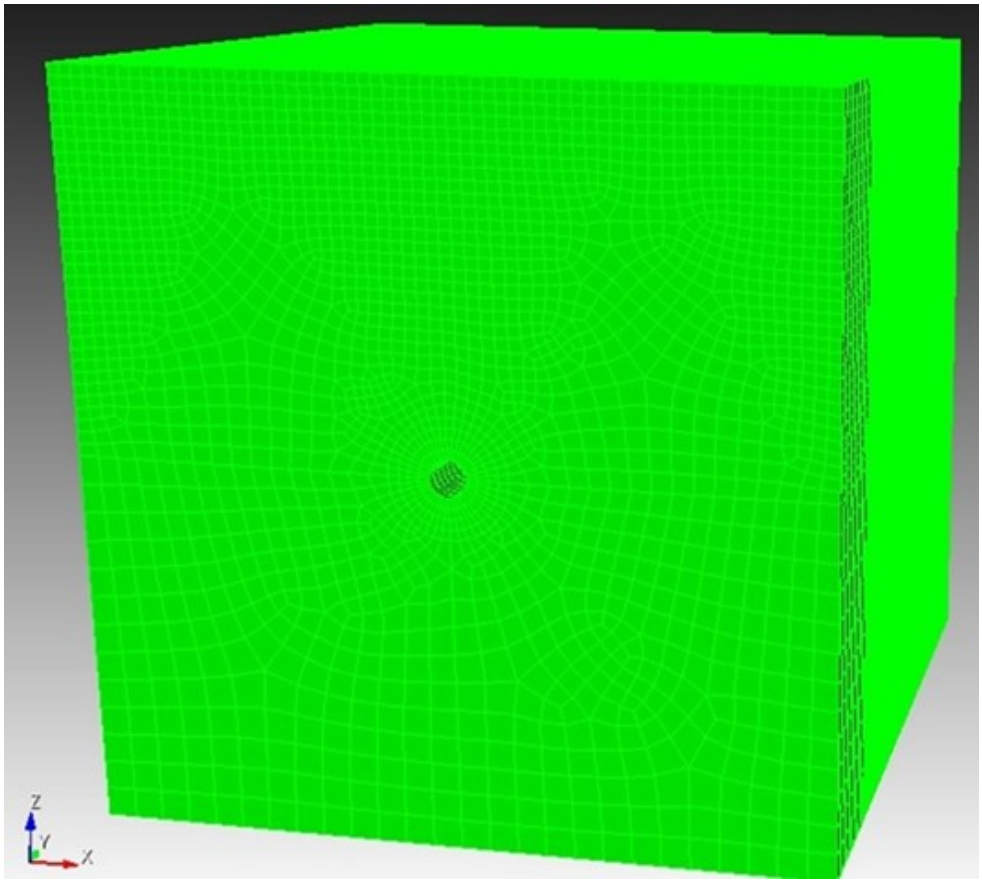


Figure 3. Geometry and meshing used for Task C, Step 0 simulations.

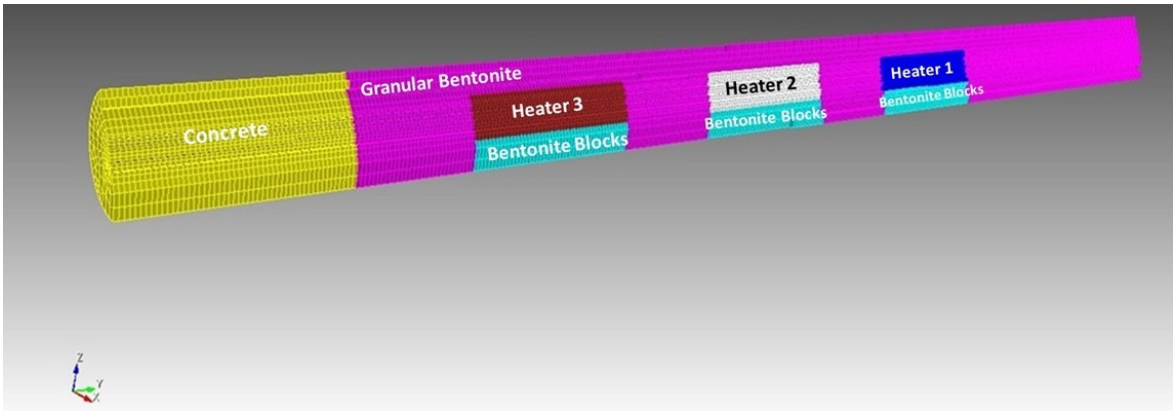


Figure 4. Representation of the experimental tunnel, Step 1 simulations.

Table 3. Heating schedule for the three heaters (Task C Specifications)

| | Date | Power (W) |
|---|---|---|
| Heater 1 | 12/15/2014<br>01/13/2015<br>02/16/2015 | 500<br>1000<br>1350 |
| Heater 2 | 02/17/2015 | 1350 |
| Heater 3 | 02/18/2015 | 1350 |

## 1.4 Step 1 Preliminary Simulation Results

Preliminary TH simulations were made for Step 1 using PFLOTRAN numerical code. Selected simulations results are shown in Figure 5 to 11. Note that these are interim results and the final results will be reported in the future.

Figure 5 shows predicted distribution of temperature after 100 days of simulation. The figure on the left is a cross-section along the tunnel axis. At 100 days Heater 1 is hotter than the other heaters due to the heating schedule (Table 3). The middle figure is a cross-section perpendicular to tunnel axis, showing the effect of the anisotropy in the Opalinus Clay.

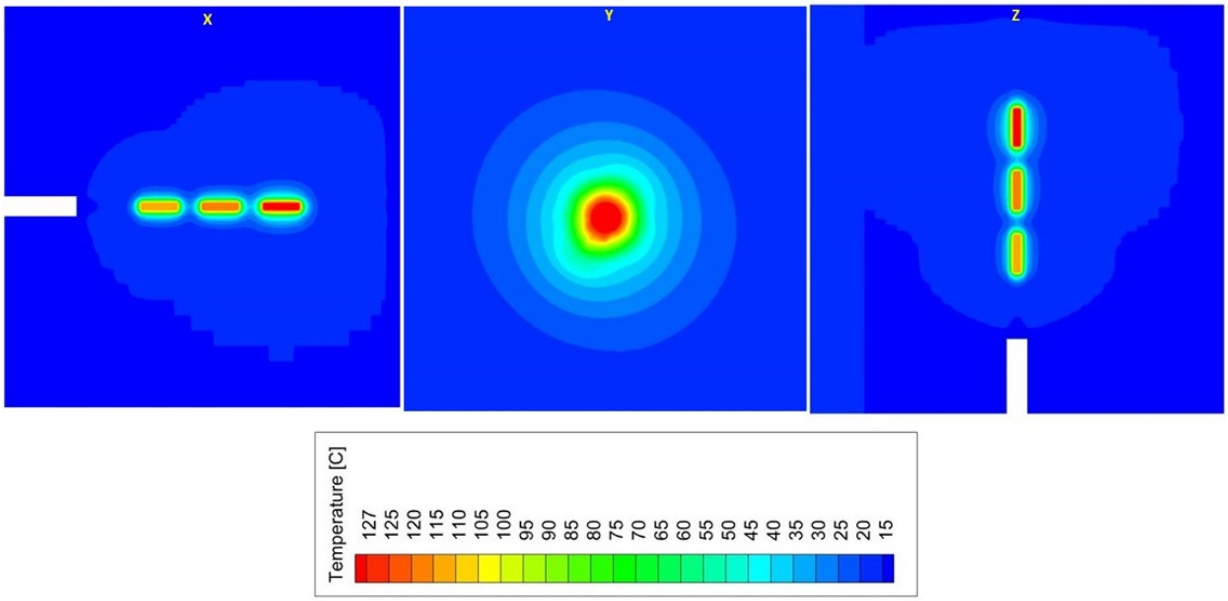


Figure 5. Prediction of temperature distribution at 100 days

Predictions of temperature evolution at selected observation points were also conducted. The selected points are given below and in Figure 6.

- H1_230_0_1 – near heater surface (H1)
- H2_230_0_1 – near heater surface (H2)
- H3_230_0_2 – near heater surface (H5)
- BH2_230_6 – 20 cm from heater surface (T6a)
- BFEA 002_TEM_03 – on Opalinus Clay (10a) – 2 m from heater surface

The predicted results were compared to experimental results as shown in Figures 7 to 11. For most of the plots the predicted results are close to the experimental. The initial temperatures in the experimental data are below the 15 °C assumed for the simulations. This could be due to ventilation prior to the heating phase. That is not captured in the current simulations.

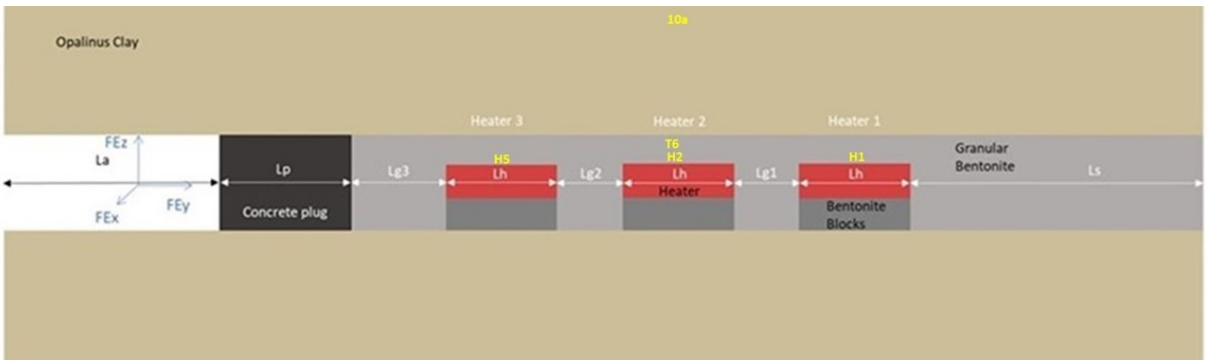

Figure 6. Locations of selected observation points (H1, H2, H5, T6, 10a)

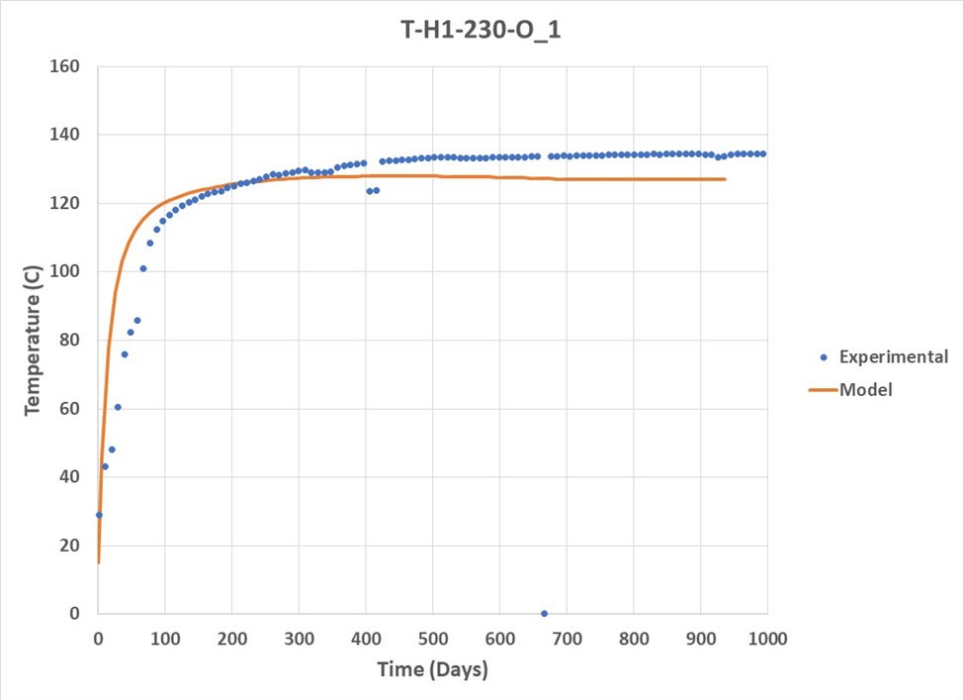


Figure 7. Temperature comparison at Observation Point H1 (Model and Experimental)

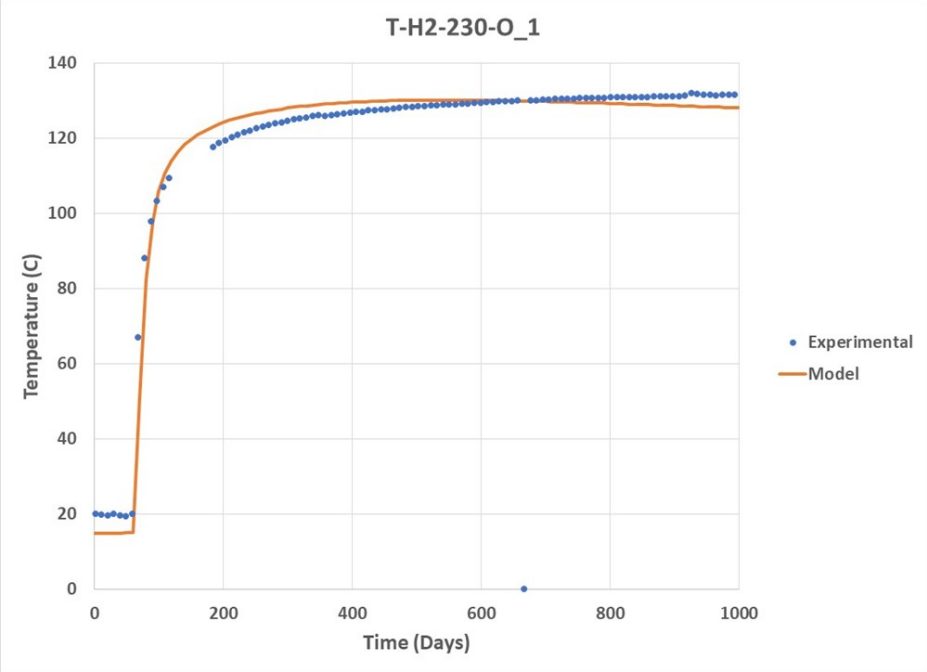

Figure 8. Temperature comparison at Observation Point H2 (Model and Experimental)

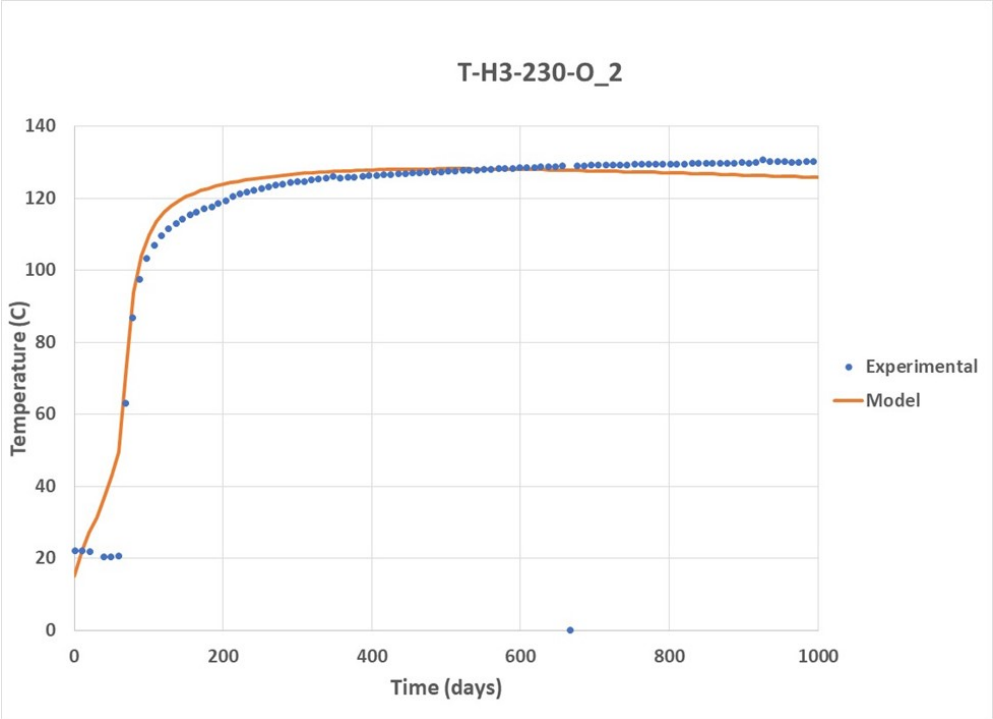


Figure 9. Temperature comparison at Observation Point H5 (Model and Experimental)

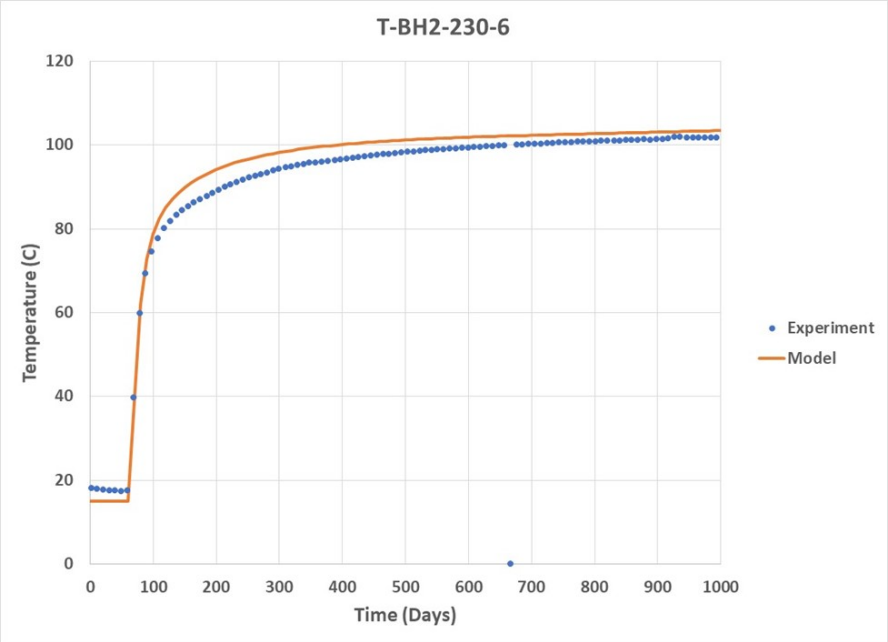

Figure 10. Temperature comparison at Observation Point T6a (Model and Experimental)

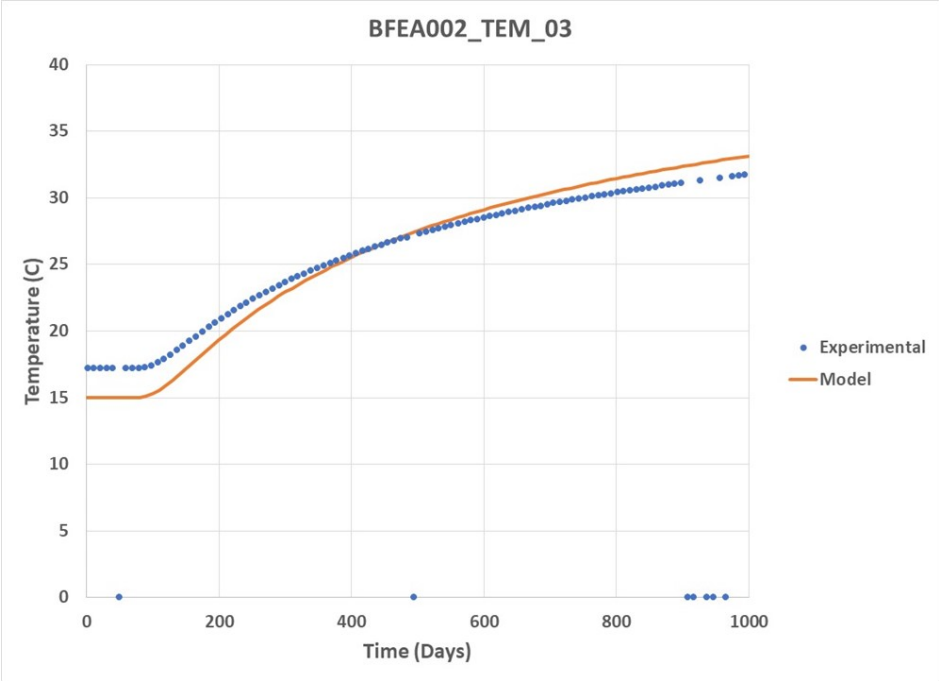


Figure 11. Temperature comparison at Observation Point 10a in the Opalinus Clay (Model and Experimental)

## 1.5 Summary and Future Work

Preliminary TH simulations of Task C, Step 1 were conducted using PFLOTRAN numerical code and a 3-D geometry. Comparison of predicted temperature evolution at a few selected observation points and the experimental data were very close.

The simulations will continue with the calibration phase where predicted temperature, pressure and RH at specified locations will be compared with experimental data. Future simulations will also look at the discrepancy in initial conditions between the predicted and experimental data, likely a result of ventilation.

## 1.6 References

COMSOL Multiphysics® v. 5.6. www.comsol.com. COMSOL AB, Stockholm, Sweden.

Hammond, G.E., P.C., Lichtner, and R.T., Mills. 2014. Evaluating the Performance of Parallel Subsurface Simulators: An Illustrative Example with PFLOTRAN. *J. Water Resources Research*. 50, doi:10.1002/2012WR013483.

Nagra, 2019. Implementation of the Full-scale Emplacement Experiment at Mont Terri: Design, Construction and Preliminary Results. Nagra Technical Report 15-02.

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