Analysis of key thermal coupled factors in modelling of bentonite barriers

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ABSTRACT

Bentonite is a material considered to be used as a component of a barrier in deep geological repositories for nuclear waste. Its behaviour is affected by temperature, humidity and chemical composition of water saturating its pores. Reproduction of bentonite behaviour in such thermo-hydro-mechanical (THM) conditions involves extensive use of empirical and physical coupled relationships. This paper investigates parameters, which influence the bentonite behaviour in THM experiments relevant to the conditions in the repositories. For the study, a numerical investigation is performed based on test simulation computed with the finite element code Thebes (Abed and Sołowski 2017). A numerical simulation by Abed and Sołowski (2017) of a non-isothermal infiltration experiment (Villar and Gomez-Espina 2009) has been taken as a basis for the investigation. The results of this simulation were compared with a series of 7 other simulations that are set up by inactivating the selected thermally coupled variables, one at a time. Presented results identify the key parameters the simulation is sensitive to and provide insights on the relevance of the underlying coupled processes.

Keywords: Bentonite, nuclear repository, thermo-hydro-mechanical coupling, net mean stress.

1   INTRODUCTION

Unsaturated expansive clays, such as bentonite, considered to be an ideal material to be used as a barrier to isolate the radioactive waste in deep geological repositories (Chapman and McCombie 2003; NDA 2014; Sellin and Leupin 2014) due to its properties such as low permeability, self-sealing ability and long-term stability (Sellin and Leupin 2014). As radioactive waste takes thousands of years to decay (United States Nuclear Regulatory Commission 2019), to ensure safe disposal, one has to have confidence in the prediction of the expansive clay barrier behaviour over a very long time. The prediction is typically achieved based on Finite Element (FE) simulation (e.g., Navarro and Alonso 2000; Guimarães et al. 2006; Seetharam et al. 2007; Abed and Sołowski 2017). Although expansive clay is a structurally complex material, modelling repository conditions is particularly challenging due to the presence of coupled THMC processes (thermal, hydraulic, mechanical, and chemical). A model thus usually relies on several empirical and physical relationships, requiring many input variables.

The study aim is to identify the variables that majorly influence bentonite behaviour in thermally coupled simulation. This may be further extended in the future to other variables, ultimately leading to more accurate predictions of repository safety.

This study uses the finite element code Thebes (Abed and Sołowski 2017) to model fully coupled THMC behaviour of bentonite. The research runs series of analysis with certain parts of the coupled equations inactive. Those were compared to an original analysis (Abed and Sołowski 2017), simulating a non-isothermal infiltration experiment on FEBEX bentonite (Villar and Gomez-Espina 2009). It is worth mentioning that even though the coupling equations evaluated can be specific to Thebes, they still provide valuable general insights, as the physical phenomena modelled are the same as in the other THM frameworks. The undertaken research approach is less methodical than e.g. Taguchi's experimental design method or Monte Carlo simulations (Wang et al. 2010; Lafifi et al. 2019). Those approaches usually require a large number of simulations, not feasible to do in this study. Yet, we believe that the results offer some interesting insights related to the key parameters in the simulation and to the corresponding physical processes.

2   CODE THEBES AND SELECTED COUPLING VARIABLES

2.1   Thebes overview

Due to space constraints, the reader should refer to Abed and Sołowski (2017, 2018) for the description of the Thebes numerical framework. In this study Thebes models bentonite as a porous material, which includes three components: a) soil particles b) water and c) air.

These components are in 3 phases: the solid phase consists of soil particles, the liquid phase consists of liquid water and dissolved air, and the gas phase is the gaseous air. The framework, among others, includes: mass balance of the components, heat conservation and balances of mechanical forces and laws for transport of species and phase changes: Darcy's law (fluid flow), Philip and De-Vries (1957) vapour diffusion law and Fourier's law (heat flow).

2.2 Studied coupled variables

The study focuses on thermally coupled variables associated with mechanical behaviour and water components. The gas pressure head (Hg) is taken as zero in this work and hence the associated terms are neglected here. However, the study considers phase changes and water transport as vapour.

2.2.1 Mechanical related coupling terms

Thebes uses a modified version of the Barcelona Basic Model (BBM) incorporating pressure dependent elastic parameters to address the expansive nature of bentonite (Alonso et al. 1990; Hoffmann et al. 2007). Additionally, the model considers an extra temperature effect in BBM (Gens 1995; Laloui and Cekerevac 2003; Sánchez et al. 2012).

The thermo-mechanical coupling relations used in the constitutive model along with the variables evaluated in the study are described below:

a) Thebes incorporates an expression for thermal induced elastic volumetric strain rate ($\dot{\varepsilon}_e^T$) in soil, i.e. as follow (Gens 1995):

$$\dot{\varepsilon}_e^T = \frac{\left(\alpha_0 + \alpha_2\left(T - T_0\right)\right)\dot{T}}{3} \tag{1}$$

where α_0 and α_2 are material constants. In the original simulation α_2 is 0 (Abed and Sołowski 2017), hence only α_0 is investigated.

b) The suction induced strength increase p_s of BBM is temperature dependent (Gens 1995):

$$p_s = kse^{-\rho^T \Delta T} \tag{2}$$

where ρ^T is a material constant that is evaluated in the study.

c) The saturated pre-consolidation pressure (p_0^* at suction (s) = 0) is also thermally coupled (Laloui and Cekerevac, 2003):

$$p_{0T}^* = p_0^*\left[1 - \gamma_T \log\left(\frac{T - T_{ref}}{T_0 - T_{ref}}\right)\right] \tag{3}$$

where γ_T is a material constant investigated in this study, T_0 is an initial temperature and T_{ref} is a reference temperature.

2.2.2 Hydraulic behaviour related terms

The mass balance of water used in this study is (Abed and Sołowski, 2017):

$$[n(\rho_w^l - \rho_w^g)\frac{\partial S^l}{\partial T} - (1-n)(S^l\rho_w^l + S^g\rho_w^g)\beta_{sT} \tag{4}$$
$$-nS^l\beta_{wT}\rho_w^l + nS^g\frac{\rho_w^g}{T^2}(4974 + g\frac{M_w\psi}{R})]\frac{\partial T}{\partial t}$$
$$+[nS^g\frac{\rho_w^g gM_w\psi}{RT} - n(\rho_w^l - \rho_w^g)\frac{\partial S^l}{\partial \psi} + nS^l\beta_{wP}\rho_w^{l2}]\frac{\partial h_w}{\partial t}$$
$$+(S^l\rho_w^l + S^g\rho_w^g)\frac{\partial \varepsilon_v}{\partial t} + \nabla . j_w^g + \nabla . (\rho_w^l q^l) = 0$$

The reader finds the symbol description in Abed and Sołowski (2017). With respect to Eq. (4), the thermally coupled hydraulic relationships and the associated variables evaluated in the study are:

a) Thermal coupling of van Genuchten water retention curve (van Genuchten 1980; Jacinto et al. 2009), given as:

$$S^l = (S_{sat}^l - S_{res}^l)[1 + g_\alpha |\psi|^{g_n}]^{g_m} + S_{res}^l \tag{5}$$

where S_{sat}^l and S_{res}^l are the degree of saturation at full saturation and at residual state respectively, g_α, g_n and g_m are the temperature dependent curve fitting parameters, expressed in terms of reference values ($g_{\alpha 0}$, g_{n0}) at the reference temperature T_0 as:

$$g_\alpha = (\sigma_0^t / \sigma^t)g_{\alpha 0}; \ g_n = \frac{g_{n0}}{1 - \xi_n^T g_{n0}(T - T_0)}; \tag{6}$$
$$g_m = \frac{1}{g_n} - 1$$

where σ_0^t and σ^t are the surface tensions at temperatures T_0 and T, respectively and ξ_n^T is a material constant. The degree of saturation at zero suction (S_{s0}^l) is coupled with temperature as:

$$S_{s0}^l = S_{sat}^l + \xi_w^T(T - T_0) \tag{7}$$

where, ξ_w^T is a material constant.

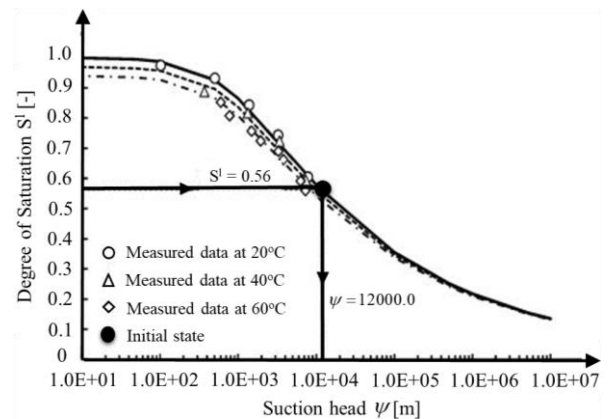The soil water retention curve shown in Fig. 1, at different temperatures is fitted in the above expressions.

Fig. 1. Retention curve at different temperatures fitted in Thebes for the simulation (Abed and Sołowski 2017).

b) Equation (4) is dependent on the coefficient for thermal expansion of water (β_{wT}). The factor leads to water density changes with temperature and thereby results in a change in water mass. Its influence in the model is thus assessed.

c) Another temperature dependency of Eq. (4) evaluated in this study is due to the coefficient for thermal expansion of solids (β_{sT}), see Fig 2.
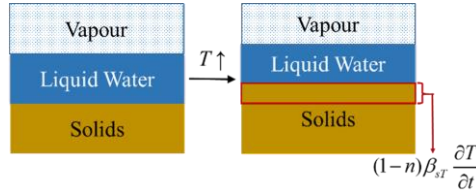

Fig. 2. Change in water and vapour masses due to change in solids via its thermal expansion.

2.3 Test configuration

Based on the identified thermal coupled variables in the earlier section, Table 1. gives the thermal couplings deactivated in 7 numerical test cases (T1 – T7).

3 NON-ISOTHERMAL INFILTRATION EXPERIMENT SIMULATION

Villar and Gomez-Espina (2009) provides detailed description and results of a non-isothermal hydration experiment with FEBEX bentonite. The test setup consisted of an insulated cylindrical cell of 40 cm in length and 7 cm in diameter, containing 5 blocks (3 blocks of 10 cm and 2 blocks of 5 cm in length) of compacted bentonite (dry density of 1.65 g/cm^3). This study uses Abed and Sołowski (2017) simulation to investigate the effects of thermo-mechanical coupling. The axisymmetric FE mesh consists of 250 quadrilateral 4-noded elements, see Figure 3c. The bentonite layer is 0.4m long and 0.035m wide, modelled by a thermally extended version of BBM constitutive model (Abed and Sołowski 2017).

The bentonite is surrounded by a Teflon layer, triaxial cell steel and foam. The latter materials are taken as a non-porous linear elastic, with different mechanical and thermal properties (refer to Table 2). The only difference with comparison to the simulation

in Abed and Sołowski (2017) is an additional, approximately 2e-6m wide interface layer between the Teflon and bentonite. This allows for a more realistic modelling of low friction of the Teflon layer. The interface is taken as a non-porous linear elastic material with Young's modulus of 100 kPa & Poisson's ratio equals to 0.499.

The simulation assumed the initial conditions: temperature 22ºC, the mean net stress 1.0 kPa and suction 120 MPa. Simulation maintained the temperature of 22ºC at the top and side boundaries, and 100 ºC at the bottom boundary (Fig. 3a). At time 65h, a constant water pressure head of 122.32 m is applied at the top boundary (Fig. 3b). The other boundaries are closed to the flow. The simulation assumes a fully rigid cell, by setting the displacements on the right side of the interface layer (adjacent to Teflon) to zero in x-direction and restricting other displacement boundaries of the bentonite layer in normal directions. The results (Fig. 3c) are read at points on the axis of symmetry at Y= 0.3m (A), 0.2m (B) and 0.1m (C).

For more information on all the other test parameter settings, refer to Table 3 in Abed and Sołowski (2017). The test simulations assume gas pressure head (h$_g$) = 0 and no gravity effect over the liquid flow.
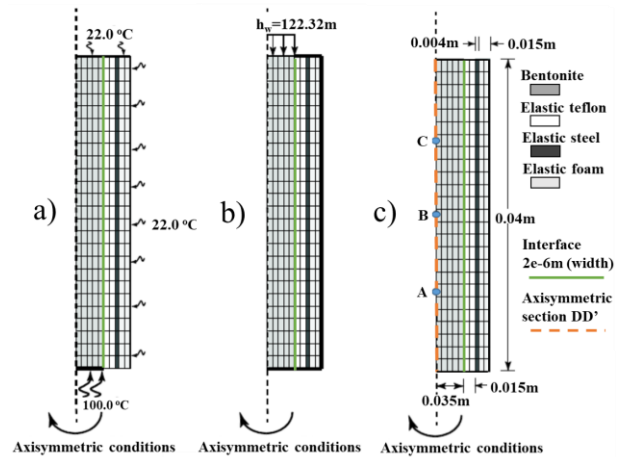

Fig. 3. Finite element model for non-isothermal infiltration test: a) thermal boundary conditions, b) hydraulic boundary conditions, c) dimension of the geometry, controlled points and section. (Modified from Abed and Sołowski 2017).

Table 1. Type of tests simulated.

Remarks	Parameter	Test							
		Original	T1	T2	T3	T4	T5	T6	T7
Thermal Coupling	-	Y	Y	Y	Y	Y	Y	Y	N
Thermal effect of BBM	α_0	Y	N	Y	Y	Y	Y	Y	N
	ρ^T	Y	Y	N	Y	Y	Y	Y	N
	γ_T	Y	Y	Y	N	Y	Y	Y	N
Van Genuchten Temp. coupling	Van G.Temp.	Y	Y	Y	Y	N	Y	Y	N
Thermal expansion of water	β_{wT}	Y	Y	Y	Y	Y	N	Y	N
Thermal expansion of solid	β_{sT}	Y	Y	Y	Y	Y	Y	N	N

Table 2. Material properties (Abed and Sołowski 2017).

Material	Young's modulus (E) [kPa]	Poisson ration (υ)	Thermal conductivity (λ_T) [W/m/K]
Teflon	5.0e+5	0.46	0.25
Steel	2.0e+8	0.3	12
Foam	1.0e+4	0.3	0.17

4   RESULTS AND DISCUSSION

4.1   General simulation analysis

Figure 4 shows the evolution of mean effective stresses along the axis of symmetry (section DD', Fig. 3), after 20, 173, 506, 838 and 1176 days while Fig. 5 shows the suction profiles in time at the selected points (A, B & C). Upon analysing these results for the original simulation, it seems that there are 3 stages of the experiment:

a) Initial stage: This stage is marked by a sharp initial dip in suction profiles, especially closer to the drying boundary (see section e-f from Fig. 5a, at Point A). As during the initial 65h wetting boundary is inactive, the change in the water content and suction is mainly due to the vapour movement from the bottom.

b) Transitional stage: This stage is marked by a rise in suction values closer to the drying side, at Point A (see part f – g in Fig. 5a), whereas at the other two locations (Points B & C) suction drops. In this stage, the water from the wetting side boundary has not yet reached the lower regions of the bentonite domain, whereas the drying from the heated bottom boundary progresses upwards.

c) Post transitional stage: At this stage the water from the wetting side gradually penetrates the lower regions of the domain, and the suction drop at point A (see Fig. 5a), part g-h. Also, later at this stage a peak is observed in the mean effective stress plots (Fig. 4 at T=506, 838 and 1176 days). This is due to the fact that the part of a soil closer to the wetting boundary achieves full saturation and starts generating excess pore pressures. This is apparent from the pressure head result of the original test, shown in Fig. 6.

4.2   Sensitivity analysis

Examination of Fig. 4 reveals that two main variables affect the results most significantly: a) the thermal component in the van Genuchten water retention expression and b) the thermal expansion of water (β_{wT}).

Table 3. Properties associated with selected variables.

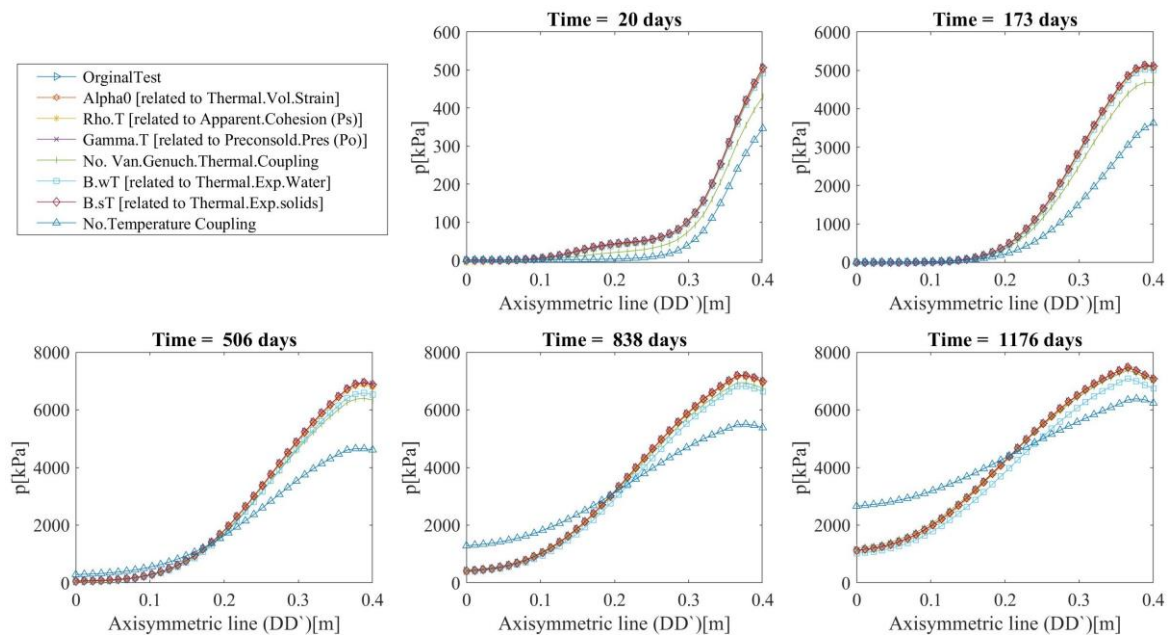| BBM thermal coupled parameters					van Genuchten thermal coupled parameters						Thermal expansion of materials	
α_0	k	ρ^T	ρ_0^* [kPa]	γ_T	$g_{\alpha 0}$ [1/m]	g_{n0}	S_{res}^l	S_{sat}^l	ξ_n^T [1/K]	ξ_w^T [1/K]	β_{wT} [1/K]	β_{sT} [1/K]
1.5e-4	0.1	0.2	1.4e+4	0.25	12e-4	1.22	0.01	1	-1e-4	-1.5e-3	2.1e-4	7.8e-6

Fig. 4. Mean effective stresses at the axisymmetric line (section DD'), at different times.

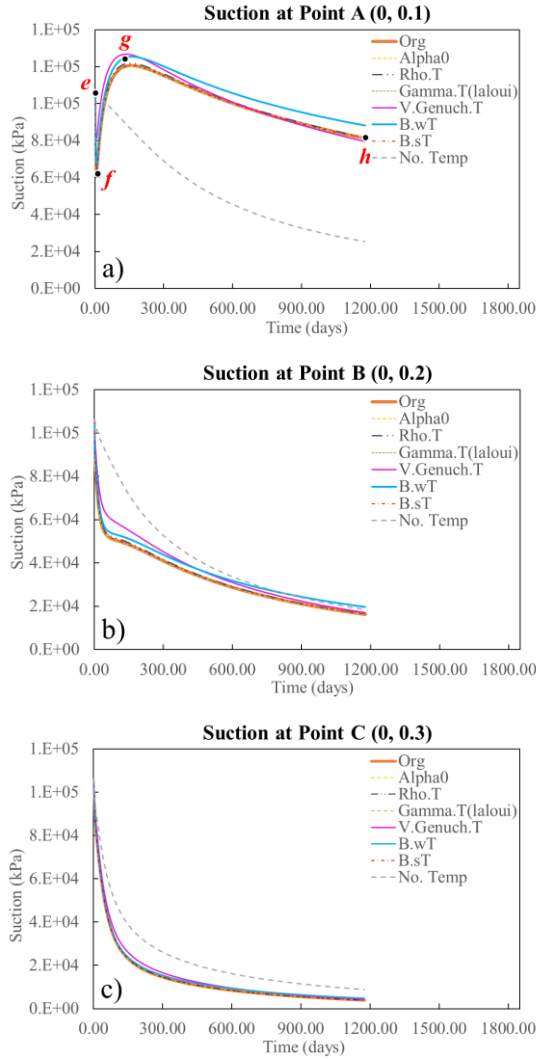Fig. 5. Suction response in time at selected points on the axisymmetric line: a) at Point A, b) at Point B and, c) at Point C.

yielding occurs and thus the value of γ_T parameter does not affect the simulation results.

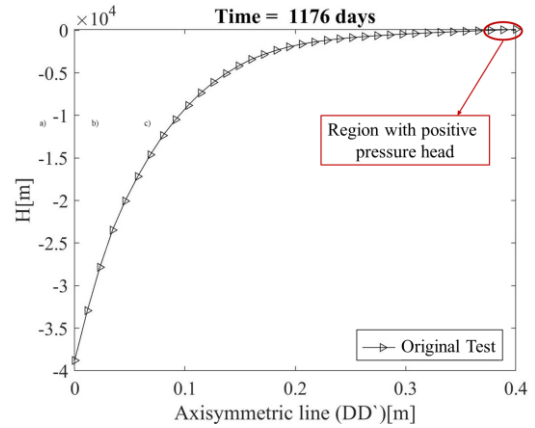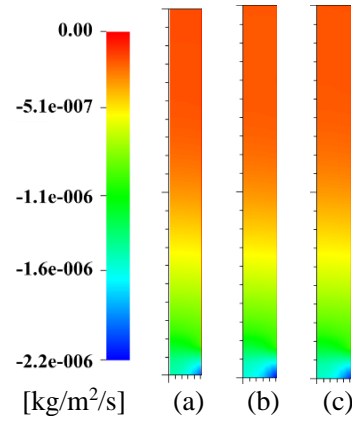Fig. 6. Original test pressure head at T=1176 day.

Fig. 7. Water flux in bentonite layer at T= 506 days: a) Original test (max: -2.0e-6 kg/m^2/s), b) Van.G temp coupling test (max: -2.2e-6 kg/m^2/s), and c) Thermal expansion coupling test (max: -2.1e-6 kg/m^2/s).

In order to satisfy water mass balance Eq. (4), the absence of these couplings under the same boundary conditions leads to a slightly higher flux (see bottom regions of Fig. 7) and higher suctions (see, Fig. 5). In the case of simulation with a constant van Genuchten water retention curve, the result deviates more from the original case closer to the beginning of the experiment, with the peak difference of approximately 15% at day 20 (see Fig. 8). This difference gradually reduces to about 8% at mid-stages (T= 838 days) and later to less than 2%, at the end of the simulation. In contrast, the influence of the thermal expansion of water becomes more evident in the later stages of the situation, with a 6% difference vs the original result at day 1176. This is likely because of the increase of saturation and hence the amount of water affected by thermal expansion.

The simulations involving variables such as ρ^T, α_0, γ_T, and β_{sT} show less than 1% difference (Fig. 4) and thus can effectively be considered as insignificant. However, as the soil does not reach the reference pre-consolidation pressure value (p_o), no
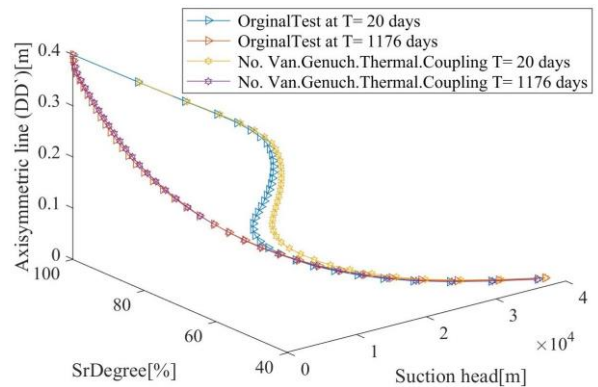

Fig. 8. Retention curve along the axisymmetric line for original test vs constant (T) van Genucten test at T= 20 & 1176 days.

Lastly, in case of no thermal coupling obvious large differences in mean stress values are observed (see, Fig. 4). Right from the initiation of the wetting boundary the suction in the system steadily decreases. As there is no active soil drying process involved, even the bottom of the sample gets saturated (see, Fig. 5a). There are also

higher mean stresses near the bottom side and lower at the wetting side (Fig. 4), with the maximum difference of about 44% observed at T= 1176 days.

5   CONCLUSIONS

A pre-validated non-isothermal infiltration test in bentonite, simulating THM conditions similar to that in a nuclear repository, was used to analyse 7 different case scenarios, with 6 simulations removing individual coupling components, while the last case investigated an isothermal scenario. As swelling pressure is key for the safety of the repository, we primarily focused on the evolution of net mean stresses in bentonite. The main outcomes of the study are:

- The van Genuchten thermal coupling is one of the most influential parameters. It causes a difference in mean net stress in the range 2% - 15%, depending on the simulation stage. This coupling affects the results more in the early stages of the simulation.
- Thermal expansion of water (β_{wT}) is the other important factor that influences the results, leading to a peak difference of 6% in the net mean stress values. Thermal expansion of water leads to the most variation in the later stages of simulation since its contribution is associated with saturation levels, which increases in time.
- The van Genuchten thermal coupling and thermal expansion of water both contribute to the partial conservation of water mass due to temperature change. It may be speculated that other factors affecting the water mass transport due to temperature would also lead to visible differences in the results.
- The differences in mean stress values involving parameters, ρ^{T}, α_0 and β_{sT} are insignificant. As there is no yielding in the simulated test, the influence of the parameter γ_T cannot be assessed.
- The isothermal test shows a difference of about 44% in mean stress values. This is a much larger variation than one resulting from the combination of all the investigated factors. It indicates the presence of other critical thermal couplings (such as in vapour densities, viscosity etc.).

This study investigated only a single test; thus, the results are preliminary and require further validation. In particular, further research may show that the variables not important in this study are influencing the results in other scenarios. Nonetheless, the conclusions give insight into the importance of thermal coupling during wetting and heating of bentonite. The couplings related to water expansion and thermal effects on the water retention curve are essential and should be accounted for in any future THM calculations.

REFERENCES

1) Abed AA, Sołowski WT (2017): A study on how to couple thermo-hydro-mechanical behaviour of unsaturated soils: Physical equations, numerical implementation and examples. Comput Geotech 92:132–155. https://doi.org/10.1016/j.compgeo.2017.07.021

2) Abed AA, Sołowski WT (2018): Applications of the new thermo-hydro-mechanical-chemical coupled code "Thebes." Environ Geotech 7:3–16. https://doi.org/10.1680/jenge.18.00083

3) Alonso EE, Gens A, Josa A (1990) A constitutive model for partially saturated soils. Géotechnique 40:405–430. https://doi.org/10.1680/geot.1990.40.3.405

4) Chapman N, McCombie C (2003) Principles and standards for the disposal of long lived radioactive wastes. 3:292

5) Gens A (1995): Constitutive Laws BT - Modern Issues in Non-Saturated Soils. In: Gens A, Jouanna P, Schrefler BA (eds). Springer Vienna, Vienna, pp 129–158

6) Guimarães L do N, Gens A, Sánchez M, Olivella S (2006): THM and reactive transport analysis of expansive clay barrier in radioactive waste isolation. Commun Numer Methods Eng 22:849–859. https://doi.org/10.1002/cnm.852

7) Hoffmann C, Alonso EE, Romero E (2007): Hydro-mechanical behaviour of bentonite pellet mixtures. Phys Chem Earth 32:832–849.

8) Jacinto AC, Villar MV, Gómez-Espina R, Ledesma A (2009): Adaptation of the van Genuchten expression to the effects of temperature and density for compacted bentonites. Appl Clay Sci 42:575–582. https://doi.org/10.1016/j.clay.2008.04.001

9) Lafifi B, Rouaiguia A, Boumazza N (2019): Optimization of Geotechnical parameters using Taguchi's design of experiment (DOE), RSM and desirability function. Innov Infrastruct Solut 4:1–12.

10) Laloui L, Cekerevac C (2003): Thermo-plasticity of clays: An isotropic yield mechanism. Comput Geotech 30:649–660.

11) Navarro V, Alonso EE (2000): Modeling swelling soils for disposal barriers. Comput Geotech 27:19–43.

12) NDA (2014) A Review of the Development of Bentonite Barriers in the KBS 3V Disposal Concept. NDA Tech Note no 21665941 March:1–74

13) Philip J, Vries D De (1957): Moisture movement in porous materials under temperature gradients. Eos, Trans Am Geophys Union 38(2):222–232.

14) Sánchez M, Gens A, Olivella S (2012): THM analysis of a large-scale heating test incorporating material fabric changes. Int J Numer Anal Methods Geomech 36:391–421.

15) Seetharam SC, Thomas HR, Cleall PJ (2007): Coupled thermo/hydro/chemical/mechanical model for unsaturated soils—Numerical algorithm. Int J Numer Methods Eng 70:1480–1511. https://doi.org/10.1002/nme.1934

16) Sellin P, Leupin OX (2014): The use of clay as an engineered barrier in radioactive-waste management - A review. Clays Clay Miner 61:477–498.

17) United States Nuclear Regulatory Commision (2019): Backgrounder on Radioactive Waste. 1–5

18) Van Genuchten MT (1980): A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils. Soil Sci Soc Am J 44:892–898.

19) Villar MV, Gomez-Espina R (2009): Report on Laboratory Tests Performed by CIEMAT on Febex Bentonite. 67

20) Wang Y, Cao Z, Au SK (2010): Efficient Monte Carlo Simulation of parameter sensitivity in probabilistic slope stability analysis. Comput Geotech 37:1015–1022. https://doi.org/10.1016/j.compgeo.2010.08.010