Coupled Thermo-Hydro-Mechanical Modeling of Saturated Boom Clay

Mohammadreza Mir Tamizdoust, S.M.ASCE¹; and Omid Ghasemi-Fare, Ph.D., A.M.ASCE²

ABSTRACT

Temperature variations in low permeable soil (e.g. clay) induce pore pressure, which is known as thermal pressurization. Previous research showed that thermal pressurization highly depends on thermal pressurization coefficient. This coefficient depends on the soil type and changes with temperature due to temperature dependency of thermal expansion coefficient of water. Thermal pressurization is often investigated through thermo-hydro-mechanical (THM) numerical modeling. THM process, with respect to thermal loading, has been examined in the literature to justify the field observations by incorporating advanced thermo-mechanical constitutive models. However, result of numerical simulations using advanced thermoelastoplastic models still show some discrepancies with experimental and field observations. In this study, the assessment of thermal pressurization in Boom clay is scrutinized through employing a relatively simple while practical thermo-poroelastic finite element model with careful consideration of the temperature-dependent thermal, hydraulic, and mechanical properties of the medium and saturating fluid (i.e. water). The numerical model is carried out using COMSOL Multiphysics and the results of the numerical simulations are compared and validated with the ATLAS project, a large-scale experimental facility in Belgium. The results confirm that thermal and hydraulic coupling parameters are the key factors to change thermal pressurization.

Keyword: Multiphase flow; Heat transfer; THM process; Thermal pressurization

INTRODUCTION

In the last few decades, much attention has been given to the non-isothermal process in saturated and variably saturated soils and rocks in the field of energy geotechnics as thermal loading may induce pore fluid pressure, and/or pore fluid flow (Ghasemi-Fare and Basu 2016, 2019; Sánchez et al. 2016; Tamizdoust and Ghasemi-Fare 2020). Therefore, in order to analyze coupling effects of temperature, pore pressure, pore fluid flow, and mechanical response, thermo-hydro-mechanical (THM) analysis must be performed (Braun et al. 2018; McCartney et al. 2016; Tamizdoust and Ghasemi-Fare 2019). Thermo-poromechanics theory has been used to predict the THM behavior in rocks (Gens Solé et al. 2007; Ghabezloo and Sulem 2009) and normally consolidated and overconsolidated clays (Abuel-Naga et al. 2007; Hueckel and Borsetto 1990). To justify the thermo-mechanical behavior of clays in experimental observations, advanced thermo-elastoplastic constitutive models such as TEAM (Cui et al. 2000) and ACMEG-T (Laloui and François 2009) have been proposed. These models consider reduction of preconsolidation pressure due to thermal loading and softening of the yield surface.

In general, temperature variations can change hydraulic and mechanical features of the porous medium through altering the fluid density and porosity of the medium (Coussy 2004; Joshaghani et al. 2018; Joshaghani and Ghasemi-Fare 2019; and Ghasmei-Fare and Basu 2019),

¹Ph.D. Candidate, Dept. of Civil and Environmental Engineering, Univ. of Louisville, USA. E-mail: m.mirtamizdoust@louisville.edu

²Assistant Professor, Dept. of Civil and Environmental Engineering, Univ. of Louisville, USA. E-mail: omid.ghasemifare@louisville.edu

which consequently can change the stress state through thermal deformation of the medium. One of the most interesting yet challenging problems involving THM process in porous media, is the management of geological waste repositories. Since 1980s, many experimental, theoretical, and numerical research have been carried out to investigate time-dependent heat transfer and thermal pressurization in deep geological waste repositories due to the low permeability of the host rock (Bernier and Neerdael 1996; Chen et al. 2017; François et al. 2009; Hueckel et al. 2011; Nguyen et al. 2017). Much attention has been given to the consideration of thermo-plastic response of the soil medium with respect to THM process, yet some major coupling features between stress equilibrium and mass balance law have been simplified or completely neglected.

In this study, accurate prediction of the THM process in Boom clay has been facilitated by incorporating a thermo-poroelastic model with careful consideration of the thermal, hydraulic, and mechanical coupling features of the soil along with the saturating fluid (*i.e.* water). The developed model is used to numerically simulate the heat transfer and pore pressure generation in Boom clay surrounding a heat source deep into the soil. The results are compared with the in situ measurements of the large-scale experiment called ATLAS in an underground research facility (HADES-URF) in Belgium (De Bruyn and Labat 2002). Also, the effect of thermal properties of water and hydraulic properties of the medium on thermal pressurization are discussed.

THERMO-PORO-ELASTIC FORMULATION

The governing equations for THM modeling are stress equilibrium, mass balance, energy balance (Coussy 2004). These three sets of coupled field equations are solved for a saturated and deformable porous medium using COMSOL Multiphysics. In the following, Equations (1) through (3) are stress equilibrium, mass balance of fluid, and energy balance of the medium, respectively:

$$\nabla \cdot \left(\sigma' + p_f I\right) + \rho_m g = 0 \tag{1}$$

$$\frac{\partial (n\rho_f)}{\partial t} + \nabla \cdot \left[-\rho_f \frac{K}{\mu} (\nabla p_f + \rho_f g) \right] = 0$$
 (2)

$$\left(\rho C\right)_{m} \frac{\partial T}{\partial t} + \nabla \cdot \left[-\left(\rho C\right)_{f} \frac{\mathbf{K}_{int}}{\mu} \nabla p_{f} T - \lambda_{m} \nabla T \right] = 0$$
(3)

Where σ' , p_f , and T are effective stress, fluid pore pressure, temperature, respectively. $\rho_m = n$ $\rho_f + (1-n) \rho_s$ is the density of the medium while ρ_f is the density of water, ρ_s is the density of the solid grains, n and is the porosity, μ is viscosity of water and K_{int} is intrinsic permeability of the soil and is related to porosity through Kozeny-Carman equation (Chapuis and Aubertin 2003; Chen et al. 2017; Han and Dusseault 2003). The fluid velocity is governed by Darcy's law. In equation (3), the properties of the medium can be predicted using: $(\rho C)_m = n\rho_f C_f + (1-n)\rho_s C_s$ and $\lambda_m = n\lambda_f + (1-n)\lambda_s$, where, C_m , C_f , and C_s are the specific heat capacity of the medium, water, and solid grains at constant stress, respectively. λ_m , λ_f , and λ_s are the thermal conductivity of the medium, water, and solid grains, respectively.

Additional state variable equations are needed in order to study fluid mass conservation considering the soil deformation and temperature increments. Equations (4) and (5) express variations of the fluid density and the medium porosity with temperature and pore pressure; note that in Equation (5), the change in porosity is governed by the linear thermo-poroelastic constitutive law:

$$\frac{\partial \rho_f}{\partial t} = \rho_f \left(\left(\frac{1}{K_f} \right) \frac{\partial p_f}{\partial t} - \alpha_f \frac{\partial T}{\partial t} \right) \tag{4}$$

$$\frac{\partial n}{\partial t} = (1 - n) \left(\left(\frac{1}{K} \right) \frac{\partial \sigma'}{\partial t} - \alpha_s \frac{\partial T}{\partial t} \right)$$
 (5)

Where K_f and α_f are the bulk modulus and thermal expansion coefficient of Fluid, respectively. K is the drained bulk modulus of medium, and α_s is the thermal expansion coefficient of solid grains.

In this study, variations of the thermal expansion coefficient, compressibility, dynamic viscosity of water, thermal conductivity, and heat capacity with the temperature ranging from 10 to 100 °C according to Spang 2002 are precisely considered. The temperature values beyond this range are extrapolated. Thermo-poroelastic model described above is used to simulate the ATLAS experiment. A brief discerption of the experiment and the Numerical setup of THM modeling is presented in the next section.

DESCRIPTION OF THE PROBLEM

ATLAS experiment

The underground research facility HADES-URF was designed and built in Mol, Belgium at a depth of 223 m in Boom clay where the ATLAS test was conducted. The Boom clay is a deposit of overconsolidated clay which is considered as a host rock for the Belgian disposal of radioactive waste. The ATLAS experiment consists of a horizontal main borehole (19 m long) with heaters and two parallel boreholes (15.65 m long) with instrumentation, which have been drilled at 1.184 m and 1.515 m of the main borehole in the same horizontal plane. The changes in the temperature, pore water pressure, and radial stress have been measured in observation boreholes (De Bruyn and Labat 2002). Figure 1 shows the thermal loading in the main borehole which was used in this model. The first heating phase started at a power of 900 W. This phase lasted nearly 3 years. The second heating phase started at 1800 W and maintained for almost one year later, then the power was shut down which initiated the cooling phase. Moreover, the properties of the Boom clay used in this study are presented in Table 1 which is according to the reported literature (Baldi et al. 1991; Bernier et al. 2007; Delage et al. 2008; Delage et al. 2000; Horseman et al. 1987).

Numerical setup and conditions

A 2D axisymmetric domain in the horizontal plane is considered with a heat source on the symmetry boundary. The domain geometry (100 m in radial and perpendicular distances from the heater) has been considered such that the effect of boundary conditions on soil response is negligible. Constant temperature and pore pressure equal to the initial values are considered for all boundaries except the axisymmetric one. The schematic view of the finite element mesh and the boundary conditions are illustrated in Figure 2. In the numerical simulations, the solutions of partial differential equations are obtained using direct linear solver in COMSOL with fully coupled approach where the relative tolerance is set to 0.01%. Moreover, the in situ stress, initial pore water pressure, and temperature are brought in Table 2.

Table 1.1 hysical Properties of Boom clay										
Parameters	$ ho_{f0}$	$ ho_{s}$	n_0	k_0	$oldsymbol{E}^*$	υ	λ_{s}	C_s	α_s	
(dimensions)	(kg/m^3)	(kg/m^3)	(m^3/m^3)	(m^2)	(MPa)	(1)	(W/m°C)	(J/kg°C)	(1/°C)	
Values	1000	2670	0.39	2.5×10 ⁻¹⁹	350	0.125	1.65	730	1.3×10 ⁻⁵	

Table 1. Physical Properties of Boom clay

^{*} $K = E/3(1-2\nu)$

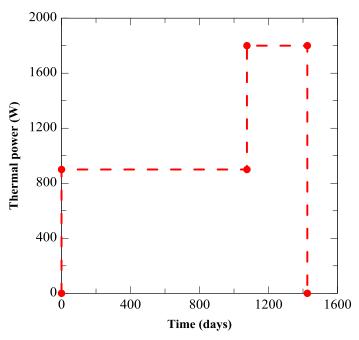


Figure 1. Thermal loading in ATLAS experiment

Table 2. Initial condition of the field variables

Parameters (dimensions)	Values
$\sigma_z = \sigma_r (MPa)$	4.5
$p_f(MPa)$	2.025
OCR	2.4
<i>T</i> (°C)	16.5

RESULTS AND DISCUSSION

The results of 2D axisymmetric numerical model are presented in Figures 3 and 4. All the results are showing at 1.515 m from the heat source at the observation borehole. The comparison of the numerical and experimental results (the variations of temperature and pore water pressure with time) are presented in Figure 3 and 4. As it can be seen in Figure 3, temperature changes obtained using the developed model matches well with the results at the observation borehole. Figure 4 shows thermal pressurization prediction using the thermo-poroelastic model reasonably matches with the experimental observation. The model slightly underestimates the thermal pressurization in the first heating phase. However, the maximum pore pressurization happens in the second heating phase is captured well with the thermo-poroelastic model while in cooling phase, the simulations are marginally overpredicted.

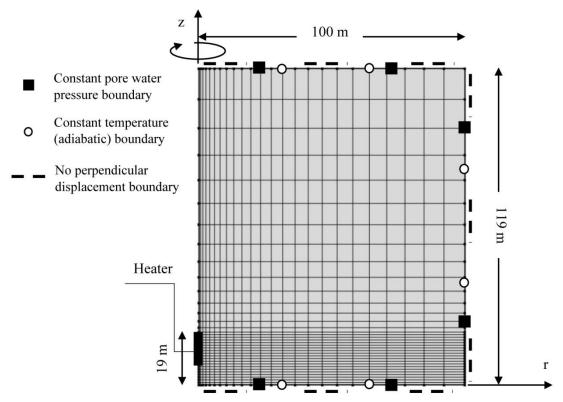


Figure 2. Schematic view of the numerical domain and boundary conditions

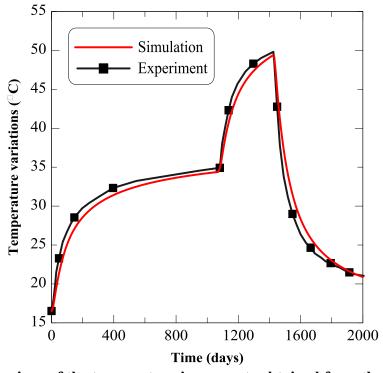


Figure 3. Comparison of the temperature increments obtained from thermo-poroelastic model and experimental observation at r=1.515 m from the heater

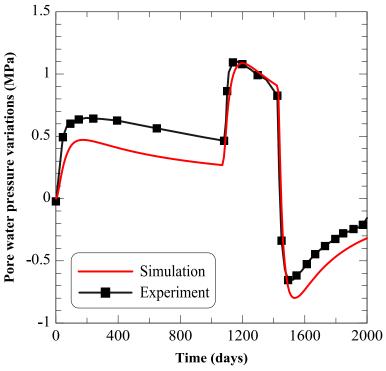


Figure 4. Comparison of the thermal pressurization variations at r=1.515 m from the heater

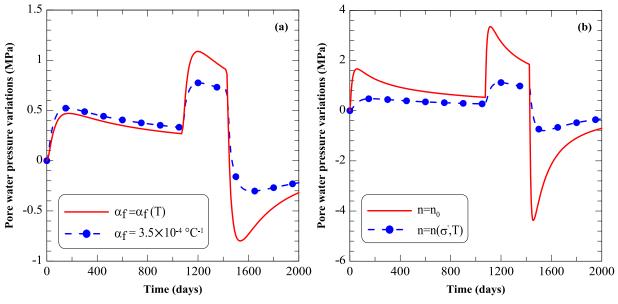


Figure 5. Prediction of pore water pressure variations versus time with (a) consideration of different thermal expansion coefficients of water (temperature-dependent and constant) and, (b) consideration of constant and variable porosity

The thermally-induced pore fluid pressure is mainly due to difference between the thermal expansion coefficient of water and solid grains (Ghabezloo and Sulem 2009). The precise evaluation of α_f shows a strong dependency of this parameter on temperature variations; however, in numerous studies, this parameter has been set to a constant value (Chen et al. 2017;

Hueckel et al. 2011). Furthermore, intrinsic permeability as a function of porosity can inversely affect the thermally-induced pore fluid pressure since excessive pore pressure is higher in low permeable soils. Therefore, it can be concluded that the intrinsic and hydraulic properties of the soil medium and the thermal properties of the saturating fluid (water in this case) should have profound effects on thermal pressurization. Here, the impact of the thermal expansion coefficient of water and the variations of porosity on the thermal pressurization have been investigated in detail. Figure 5(a) shows the result of a secondary numerical simulation considering a constant thermal expansion coefficient of water (α_f) and compares the results with the temperature-dependent one. The pore pressure variations are strongly underestimated in the second heating phase and the cooling phase where the temperature variation reaches to the maximum and minimum values, respectively. In the first heating phase, the results of both simulations are fairly close. In Figure 5(b), the effect of porosity variations (Equation 5) on the thermal pressurization is presented, the maximum elastic porosity change is Δn =+0.24% and Δn =-0.11% during second heating phase and cooling phase, respectively. It is shown that neglecting the porosity changes, even though very small, results in enormous error in the predictions of thermal pressurization.

CONCLUSION

In this study, a simple while practical thermo-poroelastic model was considered to analysis the thermal pressurization in Boom clay through a coupled thermo-hydro-mechanical process. The intrinsic properties of the medium along with the thermal and hydraulic properties of water were considered carefully. The results of the numerical simulations were compared and validated with the experimental data obtained from ATLAS experiment. It was found that the variations of temperature and pore water pressure can be captured with enough accuracy through a simple while practical thermo-poroelastic model. Results showed that in order to accurately predict the THM process in the soil media, temperature dependent properties of the soil and saturating fluid must be considered.

ACKNOWLEDGEMENT

The authors would also like to gratefully acknowledge the financial support by the National Science Foundation under Grant No. CMMI-1804822.

REFERENCES

- Abuel-Naga, H. M., Bergado, D. T., and Bouazza, A. (2007). "Thermally induced volume change and excess pore water pressure of soft Bangkok clay." *Engineering Geology*, 89(1-2), 144-154.
- Baldi, G., Hueckel, T., Peano, A., and Pellegrini, R. (1991). "Developments in modelling of thermo-hydro-geomechanical behaviour of boom clay and clay-based buffer materials. Commission of the European Communities." *Nuclear science and technology*.
- Bernier, F., Li, X. L., and Bastiaens, W. (2007). "Twenty-five years' geotechnical observation and testing in the Tertiary Boom Clay formation." *Géotechnique*, 57(2), 229-237.
- Bernier, F., and Neerdael, B. (1996). "Overview of in situ thermomechanical experiments in clay: Concept, results and interpretation." *Engineering geology*, 41(1-4), 51-64.
- Braun, P., Ghabezloo, S., Delage, P., Sulem, J., and Conil, N. (2018). "Theoretical analysis of pore pressure diffusion in some basic rock mechanics experiments." *Rock Mechanics and Rock Engineering*, 51(5), 1361-1378.

- Chapuis, R. P., and Aubertin, M. (2003). "On the use of the Kozeny Carman equation to predict the hydraulic conductivity of soils." *Canadian Geotechnical Journal*, 40(3), 616-628.
- Chen, W., Ma, Y., Yu, H., Li, F., Li, X., and Sillen, X. (2017). "Effects of temperature and thermally-induced microstructure change on hydraulic conductivity of Boom Clay." *Journal of Rock Mechanics and Geotechnical Engineering*, 9(3), 383-395.
- Coussy, O. (2004). *Poromechanics*, John Wiley & Sons.
- Cui, Y. J., Sultan, N., and Delage, P. (2000). "A thermomechanical model for saturated clays." *Canadian Geotechnical Journal*, 37(3), 607-620.
- De Bruyn, D., and Labat, S. (2002). "The second phase of ATLAS: the continuation of a running THM test in the HADES underground research facility at Mol." *Engineering Geology*, 64(2-3), 309-316.
- Delage, P., Le, T. T., Tang, A.-M., Cui, Y.-J., and Li, X.-L. (2008). "Suction effects in deep Boom clay block samples." *arXiv preprint arXiv:0801.2105*.
- Delage, P., Sultan, N., and Cui, Y. J. (2000). "On the thermal consolidation of Boom clay." *Canadian Geotechnical Journal*, 37(2), 343-354.
- François, B., Laloui, L., and Laurent, C. (2009). "Thermo-hydro-mechanical simulation of ATLAS in situ large scale test in Boom Clay." *Computers and Geotechnics*, 36(4), 626-640.
- Gens Solé, A., Vaunat, J., Garitte, B., and Wileveau, Y. (2007). "In situ behaviour of a stiff layered clay subject to thermal loading: observations and interpretation." *Géotechnique*, 57(2), 207-228.
- Ghabezloo, S., and Sulem, J. (2009). "Stress dependent thermal pressurization of a fluid-saturated rock." *Rock Mechanics and Rock Engineering*, 42(1), 1.
- Ghasemi-Fare, O., and Basu, P. (2016). "Thermally-induced pore pressure fluctuations around a geothermal pile in sand." *Geo-Chicago*, *GSP*, 270, 14-18.
- Ghasemi-Fare, O., and Basu, P. (2018). "Influences of ground saturation and thermal boundary condition on energy harvesting using geothermal piles." *Energy and Buildings*, 165, 340-351.
- Ghasemi-Fare, O. and Basu, P. (2019). "Thermal performance of heat exchanger piles in the presence of temperature-induced buoyant pore fluid flow," Computers and Geotechnics, 116, 103211.
- Han, G., and Dusseault, M. B. (2003). "Description of fluid flow around a wellbore with stress-dependent porosity and permeability." *Journal of petroleum science and engineering*, 40(1-2), 1-16.
- Horseman, S., Winter, M., and Enwistle, D. (1987). "Geotechnical characterization of Boom clay in relation to the disposal of radioactive waste." Commission of the European Communities.
- Hueckel, T., and Borsetto, M. (1990). "Thermoplasticity of saturated soils and shales: constitutive equations." *Journal of Geotechnical Engineering*, 116(12), 1765-1777.
- Hueckel, T., Francois, B., and Laloui, L. (2011). "Temperature-dependent internal friction of clay in a cylindrical heat source problem." *Géotechnique*, 61(10), 831-844.
- Joshaghani, M., Ghavami, M., Ghasemi-Fare, O. (2018). "Experimental investigation on the effects of temperature on physical properties of sandy soils", IFCEE, ASCE, March 5-10.
- Joshaghani, M., Ghasemi-Fare, O. (2019). "A Study on thermal consolidation of fine grained soils using modified triaxial cell", Geo-congress, ASCE, March 24-27.
- Laloui, L., and François, B. (2009). "ACMEG-T: soil thermoplasticity model." *Journal of engineering mechanics*, 135(9), 932-944.
- McCartney, J. S., Sanchez, M., and Tomac, I. (2016). "Energy geotechnics: Advances in subsurface energy recovery, storage, exchange, and waste management." *Computers and*

- Geotechnics, 75, 244-256.
- Nguyen, T. S., Li, Z., Barnichon, J., and Garitte, B. (2017). "Modelling a heater experiment for radioactive waste disposal." *Environmental Geotechnics*, 4(2).
- Sánchez, M., Gens, A., Villar, M. V., and Olivella, S. J. I. J. o. G. (2016). "Fully coupled thermo-hydro-mechanical double-porosity formulation for unsaturated soils." 16(6), D4016015.
- Spang, B. (2002). "Excel add-in for properties of water and steam in SI-units." *Water97_v13*. *xla*. *Hamburg*.
- Tamizdoust, M. M., and Ghasemi-Fare, O. (2019). "Numerical Analysis on Feasibility of Thermally Induced Pore Fluid Flow in Saturated Soils." *Eighth International Conference on Case Histories in Geotechnical Engineering*, ASCE, Philadelphia, Pennsylvania, 73 82.
- Tamizdoust, M. M., and Ghasemi-Fare, O. (2020). "A fully coupled thermo-poro-mechanical finite element analysis to predict the thermal pressurization and thermally induced pore fluid flow in soil media." *Computers and Geotechnics*, 117, 103250.