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Modelling the behaviour of swelling clays in a Geological Disposal Facility (GDF)

La modélisation du comportement des argiles gonflantes dans les structures pour le stockage géologique profond

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ABSTRACT: This paper discusses the numerical modelling of the buffer material in a Geological Disposal Facility (GDF), by simulating the FEBEX in-situ experiment. The test was conducted over 18 years at the Grimsel site in Switzerland, under the conditions of a real GDF, with compacted bentonite blocks used as the buffer material and a heater replacing the nuclear waste canister. Particular emphasis in the paper is given to the constitutive modelling of the FEBEX bentonite, highlighting the importance of accounting in the model for the double porosity structure of the compacted bentonite. Furthermore, the coupled thermo-hydro-mechanical (THM) finite element analysis also emphasises the importance of realistic modelling of the evolution of the hydraulic permeability of the bentonite with the changing suctions. The analysis results demonstrate substantial agreement between numerical predictions and FEBEX field measurements in terms of the buffer's THM evolution. The area of the host formation affected by the test is also defined and investigated in order to provide useful information for the design of a GDF.

RÉSUMÉ: Cet article discute de la modélisation numérique du comportement du bouchon de bentonite en simulant le test FEBEX. Ce test a eu lieu pendant 18 ans au Grimsel en Suisse : les conditions d'une vraie structures pour le stockage géologique profond ont été reproduites, avec un bouchon fait par des blocs compactés de bentonite et les déchets simulés par des appareils de chauffage. Une attention particulaire est portée à la modélisation constitutive du bouchon de FEBEX bentonite : le rôle de la double structure dans la bentonite compactée est très important. En outre l'analyse numérique thermo-hydro-mécanique (THM) aux éléments finis souligne l'importance de prendre en compte le changement de la perméabilité de la bentonite avec la succion. Les résultats de l'analyse numérique sur l'évolution thermo-hydro-mécanique du bouchon sont en accord avec les mesures prises par les capteurs situés dans la bentonite. La région de la roche dans laquelle la structure pour le stockage géologique profond est creusée est étudiée afin de définir les contours de la partie la plus influencée par le test FEBEX et de fournir des indications utiles en phase d'étude.

Keywords: Geological Disposal Facility; FEBEX; buffer; double-structure

1 INTRODUCTION

The solution proposed in many European countries for the long-term storage of high-level radioactive waste comprises the construction of a Geological Disposal Facility (GDF) infrastructure. Within these underground facilities the radioactive material would be placed inside a drift or borehole where, sealed inside corrosion-resistant copper or steel canisters, it would be protected by a buffer material. Made of compacted, unsaturated blocks, the buffer is a highly expansive clay capable of developing high swelling pressures upon contact with groundwater supplied by the host formation in which the drift or borehole is excavated. Upon resaturation the swelling of the buffer provides an additional and fundamental layer of protection for the waste, which must be isolated at all times from the host formation in order to avoid a potentially disastrous leakage of contaminants. A numerical study of the Thermo-Hydro-Mechanical (THM) evolution of the buffer upon resaturation is therefore an essential tool to investigate the effectiveness of GDFs.

The FEBEX in-situ experiment is a repository mock-up test conducted at real scale that was conceived with the purpose of demonstrating the feasibility of constructing a GDF. The structure was kept in operation for nearly 20 years, providing an adequate time period for the interpretation and prediction of the THM processes that concur in the evolution of the buffer. The experiment generated a large amount of data which can be, and has been, employed in the development and validation of numerical tools.

In this paper the FEBEX in-situ experiment is numerically reproduced using the finite element code ICFEP (Imperial College Finite Element Program, Potts & Zdravkovic, 1999). In particular, the constitutive framework IC DSM (Imperial College Double Structure Model, Ghiadistri et al., 2018) is employed to simulate the buffer. Its performance is evaluated through a comparison of the numerical predictions and the field measurements collected in the documentation of the FEBEX in-situ test (ENRESA, 2000; FEBEX, 2017).

2 THE FEBEX IN-SITU EXPERIMENT

The FEBEX (Full-scale Engineered Barriers Experiment in Crystalline Host Rock) in situ test was conducted over a period of 18.4 years, from 1997 to 2015, at the Grimsel test site in Switzerland (FEBEX, 2017). Excavated below 450 meters of granitic rock, which constitutes the host formation, the FEBEX drift is 20 m long, with a circular cross-section 2.28 m in diameter. Two electrical heaters were placed inside the drift, each with a circular section 0.9 m in diameter, which were designed to simulate real waste-containing canisters. In reality, the radioactive material would decay over time, hence giving off heat that affects both the buffer and a portion of the host rock.

The space between the canisters and the drift walls was filled with the buffer material. In this case several rings of compacted FEBEX bentonite blocks were emplaced around the heaters. A transverse section of the drift which includes either of the two heaters presents three rings of blocks: the inner ring, which is closest to the heater, the middle ring and the outer ring, which is closest to the rock. Non-heater transverse sections present an additional central zone of bentonite blocks. The drift is closed with a 2.7 meter long concrete plug.

The buffer was heavily instrumented with sensors, providing continuous measurements of relative humidity, temperature and stress at numerous transverse sections of the drift.

The FEBEX in-situ test was articulated in several different stages. The first, called Stage 1A, included the first five years of operation of the facility, in which the heaters were heated up from 12°C to 100°C within two months from installation and, subsequently, maintained at a constant temperature of 100°C. Stage 1A ended with the first dismantling in 2002 (i.e. Stage 1B), in which one of the two heaters was removed. Afterwards, an additional 13 years of operation of the remaining heater constituted Stage 2 and lead to the final dismantling in 2015. Details of the test can be found in FEBEX

(2017). This paper discusses Stage 1A analysis only.

3 NUMERICAL ANALYSIS

3.1 Domain and mesh

A three-dimensional (3D) coupled THM analysis of the FEBEX in-situ experiment was performed in ICFEP. The chosen domain is shown in Figure 1: it includes the entire drift, with the concrete plug, and the surrounding host rock, both behind the drift face and around the drift walls. A projection onto the *x*-*z* plane of the part of the domain representing the drift and the surrounding rock is presented in Figure 2. Due to the axisymmetry of the field measurements collected during the FEBEX experiment (FEBEX, 2017), it was decided to study only a quarter of the full geometry.

The dimension of the domain, namely the extension of the rock to be included in the analysis, was chosen after preliminary, two-dimensional (2D) analyses were carried out on the drift's transverse section, providing an estimation of the area perturbed by the experiment. The mesh in Figure 1 employs 15282 20-noded hexahedral elements.

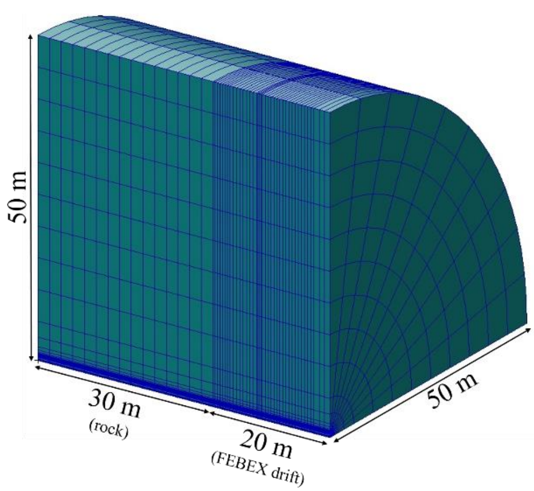

Figure 1. Finite element mesh for the analysis of the FEBEX in-situ experiment.

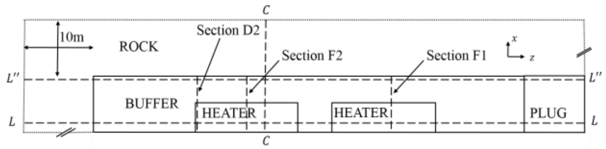

Figure 2. Part of the domain geometry projected onto the x-z plane.

3.2 Materials

There are 4 different materials included in the analysis:

- *granitic rock*. The host rock is characterised using an unsaturated Mohr-Coulomb model. From a mechanical standpoint, the material is assumed to have a purely cohesive behaviour, therefore its angle of shearing resistance is set to $\phi' = 0^{\circ}$ and its cohesion is set to a large value ($c' = 10MPa$). From a hydraulic standpoint, its permeability is assumed isotropic, constant and equal to $10^{-12}\, m/s$ (FEBEX, 2017), while its retention behaviour is modelled using the Van Genughten et al. (1980) model with parameters selected to fit the available data (FEBEX, 2017). A plot of the retention curve is omitted due to space limitations, but all model parameters are summarised in Table 1. From a thermal standpoint, the thermal conductivity is assumed to be isotropic, constant and equal to $3.2 \cdot 10^{-3}\, kW/mK$, while the specific heat capacity is equal to $920\ J/kg$℃ (FEBEX, 2017).

Table 1. Retention properties of the materials.

Parameter	Rock	FEBEX bentonite
Fitting parameter, $\boldsymbol{\alpha}$	0.4	0.00002
Fitting parameter, $\boldsymbol{m}$	0.4	0.4
Fitting parameter, $\boldsymbol{n}$	0.9	1.7
Residual degree of saturation, $\boldsymbol{S_{r0}}$	0.2	0
Suction in the long term, $\boldsymbol{s_0}$ (kPa)	10^5	10^5

- *FEBEX bentonite*. The buffer material is characterised with the IC DSM (Ghiadistri et al., 2018). This constitutive model accounts for the double porosity structure typical of compacted, expansive clays. The mechanical parameters employed in the analysis are reported in Table 2. Due to space limitations, the calibration process is not described here. In terms of hydraulic characterisation, its permeability is assumed to vary with suction according to the de-saturation permeability model available in ICFEP (Potts & Zdravkovic, 1999; Nyambao & Potts, 2010). For suctions below 2 MPa the permeability is assumed as $3 \cdot 10^{-13}\, m/s$, it reduces linearly to $6 \cdot 10^{-14}\, m/s$ for suctions between 2 and 20 MPa, remaining constant at the latter value with any further increase in suction. The material‘s retention behaviour is modelled by fitting the Van Genughten et al. (1980) model to the available data (FEBEX, 2017). All model parameters for the retention curve are reported in Table 1. In terms of thermal properties, the thermal conductivity is assumed to be isotropic, constant and equal to $0.55 \cdot 10^{-3}\, kW/mK$, while the specific heat capacity is $870\, J/kg$℃ (FEBEX, 2017).

Table 2. IC DSM parameters for the FEBEX bentonite.

Parameter	Value
Parameters controlling the shape of the yield surface, $\boldsymbol{\alpha_F}, \boldsymbol{\mu_F}$	0.4, 0.9
Parameters controlling the shape of the plastic potential surface, $\boldsymbol{\alpha_G}, \boldsymbol{\mu_G}$	0.4, 0.9
Strength parameters, $\boldsymbol{M_f}, \boldsymbol{M_g}$	0.5
Characteristic pressure, $\boldsymbol{p_c}$ (kPa)	500
Fully saturated compressibility coefficient, $\boldsymbol{\lambda(0)}$	0.2
Elastic compressibility coefficient, $\boldsymbol{\kappa}$	0.06
Maximum soil stiffness parameter, $\boldsymbol{r}$	0.61
Soil stiffness increase parameter, $\boldsymbol{\beta}$ (1/kPa)	$7 \cdot 10^{-5}$
Elastic compressibility coefficient for changes in suction, $\boldsymbol{\kappa_s}$ (kPa)	0.02
Poisson ratio, $\boldsymbol{\nu}$	0.4
Plastic compressibility coefficient for changes in suction, $\boldsymbol{\lambda_s}$	0.5
Air-entry value of suction, $\boldsymbol{s_{air}}$ (kPa)	1000
Yield value of equivalent suction, $\boldsymbol{s_0}$ (kPa)	10^6
Microstructural compressibility parameter, $\boldsymbol{\kappa_m}$	0.1
Coefficients for the micro swelling function, $\boldsymbol{c_{s1}}, \boldsymbol{c_{s2}}, \boldsymbol{c_{s3}}$	-0.1, 1.1, 2.0
Coefficients for the micro compression function, $\boldsymbol{c_{c1}}, \boldsymbol{c_{c2}}, \boldsymbol{c_{c3}}$	-0.1, 1.1, 2.0

- *canister (i.e. steel) and concrete plug*. Both materials have been assumed to be thermally inactive and non-consolidating. Their Young‘s modulus is set to a large value ($E = 2 \cdot 10^5$ MPa) to simulate rigidity and their Poisson‘s ratio is equal to 0.25.

3.3 Boundary conditions

Throughout the analysis, the mechanical boundary conditions impose zero radial displacements on the cylindrical external surface of the mesh, zero axial displacements on the front and rear surfaces, zero vertical displacements on the base of the mesh and zero horizontal displacements on the vertical symmetry plane.

In terms of hydraulic boundary conditions, the rock is assumed to be an infinite source of water, hence no change in pore water pressure is imposed on the rear and the cylindrical outer surface of the mesh. Equally, from a thermal standpoint, no change in temperature is imposed on these boundaries. The other boundaries are assumed to have no hydraulic flow or temperature flux across them.

The simulation reproduces the installation of the experiment and the entire operation of Stage 1A. It is articulated in three phases:

- *excavation*. The FEBEX drift is excavated in the rock;
- *construction*. The buffer, the heaters and the plug are installed;
- *operation*. The heaters start from a temperature of 12°C and, over a period of two months, reach 100°C. Subsequently, this temperature is kept constant and it gradually heats up the buffer.

3.4 Initial conditions

The initial conditions assumed for the in-situ rock and the bentonite on its construction are reported in Table 3.

Table 3. Initial conditions (pore water pressure is shown as negative suction).

Parameter	Rock	FEBEX bentonite
Suction, s (MPa)	-4.5	120
Vertical total stress, $\boldsymbol{\sigma_v}$ (MPa)	9	0
Horizontal total stress, $\boldsymbol{\sigma_h}$ (MPa)	28	0
Temperature, $\boldsymbol{T}$ (°C)	10	12
Initial dry density, $\boldsymbol{\rho_{dry}}$ (g/cm^3)	2	1.6
Initial void factor, $\boldsymbol{VF}$	-	0.3

4 RESULTS AND DISCUSSION

4.1 Comparison to field measurements

In Figures 3, 4 and 5 numerical predictions are compared to the respective field measurements taken by the sensors placed inside the buffer, in order to verify the general numerical model.

Figure 3 shows that the evolution of relative humidity (RH) over time is reasonably well captured by the model throughout the entire buffer at transverse section F2 (represented in Figure 2). It can also be noted that the buffer is far from being completely saturated at the end of Stage 1A.

In Figure 4, the temperature evolution at transverse section D2 (represented in Figure 2) is shown for three different sensors. The model captures very well the decreasing temperature in the outward radial direction: temperature is almost 100°C in the proximity of the heater, while it reduces to 35°C close to the rock.

Figure 5 shows the development of swelling pressures in the outer ring of the buffer at transverse section F1 (represented in Figure 2), as the hydration progresses from the host rock. The horizontal stress, which is underpredicted, has not yet reached the design value of 5MPa (FEBEX, 2017), however, since the buffer is still largely unsaturated, this value will increase during stage 2.

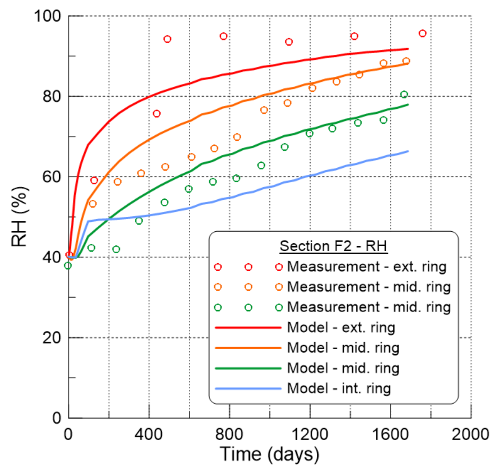

Figure 3. RH evolution over time, section F2.

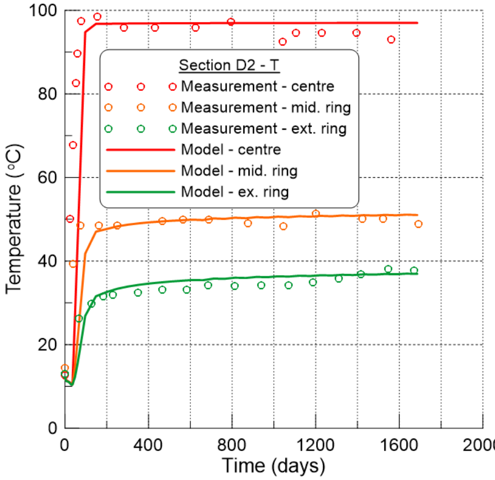

Figure 4. Temperature evolution over time, section D2.

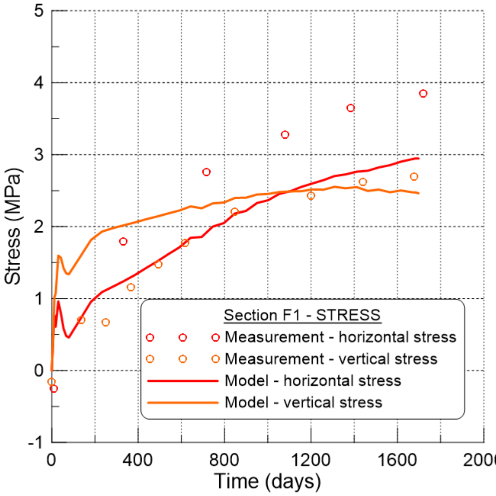

Figure 5. Stress evolution over time, section F1.

4.2 *Transverse and longitudinal sections*

In order to estimate the extent of the host formation which is perturbed by the experiment, the values of suction and temperature are interpreted across some longitudinal and transverse sections of the FEBEX drift and of the host rock. With reference to Figure 2, Figures 6 and 7 present suction and temperature changes along section LL at different time steps. Similarly, Figures 8 and 9 depict suction and temperature changes along section L''L'', while Figures 10 and 11 respectively show the same quantities along section CC, in which distance extends into the transverse *y*-direction (normal to the *x*-*z* plane).

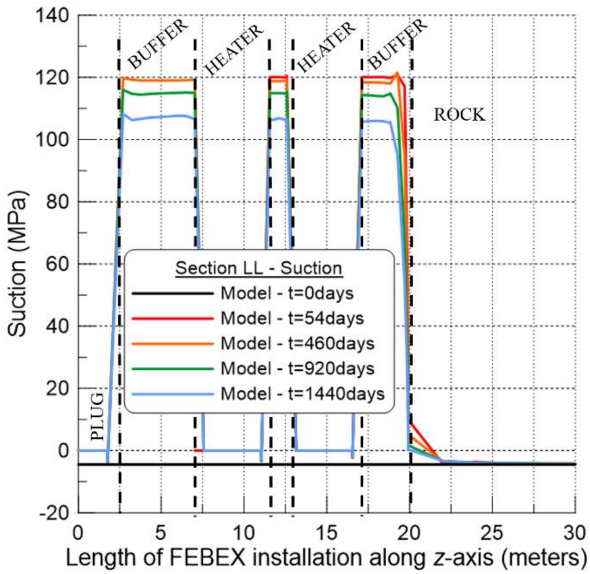

Figure 6. Suction along section LL at different time steps ($t = 54$days is during the installation phase).

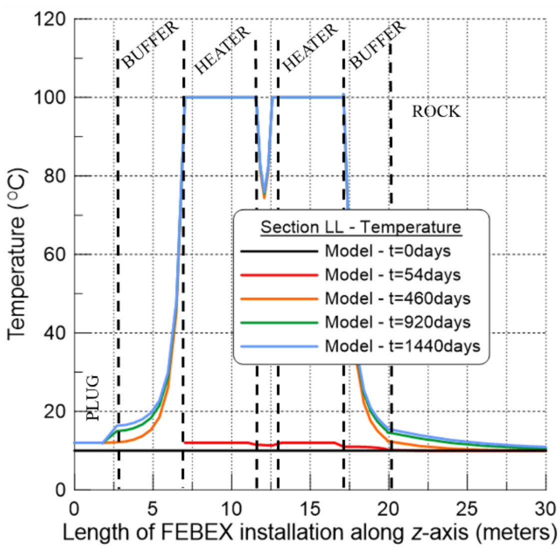

Figure 7. Temperature along section LL at different time steps ($t = 54$days is during the installation phase).

Figure 6 shows that, even at the end of stage 1A, the suction is still quite high in the bentonite that is furthest away from the host formation. On the contrary, Figure 8 presents low suction in the bentonite near the rock boundary.

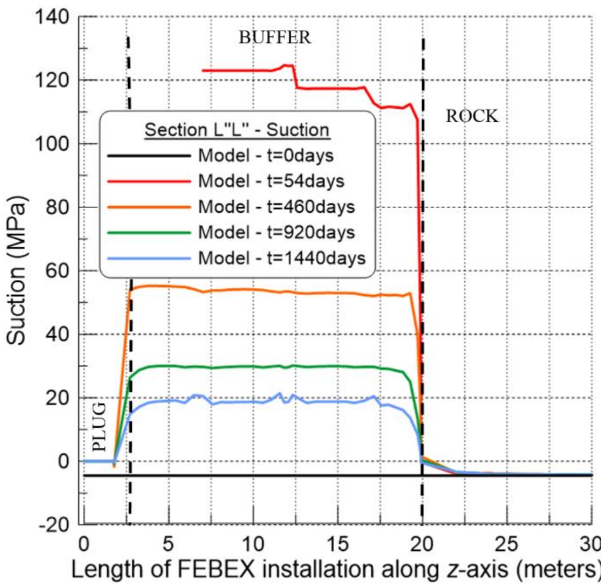

Figure 8. Suction along section L''L'' at different time steps (t = 54days is during the installation phase).

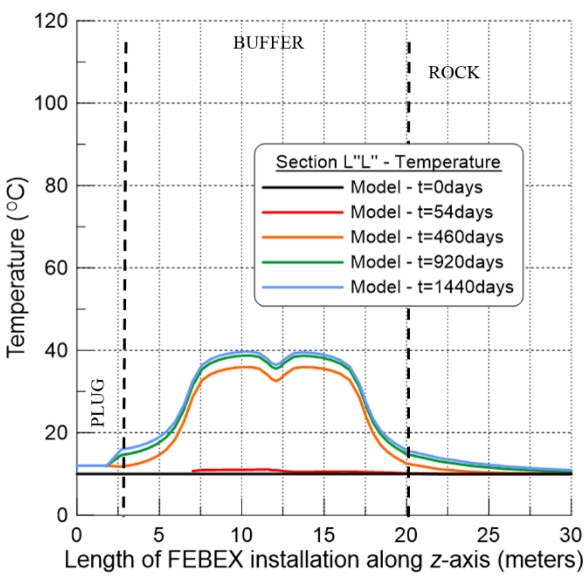

Figure 9. Temperature along section L''L'' at different time steps (t = 54days is during the installation phase).

Figure 7 shows that the temperature in the buffer increases significantly in the area between the two heaters, while it decreases rather rapidly further away from the sources of heat. Figure 9 presents temperature below 40℃ in the buffer close to the rock throughout the entire drift.

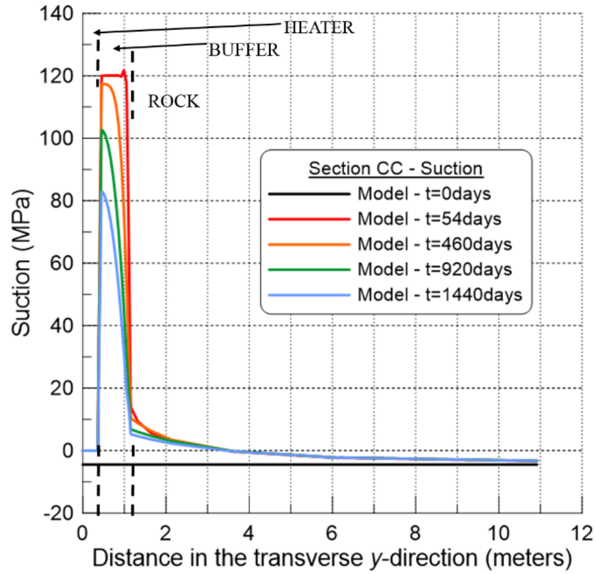

Figure 10. Suction along section CC at different time steps (t = 54days is during the installation phase).

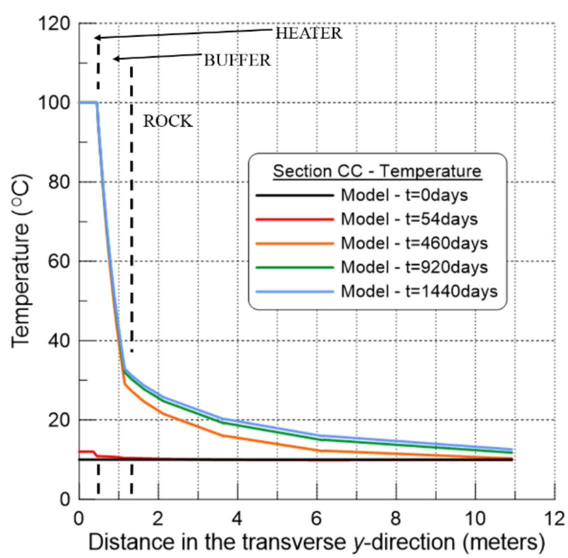

Figure 11. Temperature along section CC at different time steps (t = 54days is during the installation phase).

From Figures 10 and 11 it seems that only an area that extends over the first ten meters from the drift is significantly perturbed by the presence of the experiment. Outside this region, suction and temperature return almost perfectly to their respective values initially assigned to the host formation. Although not shown here, a similar outcome is obtained for the spatial distribution of stresses. Figures 6 to 9 corroborate this result, showing that also in the longitudinal direction the rock is mostly perturbed within 10 meters only from the face of the FEBEX drift.

5 CONCLUSIONS

A large-scale GDF mock-up test, the FEBEX in-situ experiment, has been analysed with the finite element code ICFEP. The objective was to assess the performance of the numerical tools currently at disposal for the study of unsaturated THM problems. Field measurements collected by a large array of sensors throughout Stage 1A of the FEBEX experiment have been compared to the predictions of the finite element analysis. The agreement for temperature, relative humidity and stress is very satisfying across the entire FEBEX drift. This outcome improves the confidence in the available numerical tools at Imperial College for the analysis of complex GDF scenarios. The constitutive modelling of the FEBEX bentonite buffer is carried out using the IC DSM and the satisfying results obtained from the analysis further show the importance of including the double porosity structure in the constitutive framework. In fact, preliminary analyses of the FEBEX in-situ experiment were run employing the Imperial College Single Structure Model (IC SSM) which was formulated by Georgiadis et al. (2005) as an enhancement of the BBM (Alonso et al., 1990). The comparison showed the better performance of the IC DSM, however, due to space constrains, it is not shown in this paper. At the end of stage 1A the buffer remains unsaturated, meanwhile the host formation is already affected by the presence of the experiment. Such perturbation, however, sems to be limited to the first ten meters radial distance from the drift.

6 ACKNOWLEDGEMENTS

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