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Model Development for THM Simulations of a Full-Scale Heater Emplacement in Opalinus Clay

Teklu Hadgu*, Thomas Dewers*, Edward Matteo*

*Sandia National Laboratories: MS 0747, P.O. Box 5800, Albuquerque, NM 87185, thadgu@sandia.gov, tdewers@sandia.gov, enmatte@sandia.gov

INTRODUCTION

This work describes preliminary process model development and modeling analysis for the full-scale emplacement experiment at the Mont Terri Underground Rock Laboratory, Switzerland, as part of the DECOVALEX-2023, Task C study. One of the modeling steps of Task C is benchmarking of computing methods against simplified two-dimensional test cases. The work presented here mainly focuses on benchmarking of thermal-hydrology processes using specified material properties including Opalinus Clay anisotropy. Preliminary simulations of the thermal-hydrologic processes using the numerical code PFLOTRAN [1] is presented. Development of thermal-hydrologic-mechanical models and comparison of model results to experimental data are underway.

The experiment was designed in part to investigate thermal-hydrological-mechanical (THM) processes resulting from emplacement of spent fuel and high-level nuclear waste in a geological repository in Opalinus Clay host rock [2]. The experiment involves heating of an in-situ tunnel surrounded by Opalinus Clay host rock [2]. The tunnel contains three heaters placed on pedestals made of bentonite blocks and the rest of the tunnel is filled with a granular bentonite mixture (Figure 1).

The aim of DECOVALEX-2023, Task C is to build numerical models to study the various processes such as bentonite thermal conditions and pore pressure changes in the Opalinus Clay as a result of heating, using experimental dataset. Task C is divided into steps starting from benchmarking of computing methods against simplified two-dimensional test cases, followed by three-dimensional modeling of the heating experiment and other subsequent tests. The work presented here mainly focuses on benchmarking of thermal-hydrology processes. The processes include vapor transport in the partially saturated bentonite and re-saturation.

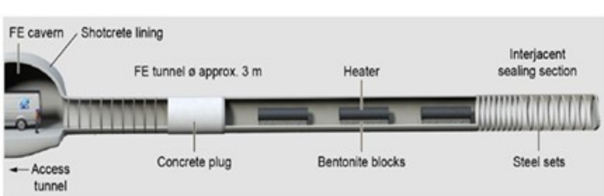

Fig. 1. Schematic diagram of the FE tunnel (DECOVALEX 2023, Task C).

MODEL SETUP

Model Geometry

For the benchmarking step a two-dimensional geometry was chosen to reduce the computing burden. The geometry consists of a cross-section through the center of the middle heater in the heater experiment (Figure 2). Note that the Opalinus Clay is bedded and has anisotropic THM properties in directions parallel and perpendicular to the 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. The heater is centered within the tunnel. A 50 m by 50 m domain outer boundary was selected, which generally avoids boundary effects. The mesh has 138,103 grid blocks (Figure 3). Measurement locations are given in Table 2. Simulation results are to be obtained at these locations.

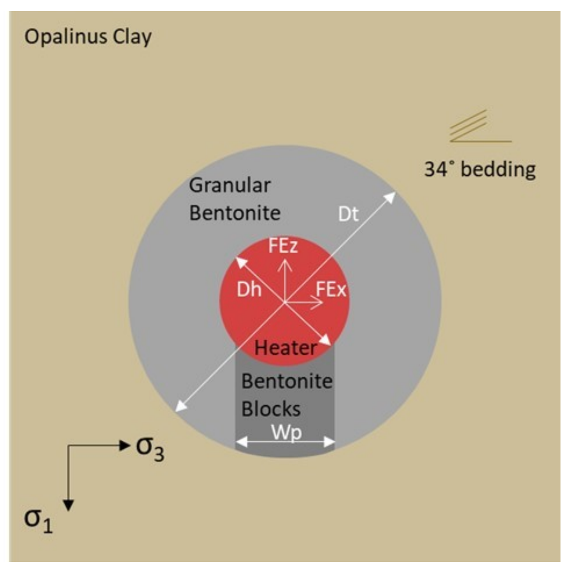

Fig. 2. Model geometry for the Benchmarking Step (Task C Specifications).

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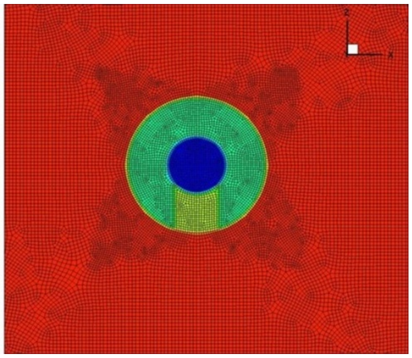

Fig. 3. Geometry and meshing used for Task C, PFLOTRAN benchmark simulations.

TABLE 1. Details of the geometry for the 2D model (Task C Specifications).

Description	Value	Reference
Diameter of tunnel (Dt)	2.48 m	[2]
Heater diameter (Dh)	1.05 m	[2]
Pedestal width at base (Wp)	0.8 m	[2]

TABLE 2. Measurement Locations (Task C Specifications)

Name	Radial distance from heater centre (m)	Angle (vertically upwards is zero and measured clockwise)
H_1	0.525	0
H_2	0.525	90
H_3	0.525	180
H_4	0.525	270
H_5	0.525	56
H_6	0.525	326
H_7	0.725	0
H_8	0.725	90
H_9	0.725	180
H_10	0.725	270
H_11	0.725	56
H_12	0.725	326
T_1	1.04	0
T_2	1.04	90
T_3	1.04	180
T_4	1.04	270
T_5	1.04	56
T_6	1.04	326
O_1	5	56
O_2	8	56
O_3	14	56
O_4	5	326
O_5	8	326
O_6	14	326

Material Properties

DECOVALEX, Task C provided material properties to be used for the simulations. Table 3 shows parameter values to be used in the benchmark simulations

TABLE 3. Material parameters for the benchmark modeling (Task C Specification)

Input parameters		Symbol	Unit	OPA [1]	GBM [3]	Bentonite blocks [4]
Thermal parameters	Dry thermal conductivity parallel and perpendicular to bedding	$\lambda_{dry,\parallel}$	W/mK	2.4	0.35	0.26
		$\lambda_{dry,\perp}$	W/mK	1.3		
	Saturated thermal conductivity parallel and perpendicular to bedding	$\lambda_{sat,\parallel}$	W/mK	2.4	1.2	0.96
		$\lambda_{sat,\perp}$	W/mK	1.3		
	Solid specific heat capacity	c_s	J/kgK	995	800	800
Hydraulic parameters	Dry Bulk Density	ρ_{bulk}	kg/m^3	2340	1490	1690
	Porosity	ϕ	-	0.13	0.331	0.331
	Intrinsic permeability	$k_{i,\parallel}$	m^2	5.0E-20	3.5E-20	1.0E-22
		$k_{i,\perp}$		1.0E-20		
	Van Genuchten Entry Pressure	p_e	MPa	20.0	28.6	30
	van Genuchten n	n	-	2.5	2.0	1.67
	van Genuchten maximum water saturation	s_{max}	-	1.0	1.0	1.0
	van Genuchten residual water saturation	s_r	-	0.0	0.0	0.0
	Pore compressibility	c_{pore}	1/Pa	8.66E-10	1.05E-07	1.13E-07
Fluid parameters	Reference water density	ρ_{fluid_ref}	kg/m^3	1000		
	Fluid compressibility	c_{fluid}	1/Pa	4.65E-10		
	Linear thermal expansion water	α_w	Pa s	4.00E-04		
	Vapour diffusivity (vapour in air)	D_v	m^2/s	2.42E-05		

Initial and Boundary Conditions

Based on the specified material properties (Table 3) and other Task C specifications, the following initial and boundary conditions were used.

- Initial condition:
  - T = 15 °C everywhere
  - Pore pressure 2 MPa. Hydrostatic pressure assumed at Opalinus Clay.
  - Bentonite blocks initial condition:
    - Initial water content 18 % [2]. Calculated liquid saturation = 0.919
  - Granular bentonite initial condition:
    - Initial water content 5 % [2]. Calculated liquid saturation = 0.227
  - Initial water saturation at Opalinus Clay = 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 vapor flow, no displacement on outer boundaries.
  - Heater power is 1350 W per heater, and each heater is 4.6 m long.
  - 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.

RESULTS

Benchmark simulations were made for the selected Task C simulation step using PFLOTRAN numerical code. As specified above the selected step involves vapor transport simulation in a two-dimensional cross-section across the experimental tunnel (Figures 2 and 3). The model includes thermal-hydrology with partial saturation in the bentonite and Opalinus Clay close to the tunnel. PFLOTRAN was run for the simulation time of 1800 days (about 5 years) using the input data described above. Some of the simulation results are presented below.

Figure 4 shows predicted distribution of temperature at end of simulation time of 1800 days. Figure 5 shows the corresponding liquid pressure distribution. The shapes of the temperature and pressure distributions reflect anisotropy in permeability and thermal conductivity that result from the orientation of the Oplinus Clay bedding planes.

Figures 6 and 7 show locations of observation points where predicted evolutions of temperature and pressure are discussed in this paper. Predicted evolution of temperature at selected locations in the Granular Bentonite and Bentonite Blocks are shown in Figure 8. Solid lines are used to indicate locations parallel to the Opalinus Clay bedding while dashed lines show locations perpendicular to the bedding. Results show that temperatures decrease at distances away from the heater, as would be expected. As shown in Figure 8 (and specified in Table 2), observation points H_5, H_11 and T_5 are located parallel to the Opalinus Clay bedding, while points H_6, H_12 and T_6 are located perpendicular to the bedding. As the results show, temperatures in the bentonite are not significantly affected by the Opalinus Clay bedding.

Predictions of temperature and pressure in the Opalinus Clay are shown in Figures 9 and 10, respectively. Solid lines are used to indicate locations parallel to the Opalinus Clay bedding while dashed lines show locations perpendicular to the bedding. As in the bentonite, temperatures in the Opalinus Clay decrease at distances away from the heater. As shown in Figure 9 (and specified in Table 2), observation points O_1, O_2 and O_3 are located parallel to the Opalinus Clay bedding, while points O_4, O_5 and O_6 are located perpendicular to the bedding. Unlike in the bentonite, the anisotropy due to the Opalinus Clay bedding does have measurable effect on temperatures and pressures in the Opalinus Clay. The increased permeability and thermal conductivity parallel to the bedding affects fluid and heat flow. Figure 9 shows higher predicted temperatures at observation points located parallel to the bedding compared to the points located perpendicular to the bedding. In Figure 10 predicted pressure values at some locations (e.g. O_1) indicate the formation of unsaturated conditions at parts of the Opalinus Clay close to the tunnel.

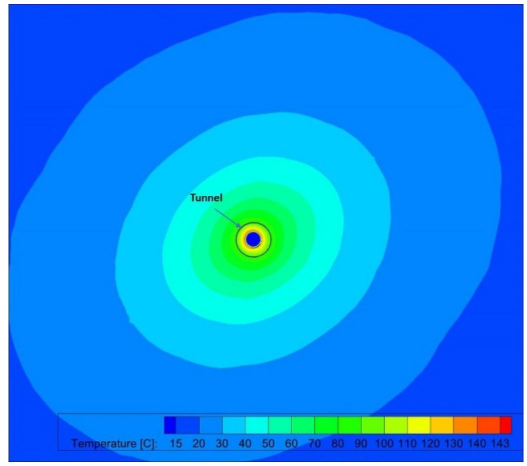

Fig. 4: Step0b Results: PFLOTRAN Predicted Temperature Distribution at 1800 Days (with anisotropy).

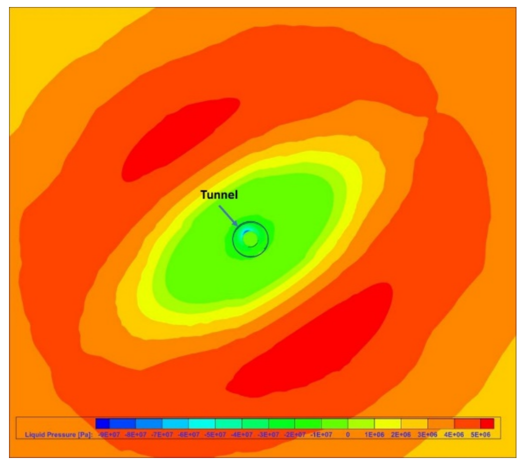

Fig. 5: Step0b Results: PFLOTRAN Predicted Liquid Pressure Distribution at 1800 Days (with anisotropy).

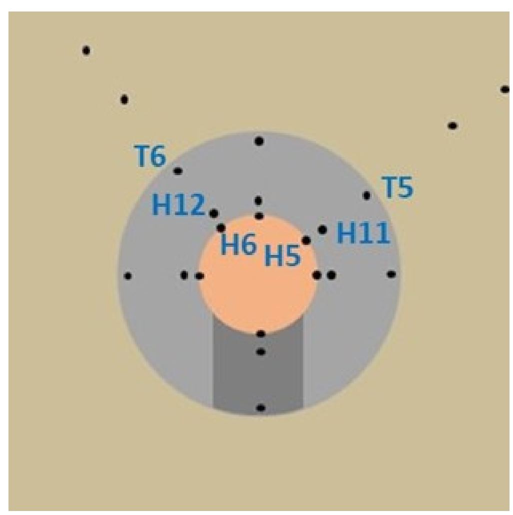

Fig. 6: Locations of observation points inside tunnel.

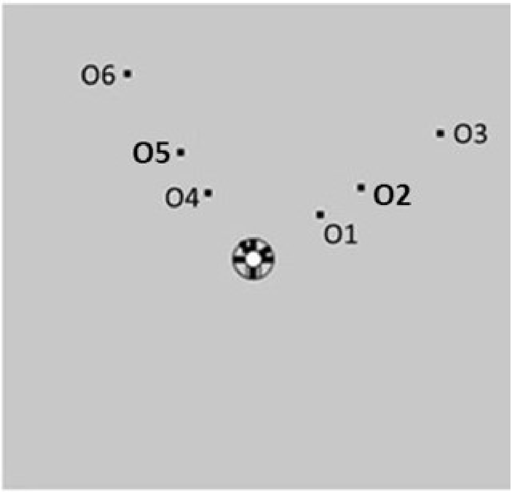

Fig. 7: Locations of observation points at Opalinus Clay

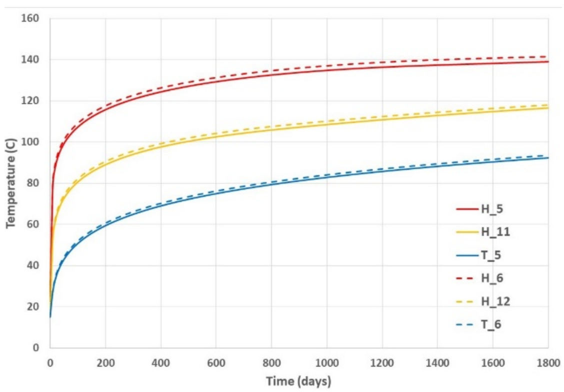

Fig. 8: PFLOTRAN Predicted Evolution of Temperature at Specified Locations in the granular bentonite and bentonite blocks.

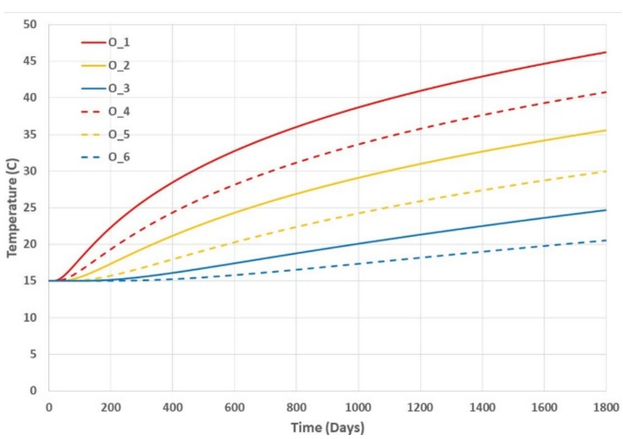

Fig. 9: PFLOTRAN Predicted Evolution of Temperature at Specified Locations in the Opalinus Clay

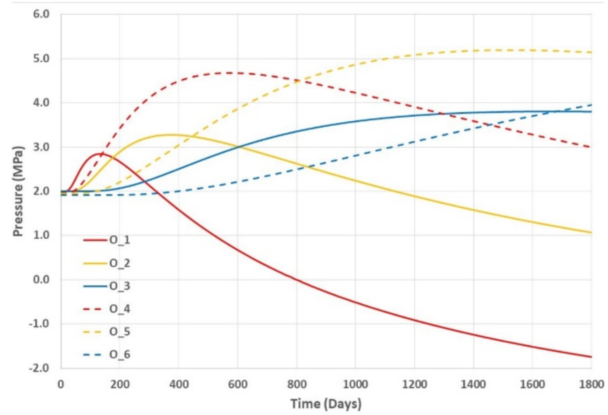

Fig. 10: PFLOTRAN Predicted Evolution of Liquid Pressure at Specified Locations in the Opalinus Clay

REFERENCES

1. 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.
2. 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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