Proceedings of the 24th UK Conference of the
Association for Computational Mechanics in Engineering
31 March – 01 April 2016, Cardiff University, Cardiff

Thermo-osmosis in saturated shale

***R. Zagorščak and H.R. Thomas**

Geoenvironmental Research Centre (GRC), School of Engineering, Cardiff University, The Queen's Buildings, The Parade, Cardiff, CF24 3AA

*ZagorscakR@Cardiff.ac.uk

ABSTRACT

An investigation of thermo-osmosis in a saturated and chemically active rock such as shale is presented. The model presented is based on an existing coupled thermal, hydraulic and mechanical model (THM) for unsaturated soils. A simplified form of a coupled THM model for saturated porous medium is developed which considers the effect of solid-fluid thermal expansion and the effects of thermal osmosis in hydraulic behaviour. An example problem dealing with pore water pressure development in saturated shale rock surrounding the bentonite buffer installed around high-level nuclear waste canister emitting heat is presented. It is demonstrated that the heat input from the waste canister can affect the pore water pressure evolution in the shale. In particular, under the conditions considered, it is shown that thermally driven liquid water flow due to thermal osmosis contributes to the convective transport of dissolved species.

Keywords: *saturated shale, hydraulic behaviour, thermal osmosis, coupled modelling*

1. Introduction

The safe storage of high-level radioactive waste is a subject of major strategic international importance. The disposal of such waste in geological repositories relies on a multi-barrier system consisting of the engineered materials placed within the repository and the natural barrier system which includes the repository rock and its surrounding subsurface environment. In the short term the heat generated by the waste will induce elevated temperatures in the engineered barrier system and the host rock [1].

During the very long lifespan of a geologic repository, the performance of the multi-barrier system is affected by a series of complex and coupled processes. Osmosis is one of the processes identified to affect the fluid pressure around the nuclear waste canisters [2]. While electro- and chemo-osmosis have been extensively identified and described in clay-rich media, a flow of water driven by temperature gradient, i.e. thermal osmosis has received less attention [2]. It is well known that an increase in temperature causes thermal expansion of mineral solids and pore water usually generating volume and effective stress changes in saturated soils [3]. The lower the hydraulic conductivity of the porous medium, the longer the time required for this pore water pressure to dissipate. However, it has been shown that in low porosity and chemically active porous media, inclusion of thermal osmosis provides further insights into pressure distribution and flow in shale layers [2].

In this work, the theoretical development of hydraulic behaviour with an emphasis on thermal osmosis is presented and implemented within an existing thermal, hydraulic and mechanical (THM) numerical model [4]. In order to assess the impact of temperature increase on pore water pressure evolution in the shale, a numerical investigation has been conducted with and without including thermo-osmotic effects.

2. Constitutive model

A constitutive model considering thermal expansion relationships, thermal osmosis and associated parameters of consolidation is implemented within an existing THM numerical model (COMPASS) developed at Cardiff University [5].

The governing equation of water flow is given by:

$$\frac{\partial}{\partial t}(\rho_l \theta_l \delta V) = -\delta V \nabla(\rho_l v_l) \tag{1}$$

where t, ρ, θ, δV and v are the time, density, volumetric water content, incremental volume of soil and the velocity of the liquid, respectively [5]. The subscript l stands for liquid. In this model, soil is deformable and the liquid phase is presented as a function of both temperature and pressure while the solid phase is presented solely as a function of temperature since the solid grains are assumed to be incompressible. Hydraulic, gravitational and thermo-osmosis potentials are considered as the mechanisms of water flow. Thermo-osmotic conductivity can be presented as a function of hydraulic conductivity:

$$k_T = k_l \frac{\Delta H}{\rho_l g T} \tag{2}$$

where ΔH is the mean value of excess enthalpy resulting from fluid-solid interactions, k_T and k_l are the thermo-osmotic conductivity and saturated hydraulic conductivity, respectively [2].

Expanding the equation 1 for a fully saturated soil with respect to its partial derivatives and using an incremental volume as a summation of the void volume and solid volume, yields:

$$\rho_l[n\beta_l + m_v]\frac{\partial u_l}{\partial t} + \rho_l[n(\beta_s^{'} - \beta_l^{'}) + \alpha]\frac{\partial T}{\partial t} = \nabla\left(\frac{k_l}{g}\nabla u_l\right) + \nabla(k_T \rho_l \nabla T) + \nabla(\rho_l \nabla z) \tag{3}$$

where n, β, β', m_v, u, α and T are the porosity, water compressibility, thermal expansion coefficient, compressibility of soil, pore water pressure, thermal expansion coefficient of the soil structure and temperature, respectively. The subscript s stands for solid.

The formulation for heat transfer is based upon the principle of conservation of energy where conduction is the primary mechanism of heat transfer [5]. The model described in this paper is a fully coupled THM model, which for the theoretical formulation presented has been tested against an analytical benchmark and a heating experiment [4].

3. Computational domain and material parameters

The properties and the stress state of the shale rock are assumed to be homogeneous for the considered area of investigation. The internal boundary of the modelled domain corresponds to the external radius of the engineered material, i.e. bentonite buffer which is placed 1.14 m from the axis of symmetry while the external boundary was placed to a sufficient distance of 200 m so the influence on the computation becomes minimal (Fig. 1). The domain was discretised into 400 quadrilateral elements with the mesh concentrated towards the heat source. A maximum time-step of 2 years was considered and the duration of the simulation was 10,000 years. The predicted temperature evolution over time at the bentonite buffer-shale interface, based on work of Lawrence Berkley International Laboratory – Earth Sciences Division [7], was prescribed at the internal boundary where the temperature slowly increases from initial ground temperature up to a temperature of 354 K over 65 years and then slowly and non-linearly decreases to 326 K by the end of the simulation. An axisymmetric analysis was performed.

Boundary Conditions	*Initial Conditions*	*Boundary Conditions*
$\partial u_l / \partial x = 0$	$u_l = 5\ MPa$	$u_l = 5\ MPa$
$T = T_{imposed}$	$T = 298\ K$	$T = 298\ K$

Figure 1: Schematic of the initial and boundary conditions

The parameters governing the thermal and hydraulic behaviour in shale were collected and established from a literature synthesis and are presented in Table 1 [2][3][6][8]. Gonçalvès et al. [2] reported that depending on the electro-chemical properties of the porous media, the thermo-osmotic conductivity for shale is between 10^{-10} and 10^{-15} m^2/sK. Hence, a value of $5x10^{-13}$ m^2/sK was adopted for this investigation.

Table 1: Material parameters

Material Parameter	**Value**
Porosity [2]	0.1
Solid density [2]	2600 kg/m^3
Thermo-osmotic conductivity [2]	$5x10^{-13}$ m^2/sK
Thermal conductivity [3]	1.5 W/mK
Hydraulic conductivity [6]	$1x10^{-13}$ m/s
Solid volumetric expansion coefficient [8]	$1.8x10^{-5}$ 1/K
Water volumetric expansion coefficient [8]	$3.0x10^{-4}$ 1/K
Water compressibility [8]	$3.0x10^{-10}$ 1/Pa
Soil compressibility [8]	$9x10^{-10}$ 1/Pa

4. Numerical results

The major heat-emitting phase from the radioactive nuclear waste is approximated to last about 10,000 years [5]. To investigate how osmotic flow modifies spatial and temporal pore water pressure field around a high-level waste, a case considering only thermal expansion of the shale constituents was compared with a case where thermo-osmotic phenomenon is included. The time evolution of the temperature can be seen in Figure 2a for different distances from the heat source. Due to the low thermal conductivity of the shale, slow heat propagation around the heat source leads to a maximum temperature difference of 15 °C between the studied locations within the domain, i.e. 2 m and 10 m from the buffer-shale interface. Hence, temperature gradient occurs in the shale around the heat source. In Figure 2b, pore water pressure evolution caused by heat emitted from the waste package is presented highlighting the thermo-osmotic and thermal expansion respective contributions. In case where only thermal expansion is considered, it can be observed that the pore water pressure in shale rock continuously increases up to the point where temperature becomes approximately constant and then the Darcian flux predominates due to pressure gradient established in the formation yielding slow pore water pressure dissipation. In case where thermo-osmosis is considered, when the temperature stabilises pore water pressure developed 2 m from the buffer-shale interface is less comparing to thermal expansion only case due to water flow induced by temperature gradient. Furthermore, due to thermo-osmotic water flow diverging from the heat source, an increase in pore water pressure is observed further in the domain, i.e. at the distance of 10 m from the buffer.

5. Conclusion

Based on observations from the current study, it can be concluded that thermo-osmosis modifies the pressure field in a natural environment subjected to heating. In the context of nuclear waste disposal and radionuclide release, thermal osmosis might contribute to the overall convective transport of water and radionuclides due to the low hydraulic permeability and low thermal conductivity of the shale rock. In this work, a value of $5x10^{-13}m^2/sK$ was chosen although higher values have been reported for shales. However, it can be concluded that for even relatively low value of thermo-osmotic conductivity, the thermal osmosis contributes to the water flow in such low permeability porous medium. This leads to a conclusion that in porous medium with higher thermo-osmotic properties, the effect of thermal-osmosis on pore water pressure evolution around the heat source could prevail over the Darcian flow.

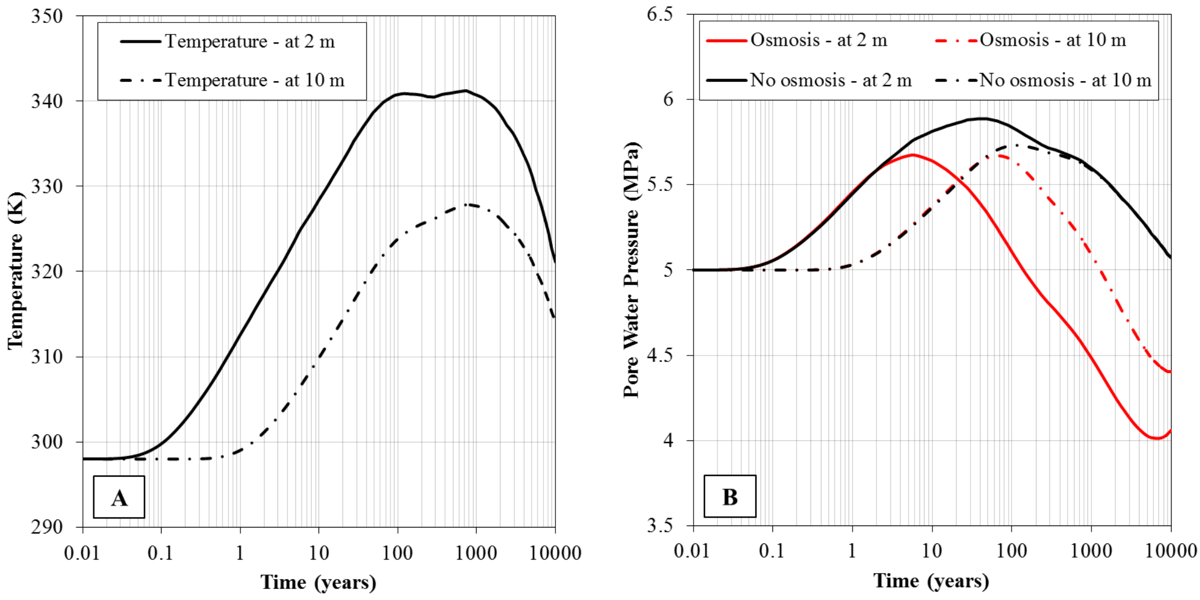

Figure 2: A) Temperature evolution with time at the distance equal to 2 m and 10 m from the buffer-rock interface, B) Pore water pressure evolution with and without the thermo-osmotic effect at the distance equal to 2 m and 10 m from the buffer-rock interface

Hence, inclusion of thermo-osmosis effect in chemically active rock such as shale for long-term numerical investigations of nuclear safety may be needed to understand the pressure distribution and flow in such porous medium.

Acknowledgements

The financial support from WEFO, for the first author, is gratefully acknowledged.

References

[1] Thomas, H.R., He, Y., Sansom, M.R. and Li, C.L.W. On the development of a model of the thermo-mechanical-hydraulic behaviour of unsaturated soils. *Engineering Geology*, 41, 197-218, 1996.

[2] Gonçalvès, J., De Marsily, G. and Trèmosa, J. Importance of thermo-osmosis for fluid flow and transport in clay formations hosting a nuclear waste repository. *Earth and Planetary Science Letters*, 339-340, 1-10, 2012.

[3] Mitchell, J. K. *Fundamentals of Soil Behavior*, 2nd Edition, John Wiley & Sons, Inc., 1993.

[4] Zagorščak, R., Sedighi. M. and Thomas, H.R. Effects of thermal osmosis on hydraulic behaviour of saturated clays. *International Journal of Geomechanics,* Accepted for publication.

[5] Thomas, H.R. and He, Y. A coupled heat-moisture transfer theory for deformable unsaturated soil and its algorithmic implementation. *International journal for numerical methods in engineering*, 40, 3421-3441, 1997.

[6] Trèmosa, J., Gonçalvès, J., Matray, J.M. and Violette, S. Estimating thermo-osmotic coefficients in clay-rocks: II. In situ experimental approach. *Journal of Colloid and Interface Science*, 342, 175-184, 2010.

[7] Lawrence Berkley National Laboratory, Earth Sciences Division. Available at: http:// http://esd.lbl.gov/used-fuel-disposition/engineered-barrier-research/, (Accessed: 9/2/16).

[8] Ghassemi, A., Tao, Q. and Diek, A. Influence of coupled chemo-poro-thermoelastic processes on pore pressure and stress distributions around a wellbore in swelling shale. *Journal of Petroleum Science and Engineering*, 67, 57-64, 2009.