On the inclusion of high temperature effects in the behaviour of buffer material

Sumi Siddiqua
Department of Civil Engineering, University of Manitoba, Winnipeg, Manitoba, Canada
H. R. Thomas
Geoenvironmental Research Centre, Cardiff School of Engineering, Cardiff University, Cardiff, UK
S.C. Seetharam
Geoenvironmental Research Centre, Cardiff School of Engineering, Cardiff University, Cardiff, UK

ABSTRACT

Bentonite is considered as the sealing/buffer material in the European Nuclear waste disposal concept due to its high swelling capacity. Therefore, the accurate prediction of the behaviour of the buffer material is crucial for the performance assessment. Consequently the modelling of the thermo-hydraulic behaviour of the buffer material is significant. This paper presents a study of thermo-hydraulic behaviour of a highly compacted bentonite subjected to an elevated thermal load and a hydraulic gradient. This is achieved via the application of a numerical model, COMPASS, which implements a coupled thermo/hydro/mechanical approach to model the behaviour of bentonite subjected to a higher temperature. The experimental work considered for the numerical simulation is a thermo-hydraulic experiment conducted on MX-80 bentonite at a temperature of 85°C in the laboratory of Cardiff University. The model is employed to solve a series of transient problems ranging from 1 day to 30 days and numerical results compared against thermal and hydraulic results from experiment.

RÉSUMÉ

La bentonite est considérée comme matériel amortisseur/étanchéité dans le concept nucléaire européen de disposition des déchets dû à sa capacité de dilatation élevée. Par conséquent, la prévision précise du comportement du matériel d'amortisseur est cruciale pour l'évaluation de sa performance. Ainsi, la modélisation du comportement thermo-hydraulique est très significative. Ce rapport présentera une étude du comportement thermo-hydraulique d'un échantillon de bentonite compactée soumis à une charge thermique élevée et à un gradient hydraulique. Ceci est réalisé à l'aide d'un modèle numérique, COMPASS, qui utilise une approche thermo/hydro/mécanique pour modeler le comportement de la bentonite soumis à une température plus élevée. Le travail expérimental qui a été considéré pour la simulation numérique est une expérience thermo-hydraulique conduit sur la bentonite MX-80 à une température de 85°C dans le laboratoire de l'université de Cardiff. Le modèle est utilisé pour résoudre une série de problèmes transitoires de 1 jour à 30 jours et les résultats numériques sont comparés aux résultats thermiques et hydrauliques de l'expérience.

1 INTRODUCTION

Numerous researches have been carried out in the recent past on bentonite clay to study the physical-chemical-mechanical behaviour when used as an engineered barrier for nuclear waste repositories (Graham et al. 1997; Dahlstrom, 1998; Huertas et al., 2000). Such studies are of vital importance as engineered barriers are expected to play a key role in the long term isolation of waste under the conditions that exist in a typical repository condition. In a typical repository, a thermo-hydraulic gradient exists due to the heat generated by the waste canisters and progressive wetting of the initially unsaturated bentonitic clay by the water table in the host rock. Since bentonitic clays are highly expansive, a thermo-hydraulic gradient can cause swelling and shrinkage (Thomas and He, 1995). It is also possible that the temperature can reach to 100°C or more in some repository condition (Gibbs, 1999). Temperature changes affect important hydraulic characteristics of compacted clay. The hydraulic responses such as water retention, liquid permeability are fundamental parameters to calculate the hydration rate of the barrier material. Any small variation in the above mentioned material properties can significantly change the performance of the buffer material. Therefore, in order to assess the performance of swelling clays at elevated thermal load, the complex couplings that exist between the thermal, hydraulic behaviour need to be investigated.

The use of thermo/hydro/mechanical models in nuclear waste repository applications to assess the long-term behaviour of clay-based buffers has been well documented (Thomas and He, 1995 and Thomas et al. 1998). There are other approaches in literature for improved prediction. Olivella and Gens (2000) suggested that gas phase permeability controls vapour concentration gradients in very low permeability soils such as swelling clays. Pintado et al. (2002) reported an inverse analysis based on a thermo-hydraulic experiment.

This paper presents a brief description of a thermo/hydro/mechanical (THM) model which can be applied at high temperature problem. The frame work of the model is based on the THM model by Thomas and He, 1997). Detail developments of the model are discussed in elsewhere (Thomas et al.2009). In the current work, the model is employed to simulate a thermo-hydraulic experiment. The work presented seeks to demonstrate the influence of the high-temperature behaviour in the prediction of moisture redistribution results.

2 TEORETICAL FORMULATION

The soil is considered a three-phase system comprising moisture, air and solid particles. The formulation is cast in terms of the principle variables of temperature (***T***), pore-water pressure ($\boldsymbol{u_l}$), pore gas pressure ($\boldsymbol{P_g}$) and displacements (**u**). The formulation follows that of Thomas & He (1997) but with a modified approach to the transport of pore gas, as presented by Thomas et al (2009).

The system of governing equations is derived with the heat conservation following Thomas and King (1991), which also includes the latent and specific heat capacities; moisture conservation take account of both liquid and vapour terms, follows the approach of Thomas and He (1997) with the exception that the diffusive term is cast in terms of the vapour mass fraction. Pore-gas is assumed to be a mixture of dry-air and vapour and the conservation equation is expressed according to Luikov, (1966). The mechanical formulation follows that of Thomas and He (1997) and uses equilibrium conditions to form the governing equation.

2.1 Governing equations

The system of equations for the above defined variables can be summarised as follows:

Deformation:

$$C_{ul}du_l + C_{uT}dT + C_{ug}dP_g + \mathbf{C_{uu}}.d\mathbf{u} + d\mathbf{b} = 0 \qquad [1]$$

Liquid and water vapour flow:

$$\begin{aligned}&C_{ll}\frac{\partial u_l}{\partial t} + C_{lT}\frac{\partial T}{\partial t} + C_{lg}\frac{\partial P_g}{\partial t} + \mathbf{C_{lu}}.\frac{\partial \mathbf{u}}{\partial \mathrm{t}}\\ &= \nabla.\left[K_{ll}\nabla u_l\right] + \nabla.\left[K_{lT}\nabla T\right] + \nabla.\left[K_{lg}\nabla P_g\right] + J_l\end{aligned} \qquad [2]$$

Bulk air flow:

$$\begin{aligned}&C_{gl}\frac{\partial u_l}{\partial t} + C_{gT}\frac{\partial T}{\partial t} + C_{gg}\frac{\partial P_g}{\partial t} + \mathbf{C_{gu}}.\frac{\partial \mathbf{u}}{\partial \mathrm{t}}\\ &= \nabla.\left[K_{gl}\nabla u_l\right] + \nabla.\left[K_{gT}\nabla T\right] + \nabla.\left[K_{gg}\nabla P_g\right]\\ &+ \mathbf{V_{gT}}.\nabla \mathrm{T} + \mathbf{V_{gg}}.\nabla \mathrm{P_g} + J_g\end{aligned} \qquad [3]$$

Heat transfer:

$$\begin{aligned}&C_{Tl}\frac{\partial u_l}{\partial t} + C_{TT}\frac{\partial T}{\partial t} + C_{Tg}\frac{\partial P_g}{\partial t} + \mathbf{C_{Tu}}.\frac{\partial \mathbf{u}}{\partial \mathrm{t}}\\ &= \nabla.\left[K_{Tl}\nabla u_l\right] + \nabla.\left[K_{TT}\nabla T\right] + \nabla.\left[K_{Tg}\nabla P_g\right]\\ &+ \mathbf{V_{Tl}}.\nabla u_l + \mathbf{V_{TT}}.\nabla T + \mathbf{V_{Tg}}.\nabla P_g + J_g\end{aligned} \qquad [4]$$

where K and C are coefficients of the governing equations, and **b** is the vector of body forces. Subscripts refer to the phase of the primary variables.

A numerical solution of the governing differential equations is achieved by the use of a continuous Galerkin weighted residual method for spatial discretisation and an implicit backward Eulerian time difference method for temporal discretisation (Thomas and He, 1997).

3 BRIEF REVEIW OF EXPERIMENTAL WORK

The tests were performed in a specially designed apparatus termed as thermal-hydraulic cell shown in Figure 1 (Singh, 2007). The top section is a hydration source maintained at a constant temperature and the bottom section contains a heating source. The samples of 100 mm diameter and 100 mm height were statically compacted in situ in the central section. Relative humidity probes were installed along the sample length at 20 mm intervals to measure the transient relative humidity and thermal distribution. The samples were subjected to fixed temperatures of 85 °C at the bottom end and 25 °C at the top end. As a hydration source deionised and de-aired water was supplied at the top end at a pressure of 0.6 MPa.

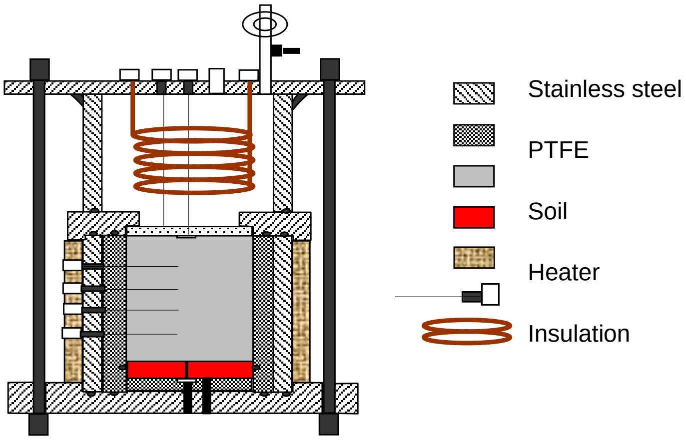

Figure 1: Schematic diagram of thermal-hydraulic test Cell (Singh, 2007)

MX-80 bentonite with an average initial density of 1.63 Mg/m^3 was chosen as the test material. Tests were performed on two similar samples with different initial water content. Sample with an initial water content of 16% corresponding to a degree of saturation of 60% is termed as dry sample and sample with an initial water content of 22% corresponding to a degree of saturation of 88% is expressed as wet sample. A number of experiments were carried out on both dry and wet soil samples, for different time intervals.

4 NUMERICAL SIMULATION

The soil sample used in the experimental work was cylindrical in shape, of size 100 mm diameter and 100 mm height. Accordingly, a 2D axisymmetric domain was employed in this study, with a height of 100mm and radius of 50mm. A uniform mesh of 500, 4 noded quadrilateral elements, and a time step of 100 seconds were found to yield converged results. Figure 2 shows the model domain, including initial and boundary conditions.

The initial temperature was specified as 25 °C. Based on the initial degree of saturation the initial suction of the material was determined from the moisture retention curve fitted using the van Genuchten model (1980). This corresponds to a pore water pressure (u_l) of 18.4 MPa and 6.85 MPa for the dry and wet samples respectively. The initial pore gas pressure is the atmospheric pressure as 0.1 MPa.

Temperature boundary conditions of a fixed temperature of 85 °C at the bottom end with 25 °C at the top were applied. A temperature dependent heat flux condition was applied to the side of the domain, to represent heat loss during the experiment via the use of heat transfer coefficient, h and reference temperature Tr. A fixed pore water pressure of 0.6 MPa was applied at the top surface. A zero flux hydraulic boundary condition was applied on all other surfaces.

4.1 Material parameters

The theoretical model requires a detailed set of thermal-hydraulic-mechanical material parameters to define the behaviour of the material present in the analysis. The material parameters concerning flow analysis are: (i) moisture retention relationship, (ii) hydraulic conductivity relationship, (iii) thermal conductivity relationship, (iv) gas conductivity relationship, (v) diffusion coefficient, (vi) Specific heat capacity for solid, liquid, vapour and air, (vii) Latent heat of vaporisation and (viii) material constants.

The thermal-hydraulic relationship to represent the material behaviour, used in the model is calibrated against the experimental results (Table 1). The detail description of material parameters are presented in Siddiqua (2008).

5 RESULTS AND DISCUSSIONS

5.1 Thermal results

Figure 3 presents a comparison of temperature profiles between the numerical and experimental results after 1 day of testing. The experimental results suggest that thermal equilibrium is reached within 1 day for both dry and wet samples. The simulated results show excellent correlation with experimental results.

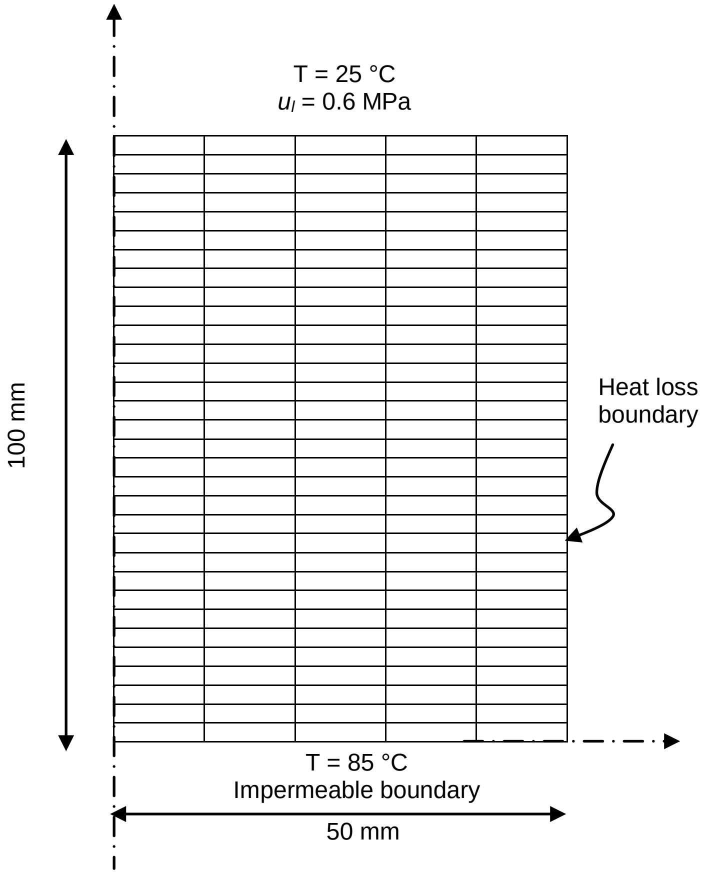

Figure 2: Schematic diagram of 2D axisymmetric mesh (500 elements)

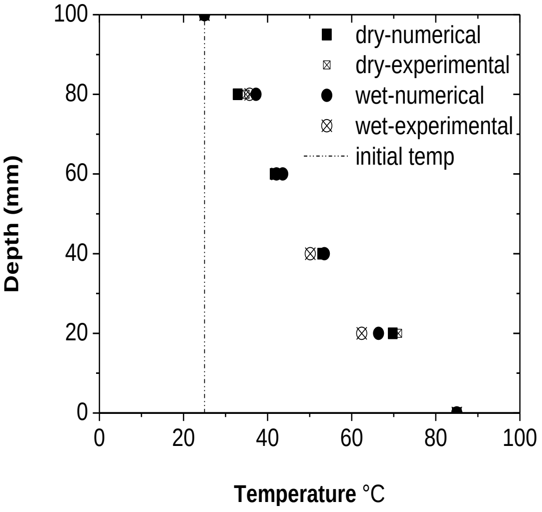

Figure 3: Temperature profile after 1 day

Table 1: Material parameters used for MX-80 bentonite for numerical analysis

Parameters	**Function/ constant**	**Reference**
<u>Hydraulic soil parameters</u>		
Unsaturated hydraulic conductivity, k_l, (m/s)	$k_l = S_r^{\delta} k_{sat}$,δ=3 k_{sat}=1.25 x 10^{-13} m/s	Huertas *et al*. (2000)
Moisture retention curve	$\frac{\theta_l - \theta_{lr}}{\theta_{ls} - \theta_{lr}} = \left[\frac{1}{1+(\alpha s)^n}\right]^m$ where $\alpha = 0.00075$, $n = 1.9$ $m = 0.474$, $\theta_{lr} = 0.0001$ $\theta_{ls} = \text{porosity} = 0.43$	Singh (2007)
<u>Thermal soil parameters</u>		
Thermal conductivity, λ, (W/mK)	$\lambda = A_2 + \frac{A_1 - A_2}{1+e(S_r - x_0)/d_x}$ where $A_1 = 1.1$, $A_2 = 1.6$ $x_0 = 0.65$, $d_x = 0.30$	Huertas *et al*. (2000)

5.2 Moisture redistribution results

Figures 4 to 6 present a comparison of profiles of moisture redistribution of dry and wet samples in terms of degree of saturation between the numerical and experimental results for 1 day, 7 days and 15 days duration.

The experiment shows drying of the sample at the hot end and consequent wetting away from the heater, at the same time wetting at the cold end due to infiltrating water. This would be expected in any standard thermo-hydraulic experiment with similar conditions (Singh, 2007). The reduction has occurred as the amount of liquid transforms to vapour due to heating. This vapour moves away with pressure gradient (advection) and concentration gradient (diffusion) to a cooler region. This process creates a significant loss of moisture in the dry zone, as a result the value of the degree of saturation in this location decreased from the initial stage. On the other hand, the amount of vapour that travels from the hot zone to a reasonably cold zone starts to condense, therefore the degree of saturation increases.

The simulated results from the above defined model show good qualitative and quantitative agreement for all times.

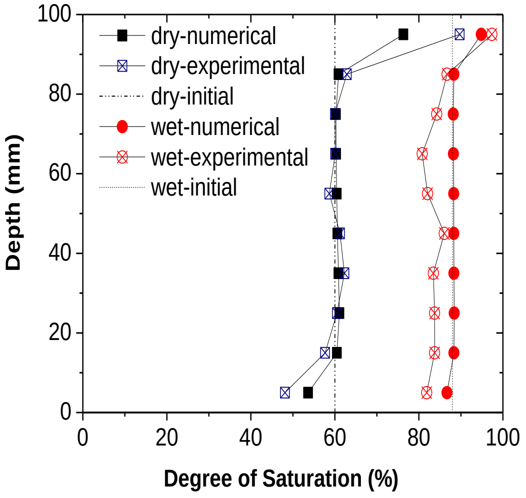

Figure 4: Comparison of degree of saturation profile between numerical and experimental results after 1 day

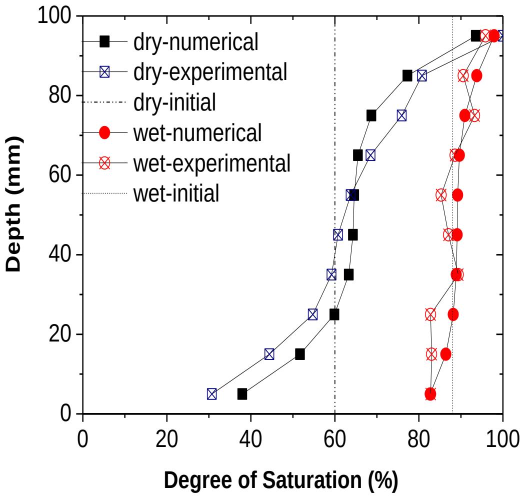

Figure 5: Comparison of degree of saturation profile between numerical and experimental results after 7 days

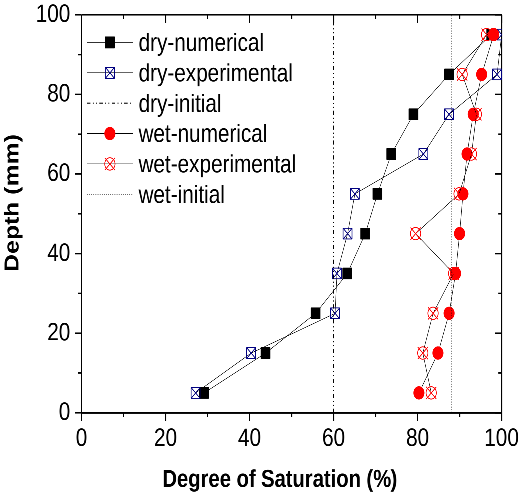

Figure 6: Comparison of degree of saturation profile between numerical and experimental results after 15 days

6 CONCLUSION

This paper has demonstrated the numerical simulation of the small cell heating and hydration experiment carried out at the geotechnical laboratory of Cardiff University .The nature of the experiment demanded that a thermo/hydro/mechanical analysis be carried out in order to successfully predict the behaviour of the material at an elevated temperature of 85°C. The response of both temperature and moisture fields is captured well offering confidence in the use of the model.

7 REFERENCES

Dahlstrom, L.O. 1998. Test plan for the prototype repository", *SKB Progress report* HRL-98-24.

Gibb, F.G.F. 1999. High temperature, very deep, geological disposal: a safer alternative for high-level radioactive waste, *Waste Manag.*,19, 207-211.

Graham, J., Chandler, N.A., Dixon, P.J., Roach, To T., and Wan, A.W.L. 1997. The Buffer/Container Experiment: results, synthesis, issues, *Technical Report* AECL-11746.

Huertas, F., Fuentes-Cantillana, J.L., Jullien, F., Rivas, P., Linares, J., Farina, P., Ghorechi, M., Jockwer, N., Kickmaier, W., Martinez, M.A., Samper, J., Alonso, E., and Elorza, F.J. 2000. Full-Scale engineered barriers experiment for a deep geological repository for high-level radioactive waste in crystalline host rock (FEBEX project) , *Euratom*.

Luikov, A.V. 1966. Heat and Mass Transfer in Capillary Porous Bodies, *Pergamon*, Oxford.

Olivella, S., and Gens, A. 2000. Vapor transport in low permeability unsaturated soil with capillary effects. *Transport in Porous Media* **40**, 219–241.

Pintado, X., Ledesma, A., and Lloret, A. 2002. Backanalysis of thermohydraulic bentonite properties from laboratory tests, *Engineering Geology* 64, 91-115.

Siddiqua, S. 2008. An investigation of the influence of elevated temperatures on the thermal-hydraulic-mechanical response of unsaturated soils, *PhD thesis*, Cardiff School of Engineering, UK.

Singh, R.M. 2007. An experimental and numerical investigation of heat and mass movement in unsaturated clays. *PhD thesis*, Cardiff School of Engineering, UK.

Thomas, H.R. and King, S.D. 1991. Coupled temperature/capillary potential variations in unsaturated soil, *ASCE, J. Eng. Mech*., 117(11), 2475-2491.

Thomas, H. R. and He, Y. 1995. Analysis of coupled heat, moisture and air transfer in a deformable unsaturated soil, *Geotechnique*, 45(4), 677-689.

Thomas, H.R. and He, Y. 1997. A coupled heat-moisture transfer theory for deformable unsaturated soil and its algorithmic implementation. *International Journal for Numerical Methods in Engineering* 40, 3421–3441.

Thomas H.R., Siddiqua, S., and Seetharam, S.C. 2009. Inclusion of higher temperature effects in a soil behavior model, Submitted for publication in *Géotechnique*.