Numerically reproduced HE-E experiment of Mont Terri project by Thermo-Hydro-Mechanical coupled model

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Abstract. In this study, numerical simulations of HE-E experiment in Mont Terri rock laboratory were performed with Thermo-Hydro-Mechanical (THM) coupled processes. The aim of this study is to validate modelling, understand THM coupled behaviour and verify applicability of material parameters obtained by a column test to the full-scale model. The results of THM and TH coupled analysis are compared, and the influence of fluid and thermal terms/factors on mechanical behaviour is discussed. The analysis code used for THM and TH coupled analysis was CODE_BRIGHT. An axisymmetric analytical model, which allowed modelling of two heaters, was used for the THM and TH coupled model, and their results were compared. As a result, a better reproducibility of relative humidity in the Engineered Barrier System (EBS) and pore water pressure of the bedrock was achieved by performing mechanical coupling. Furthermore, experimental conditions were simulated more realistically, since two heaters and different backfill materials were also modelled in the analysis.

1 Introduction

As part of an international collaborative study on radioactive waste disposal, 48 types of in-situ tests are being conducted at the Mont Terri Rock Laboratory located in the Jura Mountains, north western Switzerland [1]. One of these tests is the in-situ heater experiment (HE-E), which simulated Engineered Barrier System (EBS) in a radioactive waste disposal site with 1/2 scale, to grasp thermal, hydraulic and mechanical (THM) coupling behaviour. This experiment has been underway for about eight years since June 2011.

The HE-E experiment is performed in the microtunnel (μ tunnel in the figure) of the Mont Terri Underground Research Laboratory (URL) shown in Figure 1[1]. Microtunnel is 50 m in length and 1.3 m in diameter. The HE-E experiment is in a section, which is 10 m long and located 30 m away from the microtunnel entrance. The surrounding rock is Opalinus clay, which is a type of mudstone, and is the target host rock of the radioactive waste disposal facility in Switzerland.

A heater which models the waste in the centre of the tunnel is installed on the block bentonite, and the surrounding area is backfilled with sand-bentonite (S/B) mixture or granular bentonite, as shown in Figure 2[2]. The heating test started on 4th June 2012 after backfilling was completed. The heater temperature became steady around 7th October 2012 and until now the heater surface temperature has been kept almost constant at 140°C.

The purpose of the HE-E experiment is to construct a test database necessary for the validation of THM coupled analysis and the upscaling of parameters obtained from the element test to the field scale.

Fig 1. Layout plan of the Mont Terri test site [1]

Fig 2. Outline of HE-E experiment [2]

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The experimental setup has two types of backfill soil and these are divided by a concrete plug.

The section around Heater 1 is filled with a 65/35 S/B mixture and the section around Heater 2 is filled with pure MX80 granular bentonite as shown in Figure 2. Around these heaters, the dry density of the S/B and granular bentonite are $\rho_d=1.383 \text{ Mg/m}^3$ and $\rho_d=1.513 \text{ Mg/m}^3$, respectively. The heater is installed on block bentonite with a dry density of $\rho_d=1.806 \text{ Mg/m}^3$. The bentonite used in this experiment is Na bentonite MX-80 from Wyoming, USA.

The material parameters were set by the results obtained from the material test. Because the aim of this study is the validation for upscaling of material parameters from laboratory to field scale. An axisymmetric model was chosen as the analysis model and both the S/B and the granular bentonite section were modelled. Moreover, THM and TH coupled analysis were performed using the same material parameters, and the influence of mechanical process was discussed by comparing the results obtained from these two analyses. The analysis code used in both TH and THM coupled analysis was CODE_BRIGHT [3].

2 Analysis Code: CODE_BRIGHT

HE-E experiment is necessary to reproduce the swelling behaviour of bentonite materials due to groundwater infiltration and heat generated by the heater. Hence, THM coupled analysis is carried out. The governing equations of CODE_BRIGHT are based on the mass conservation of solid, water and gas, momentum conservation and internal energy conservation laws. The mechanical behaviour is described by the stress rate. The strong point of this code is that behaviour of swelling clay both in saturated and unsaturated state can be considered by Barcelona Basic Model [4] (BB model), which is one of the elasto-plastic constitutive models included in the code. BB Model is an extension of the modified Cam-Clay model, which also covers unsaturated soil behaviour.

The relationship between e -log p' and suction and the yield surface of the BB model are shown in Figure 3 and Figure 4, respectively.

Fig 3. The relationship of e -log p' and suction in BB Model

Fig 4. Yield surface of BB model

3 Coupled analysis by CODE_BRIGHT

3.1 Analysis model and boundary conditions

In TH and THM coupled analysis, the HE-E experiment was modelled by axial symmetry with the centre of the tunnel as the symmetry axis. Both the concrete plug and bentonite backfill inside the tunnel were modelled. There are two heaters in the HE-E experiment. Each heater is backfilled with a different material, as S/B and granular bentonite. Since thermal, hydraulic and fluid migration characteristics are different in each material, it can be considered that the response of the bedrock near the tunnel of each heater section can be different. Hence, to be able to simulate this behaviour both the S/B and bentonite sections are modelled. The analytical model is shown in Figure 5.

The analysis steps applied in this study are as follows: Step1: initial conditions of Opalinus clay is simulated, Step2: excavation of microtunnel is performed, Step3: ventilation experiment is simulated by applying 2MPa of suction pressure on the wall, Step 4: construction of EBS, Step5: reproduction analysis of HE-E experiment is performed.

In Step1, the initial conditions for the Opalinus clay were set with reference to B. Garitte et al. [1]. Hence, initial pore water pressure and the initial stress of the Opalinus clay was set to 0.8MPa and 4.9MPa [5], respectively. The initial temperature of all materials was 15°C.

Mechanical boundary conditions for the top, bottom and right side of the model were set as fixed in normal direction and free in tangential direction. To be able to create the initial state of the bedrock, the left boundary of the model on the microtunnel side was fixed in the normal direction and free in the tangential direction in this step. An initial pressure of 0.8 MPa was applied on the top, bottom and the right side of the model as fluid boundaries under the saturated condition (water pressure P_l = gas pressure P_g). On the left side of the model excluding regions where the bentonite and the plug materials were located, the initial pressure was set as 0.8MPa in the step of creating the initial state of the bedrock.

However, during the microtunnel excavation step (Step2), mechanical boundary on the left side of the model has changed to a fixed stress boundary and a surface pressure of 0.1MPa equivalent to atmospheric pressure was applied. The temperature was kept constant at 15°C in all boundaries.

To consider the influence of the ventilation experiment in the analysis, in Step3 2.0MPa of suction was loaded on the tunnel wall [6] as soon as steady state after the excavation stage has been reached.

Step 4 carried out to simulate construction of EBS. Hence, degree of saturation for S/B and granular bentonite were set as 11% and 20%, respectively. The initial saturation of the concrete plug was set as 4%. The initial stress in the whole engineered barrier was equivalent to atmospheric pressure, and the effective stress was set as 0 MPa. The water pressure (P_l) and the gas pressure (P_g) of the plug and the bentonite were set to achieve initial degree of saturation.

Fig 5. Analytical model

The heater experiment is divided into two phases. First, the heater was switched on from June 30, 2011, and the temperature was raised to 140°C over 1 year. In the second phase, the temperature was kept constant at 140°C. In the analysis, the heater experiment is simulated by applying measured temperature values during the experiment at the interface between bentonite material and the heater at the last step (Step5).

3.2 Material parameters

The thermophysical, gas-liquid two-phase flow, and mechanical properties, which are necessary to perform THM coupled analysis, are summarized in this section.

3.2.1 Physical properties

The physical properties used in this study are shown in Table 1 for solid phase [6].

Table 1. Physical properties for solid phase

	S/B	Granular bentonite	Concrete plug	Opalinus Clay
Solid grain density ρ_s (kg/m ³)	2700	2700	2700	2700
Solid phase specific heat C_s (J/kg · K)	826	893	1000	946.5
Porosity n (%)	47	45	20	13.7
Volumetric thermal expansion coefficient α (K ⁻¹)	2.5×10^{-5}	2.5×10^{-5}	1.0×10^{-5}	1.5×10^{-6}

3.2.2 Thermophysical properties

The saturation-dependent thermal conductivity in the CODE_BRIGHT analysis code is applied according to Eq. (1).

$$\lambda = \lambda_{sat} \sqrt{S_l} + \lambda_{dry} (1 - \sqrt{S_l}) \quad (1)$$

where λ_{sat} is the thermal conductivity under fully saturated condition, λ_{dry} dry is the thermal conductivity under dry condition and S_l is the degree of saturation of liquid phase. The thermoelectric coefficient of each material is listed in Table 2.

Table 2. Thermal parameters

	S/B	Granular bentonite	Concrete plug	Opalinus Clay
Dry thermal conduct. λ_{dry} (W/mK)	0.3	0.3	0.5	1.36
Saturated thermal conduct. λ_{sat} (W/mK)	1.0	1.0	1.4	1.80

3.2.3 Two-phase flow parameters

The element test results [6] were fitted with either Van Genuchten (vG)'s formula [7] or power law for two-phase flow parameters.

Table 3. Initial saturation and permeability

	S/B	Granular bentonite	Concrete plug	Opalinus Clay
Initial saturation (%)	11.0	20.0	4.0	100.0
Permeability (m ²)	3.5×10^{-20}	3.0×10^{-18}	2.5×10^{-20}	1.0×10^{-20}

Table 4. Parameter for capillary pressure

	S/B	Granular bentonite	Concrete plug	Opalinus Clay
Model	vG	vG	vG	vG
P_0 (MPa)	0.165	10.0	15.0	18.0
Shape parameter λ	0.259	0.401	0.500	0.401
Residual/max water saturation	0.01 – 1.00	0.01 – 1.00	0.01 – 1.00	0.01 – 1.00

Table 5. Parameter for relative permeability

	S/B	Granular bentonite	Concrete plug	Opalinus Clay
Intrinsic permeability (m ²)	1.0×10^{-19}	3.5×10^{-20}	1.0×10^{-20}	2.5×10^{-20}
Model	Power law	Power law	vG	vG
Parameter A	1.00	1.00	—	—
Shape parameter λ	9.00	10.0	0.500	0.401

Fig 6. Water retention curves

Fig 7. Relative permeability curves

The parameters of the initial saturation with absolute permeability, water retention and the relative permeability curves used in this study are listed in Table 3-5, respectively. Graphs of the water retention and the relative permeability curves are given in Figures 6 and 7.

3.2.4 Vapour diffusion

The water vapour diffusion in CODE_BRIGHT is based on Fick's law. The same parameters were used for all materials in the analysis, as parameter D and n are 5.9×10^{-6} and 2.3, respectively. Tortuosity was set to 0.8 for bentonite material and that 1.0 for concrete plug and Opalinus clay.

3.2.5 Mechanical parameters

The mechanical parameters for bentonite materials are listed in Table 6. The BB model was applied for S/B and Granular bentonite, which can simulate the swelling and elastoplastic behavior of expansive clay.

Table 6. Mechanical parameters for bentonite materials

Mechanical parameters	Symbol	Unit	Granular bentonite	S/B
Initial void ratio	e	—	0.80	0.86
Poisson's ratio	ν	—	0.20	0.20
Initial elastic slope for specific volume – mean stress	κ_0	—	0.06	0.06
Slope of void ratio – mean stress curve for saturated material	λ_0	—	0.170	0.170
Initial elastic slope for specific volume – mean stress	κ_{s0}	—	0.030	0.030
Parameter for expansive material	α_{sp}	—	-0.13	-0.13
Parameter for expansive material	α	—	-0.0015	-0.0015
Parameter for expansive material	α_{ss}	—	-0.016	-0.016
Parameter controlling the rate of increase of soil stiffness with suction	β	MPa ⁻¹	0.05	0.05
Parameter defining the maximum soil stiffness	γ	—	0.60	0.60
Critical state line parameter	M	—	1.30	1.30
Tensile strength in saturated conditions	P_{s0}	MPa	0.10	0.10
Parameter governing the increase of tensile strength with suction	k	—	0.10	0.10
Parameter controlling the decrease of tensile strength with temperature	ρ	°C ⁻¹	0.20	0.20
Initial preconsolidation mean stress for saturated soil	$P_{0'}$	MPa	1.00	1.00
Parameter for elastic thermal strain	α_0	°C ⁻¹	7.5×10^{-5}	7.5×10^{-5}

For Opalinus Clay, an elastic-plastic model was used, and Mohr – Coulomb yield criterion was applied as the yield surface. The concrete plug is modeled as an elastic body. For Opalinus clay and Concrete plug, Young modulus were 4000MPa and 33000MPa and Poisson's ratio were 0.24 and 0.2, respectively. The cohesion and friction angle for Opalinus clay were set to 2.2MPa and 25°, respectively.

4 Modelling results

4.1 Location of sensors

The comparison of the analysis results with the experimental results focuses on the relative humidity and temperature inside the EBS and temperature and pore water pressure for Opalinus Clay. The location of sensors inside the EBS are shown in Figure 7, and the results from sensors at all locations are to be compared.

At a larger distance from the microtunnel, the borehole BVE-91 on the S/B section side is also selected as one of the target locations for the comparison of the results (Figure8).

Fig 7. Location of the instrumented sections inside the buffer

Fig 8. Positional relationship between borehole BVE-91, Microtunnel and Gallery 98

4.2 Results of analysis

The results of THM and TH coupled analysis in comparison with experimental results are explained in this section. In all figures below, solid line, dashed line and symbols indicate results of THM analysis, TH analysis and experiments, respectively.

4.2.1 Relative humidity evaluation

In all the results (Figs. 9-10), on the heater side including the central part, the relative humidity decreases due to overheating by the heater. On the other hand, the relative humidity tends to increase with groundwater infiltration at the Opalinus Clay side and diffusion of water vapor from the center. In particular, THM coupled analysis shows good reproducibility at both the Granular bentonite and the S/B section.

On the other hand for the TH coupled analysis, although the relative humidity on the heater side decreases and on the bedrock side tends to increase, the reproducibility has lower quality than the THM coupled analysis. In particular, the reproducibility is not good until around 500 days when the relative humidity reaches a steady state, and the decrease in relative humidity is slower than the experimental results. In THM coupled analysis, since the void pressure increases with the generation of water vapour on the heater side, volume change occurs and the void ratio increases. As a result, the pores increased and the relative humidity decreased due to this volume increase.

Fig 9. Reproducibility of relative humidity in granular bentonite section by TH and THM coupled analysis

Fig 10. Reproducibility of relative humidity in S/B section by TH and THM coupled analysis

The reproducibility of relative humidity is most affected by the parameters of the water retention curve. In CODE_BRIGHT, the mass content per unit volume of moisture contained in the gas phase mass is calculated by the psychrometric law as described in Eq. (2), and the relative humidity is determined by the ratio of the mass content per unit volume with its the initial stage value as shown in Eq. (3).

$$\theta_g^w = (\theta_g^w)_0 \exp \left[\frac{-(P_g - P_l)M_w}{R(273.15 + T)\rho_w} \right] \quad (2)$$

$$RH = \frac{\theta_g^w}{(\theta_g^w)_0} \cdot 100 \quad (3)$$

where, θ_g^w is mass content per unit volume, $(\theta_g^w)_0$ is the vapour concentration in the gas phase at saturation conditions, P_g is pore air pressure, P_l is pore water pressure, M_w is molecular mass of water, R is gas constant and ρ_w is water density [6]. Although in psychrometric law denominator in exp is not $P_g - P_l$, but the total suction including osmotic suction, in this study we have defined it as referred in [6]

The difference between pore air and water pressure used in the numerator of Eq. (2), is equivalent to the suction. For this reason, relative humidity is specified according to the change of the molecular mass of water. Thus, it is clear that the setting of the water retention curve affects the reproducibility of relative humidity. On

the other hand, pore air and water pressures change according to the two-phase flow characteristics. In addition, change in volume due to mechanical changes affects gas-liquid permeability. In case that water retention characteristics are set by reproduction analysis of element test, they depend on the conditions used during the reproduction analysis. Therefore, the water retention curves used in this study are set by reproduction analysis of the element test [6] by THM coupled analysis, hence water retention characteristics are expected to have a mechanical coupling effect. As a result, it can be concluded that the THM coupled analysis was more reproducible.

4.2.2 Temperature evaluation

Comparing results of THM and TH coupled analysis (Figures 11 and 12), a high reproducibility is obtained by both, and the mechanical coupling effect is quite small. However, a higher reproducibility near the heater is achieved by THM coupled analysis. The reason of small difference between THM and TH coupled analysis is that the constitutive model of thermal conductivity, given in Eq. (1) depends on saturation and the mechanical effect contributes indirectly. Therefore, the effect of mechanical coupling on the reproducibility of heat is relatively small. However, if the mechanical term for the thermal conductivity is considered in a constitutive model, it will be affected.

Fig 11. Temperature reproducibility at granular bentonite section by TH and THM coupled analysis

Fig 12. Temperature reproducibility at S/B section by TH and THM coupled analysis

The reproducibility of THM and TH coupled analysis slightly decreases in the bedrock side. In case of both granular bentonite and S/B sections, the reproducibility decreased, which is thought to be due to the effect of inhomogeneity in the test specimen.

Depending on the above discussions, the thermophysical properties of the bentonite used in the analysis are reasonable, and the validity of the material parameters obtained from the element test is confirmed.

4.2.3 Pore water pressure evaluation

The experimental results showed that the pore water pressure reached a peak at about 500 days and then dissipated, similarly the analytical results also reproduced this trend. A smaller pore water pressure was observed in the THM coupled analysis than in the TH coupled analysis (Figures. 13-15).

As an effect of mechanical coupling, the pore pressure decreased due to the expansion of the volume in the bedrock as the pore pressure increased. As a result of mechanical coupling in THM analysis, the density distribution became inhomogeneous inside the EBS due to the generation of water vapor near the heater. Since the volume on the bedrock side became denser, the permeability on the bedrock side was decreased and the influence on the bedrock of pore pressure was reduced.

Fig 13. Reproducibility of pore water pressure by TH and THM coupled analysis at 2m away from the wall

Fig 14. Reproducibility of pore water pressure for borehole BHE-E1 located at a larger distance from the microtunnel

Fig 15. Reproducibility of pore water pressure by TH and THM coupled analysis for boreholes BVE-91 located at a larger distance from the microtunnel

5 Conclusions

In order to investigate effect of mechanical coupling, both TH and THM coupled analysis were performed on simulating HE-E test. The comparison between the analysis and the experimental results were made on the relative humidity inside the EBS, the temperature of the bedrock in the EBS and 2 m away from the tunnel wall, and the pore water pressure of the bedrock. The results are summarized below:

- A better reproducibility of relative humidity was obtained by THM coupled analysis, since the increase in pore pressure caused a volumetric change and void ratio was increased by mechanical coupling.
- The reproducibility of relative humidity is affected by the setting of the water retention curve.
- The constitutive model of thermal conductivity is an equation depending on saturation, and the influence of mechanics is but not that significantly. Hence, regarding the reproducibility of temperature inside EBS, there was no big difference between THM and TH coupled analysis results.
- The pore water pressure inside the bedrock reached a peak at about 500 days followed by a tendency to dissipate, which was reproduced also by the analysis, while the pore water pressure was smaller in the THM coupled analysis than in the TH coupled analysis.
- In order to improve the reproducibility of both analyses, it would be better to slightly change the two-phase flow parameters.

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