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Publication Date

2022-03-17

DOI

10.1061/9780784484050.033

Peer reviewed

Water retention in expansive clay under elevated temperatures and constrained conditions

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ABSTRACT

This paper focuses on the impact of elevated temperatures on the water retention of MX80 bentonite under constrained or constant volume conditions. This topic is necessary to simulate the combined heating and hydration of bentonite in engineered barrier systems for deep geological repositories for nuclear waste, where the restraint from the surrounding host rock prevents swelling. In addition to providing an evaluation of the coupled thermo-hydraulic properties of MX80 bentonite, the water retention model of Lu (2016) was extended to elevated temperatures and compared with data from the literature for compacted bentonite, with insights into the effects of the different mechanisms of water retention over the full suction range.

INTRODUCTION

The safe, long-term disposal of radioactive waste is a major international challenge. The most common disposal approach under consideration is storing waste canisters in deep geological repositories. A key component in a geological repository is the engineered barrier system, which includes a bentonite buffer placed between the waste canister and the surrounding host rock. In most geological repositories, the cylindrical waste canister is placed horizontally within a circular cavity drilled in the host rock atop a pedestal of compressed bentonite with bentonite in granular or pelletized form having low initial gravimetric water contents on the order of 10-15% packed into the space between the canister and host rock. Several field and numerical studies have shown that bentonite absorbs water from the surrounding host rock and tends to swell as it hydrates, generating stresses due to the restraint provided by the host rock and waste canister (e.g., Villar et al. 2005; Sanchez et al. 2005; Dupray et al. 2013; Zheng et al. 2017). At the same time, the waste canister will increase in temperature due to the radioactive nature of the waste, leading to thermally induced drying of the bentonite near the heater (Philip and de Vries 1957). Long-term simulations of the bentonite buffer response require a thermo-hydro-mechanical model that not only captures these coupled physical processes but also considers the highly coupled thermo-hydro-mechanical properties. A schematic highlighting the coupled processes and gradients in coupled thermo-hydro-mechanical properties is shown in Figure 1.

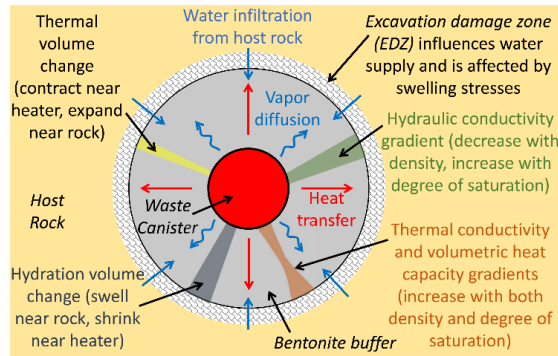


Fig. 1: Summary of coupled heat transfer and water flow processes in a bentonite buffer

Combined hydration and heating of unsaturated bentonite may lead to unexpected behavior due to coupling between the thermo-hydro-mechanical properties. For example, in field observations from the FEBEX project reported by Villar et al. (2005) where a heater reached temperatures approaching 100 °C, bentonite buffer hydration did not proceed as quickly as expected because thermally induced drying led to a decrease in thermal conductivity near the canister. More information is needed to understand the impacts of the relative rates of hydration and heating for the different heating/hydration paths experienced across the buffer radius. Although the bentonite in a repository is constrained, Villar et al. (2005) observed density gradients within the bentonite buffer as the bentonite nearest the host rock swelled as it hydrated while the bentonite closest to the canister experienced thermal volume change.

Key to understanding the relative rates of hydration and heating on bentonite buffers is knowledge of the effects of temperature and volume change on the coupled thermo-hydraulic properties of the bentonite. These include the soil-water retention curve (SWRC), the hydraulic conductivity function (HCF), the thermal conductivity function (TCF), and the volumetric heat capacity function (VHCF). Many simulations of heat transfer and water flow in bentonite buffers use thermo-hydraulic properties measured at room temperature (e.g., Sanchez et al. 2005; Zheng et al. 2017) as models to consider the effects of elevated temperatures are not yet available for expansive clays. This paper focuses on the effects of temperature on the SWRC for compacted bentonite under constrained conditions. Although this paper summarizes some of the key interrelationships between the thermo-mechanical properties of bentonite at room temperature, it focuses on the effects of temperature on the SWRC because the HCF, TCF, and VHCF are closely linked with the SWRC. For example, the HCF is often predicted from the SWRC using a bundled capillary model (van Genuchten 1980), Lu and Dong (2015) found that the parameters of their TCF are closely linked to those of the SWRC, and Baser et al. (2018) found that the VHCF has a similar form to the TCF. While the SWRC of expansive clays has been studied for temperatures up to 80 °C (e.g., Romero et al. 2003; Villar 2005; Dueck and Nillson 2010), the effects of temperature on water retention over the full suction range have not been fully studied.

Expected coupled variations in the hypothetical SWRC, HCF, and TCF (or VHCF) relationships with hydration and heating for unconstrained conditions are shown in Figure 2(a). Although this study focuses on constrained conditions where the bentonite is not allowed to

swell, it is important to show how changes in volume during swelling or heating may affect the shape of the thermo-hydraulic relationships. In general, it is expected that as bentonite hydrates under unconstrained conditions, the porosity (θ_s or n) will increase leading to an increase in water retention. It is well known that elevated temperatures are expected to lead to a reduction in capillary water retention due to changes in water-air surface tension and solid-water contact angle (e.g., Grant & Salehzadeh 1996). At higher suctions, temperature may increase the adsorption of water to the clay particles and decrease the maximum suction in the clay. The SWRC model of Lu (2016) quantifies the fundamental mechanisms of water retention in the capillary and absorptive regimes and can consider the relative roles of the bentonite micro- and macro-pore structures, and many of its constituent equations are dependent on temperature. Specifically, Luo et al. (2021) found that the suction at cavitation ψ_c is sensitive to temperature, Revil and Lu (2013) found that the adsorptive water content θ_a increases with temperature, while Lu and Khorshidi (2015) found that the maximum suction decreases with temperature. The SWRC for powdered Wyoming bentonite from Lu (2016) is shown in Figure 2(b), along with expected effects of temperature on the SWRC based on these different mechanisms.

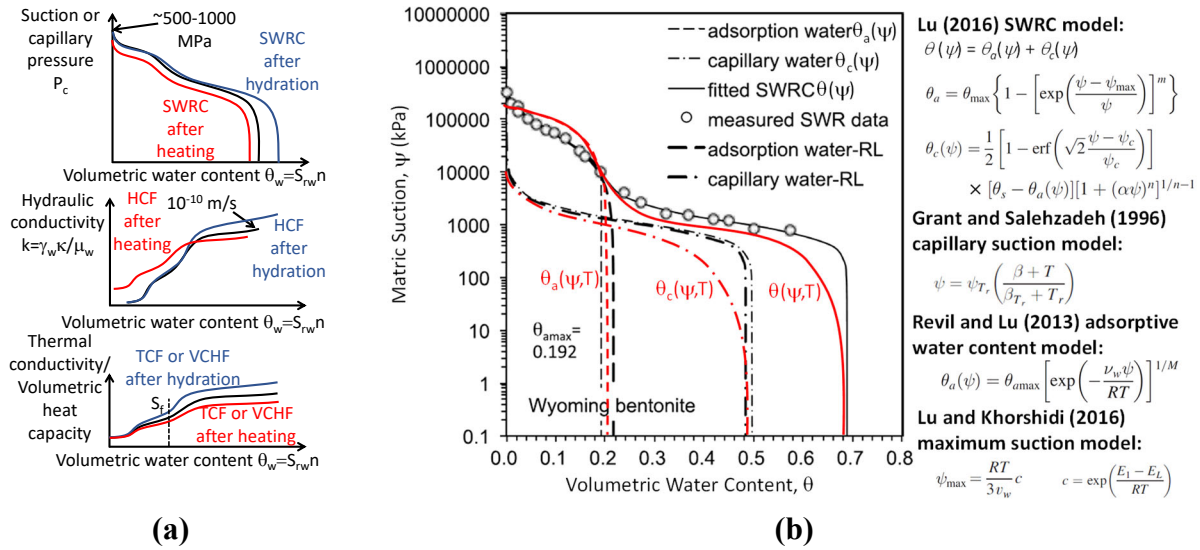


Fig. 2: (a) Expected variations in thermo-hydraulic properties during heating and hydration for unconstrained conditions; (b) SWRC for Wyoming bentonite adapted from Lu (2016) under room temperature highlighting the expected effects of temperature (T)

Regarding the other thermo-hydraulic relationships in Figure 2(a), increased temperature will result in a decrease in water viscosity which will lead to an increase in hydraulic conductivity, which may be offset by the decrease in water retention at higher suctions. The thermal conductivity will decrease with lower water retention. Unconstrained swelling will lead to an increase in hydraulic conductivity and a decrease in thermal conductivity due to the lower density. Regarding thermal volume change, several studies have found that heating may lead to plastic thermal contraction for partially hydrated bentonite having low suction magnitudes prior to heating, or to elastic thermal expansion for relatively dry bentonite having high suction

magnitudes prior to heating (Francois and Laloui 2008; Tang and Cui 2009; Dupray et al. 2013). Elevated temperatures may also result in changes in the swelling characteristics of bentonite (Zheng et al. 2017). In tests on compacted silt, Alsherif and McCartney (2015) found that the development of permanent thermal deformations may path dependent (i.e., different responses when bentonite is heated then hydrated or hydrated then heated).

MATERIAL

This paper focuses on one of the most popular types of bentonite used internationally in engineered barrier systems: MX80 bentonite from Wyoming. MX80 bentonite is a natural mined clay, so its Atterberg limits are variable, with its liquid limit ranging from 345 to 570 and its plastic limit ranging from 48 to 70. It is supplied by American Colloid Co. in granular form with a low initial gravimetric water content of approximately 9%. This section reports the basic thermo-hydro-mechanical properties of MX80 bentonite reported in the literature. The SWRCs of MX80 bentonite having different forms (compacted and powdered) are shown in Figure 3(a). The SWRC at high suctions (greater than 10 MPa) does not depend significantly upon the initial dry density of the specimen. A slight hysteresis is noted for the tests that involved wetting and drying (paths shown as solid lines), with greater water retention upon drying than upon wetting. Villar (2005) performed a suite of wetting-path SWRC tests on compacted bentonite blocks having different initial dry densities in unconstrained conditions. Fitted van Genuchten (1980) SWRCs for blocks with different initial dry densities are shown in Figure 3(b). While the SWRCs shown in terms of degree of saturation exhibit an increase in water retention with dry density, conditions close to saturation have not been fully characterized.

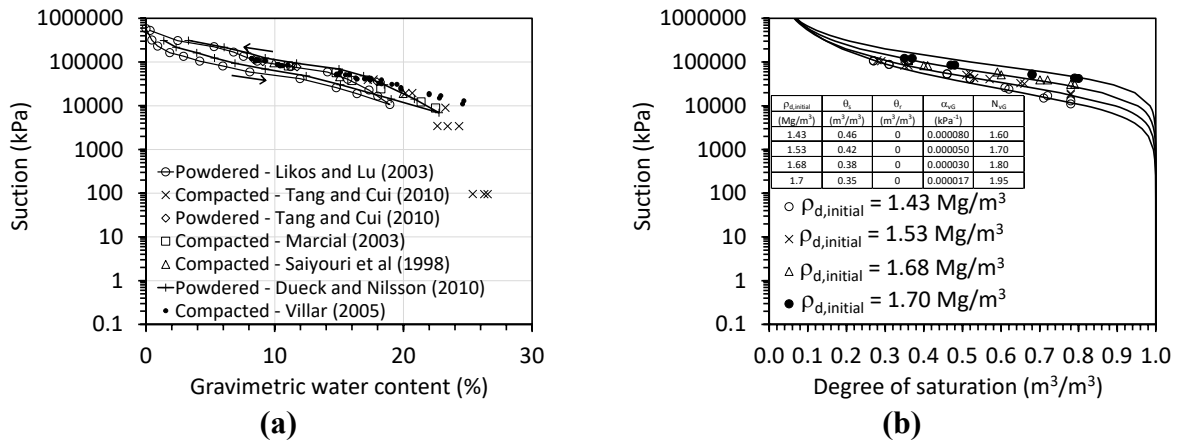


Fig. 3: (a) Comparisons of SWRCs of bentonite in powdered and granular forms; (b) Effect of initial dry density on the SWRC of compacted MX80 bentonite (Villar 2005)

Villar (2005) measured the hydraulic conductivity of saturated MX80 in constrained conditions, shown in Figure 4(a) with respect to the initial dry density. The effective stress state in these experiments is not known as swelling was prevented while high water pressures were

applied to the specimen boundaries to form a hydraulic gradient. The results in Figure 4(a) can be converted to intrinsic permeability using the density and dynamic viscosity of water at room temperature, which can then be used to predict changes in k_{sat} with temperature as noted in Figure 2(a), as both the density and dynamic viscosity of water depend on temperature. The SWRCs from Figure 3(b) can be used to predict the HCF from these k_{sat} values. Tang and Cui (2008a) performed a series of thermal needle tests on MX80 bentonite having different dry densities and compaction water contents as shown in Figure 4(b). Although this means that each of the specimens likely has a different soil structure which can affect the thermal conductivity, an effect of the compaction induced soil structure was not observed apart from the density effect.

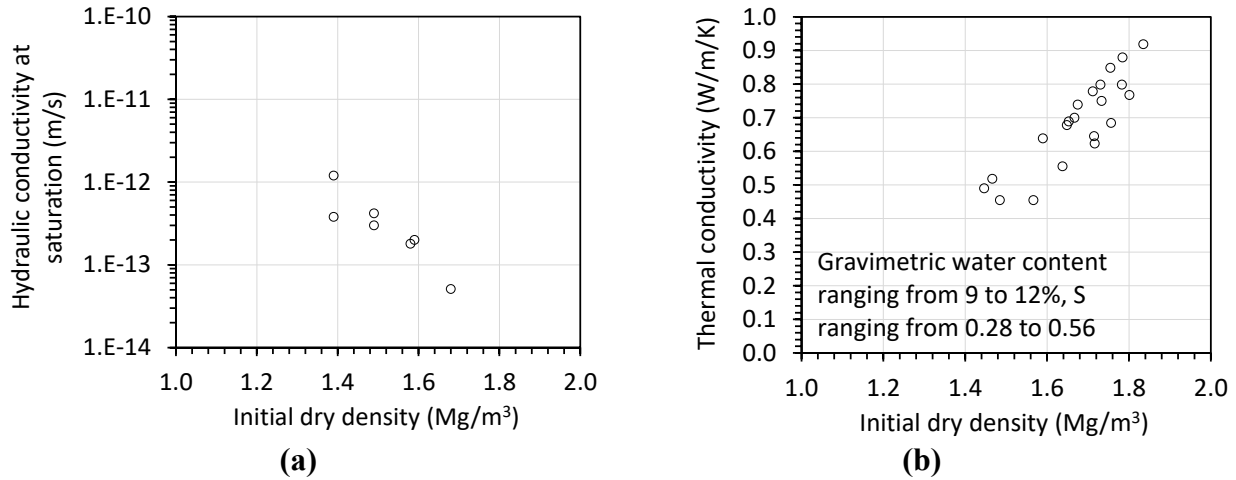


Fig. 4: Effects of dry density of MX80 bentonite: (a) Hydraulic conductivity at saturation (Villar 2005); (b) Thermal conductivity (Tang and Cui 2010)

The TCF of Lu and Dong (2015) was fitted to the data in Figure 4(b) plotted terms of the degree of saturation but separated by the initial dry density in Figure 5(a). The trend between the thermal conductivity and the initial dry density in Figure 4(b) can be used to determine the initial thermal conductivity of the compacted soil layer, and the trend in Figure 5(a) can be used to predict the impact of changing S during hydration on the thermal conductivity. It is assumed that the thermal conductivity is not sensitive to temperature, but as Lu and Dong (2015) showed that the parameters of the TCF are closely related to those of the SWRC, the TCF may be indirectly related to temperature through temperature effects on the SWRC. Relatively few studies have characterized the volumetric heat capacity of MX80 bentonite. Knutsson (1983) performed a series of heat diffusion tests on heavily compacted bentonite (not MX80 bentonite but with similar characteristics), and the results are shown in Figure 5(b). The Lu and Dong (2015) model in terms of the volumetric heat capacity was fitted to the data. Despite the different type of bentonite, the parameters for this VHCF are the same as the TCF in Figure 5(a).

Although this study is focused on understanding the SWRC under constrained conditions, it is relevant to understand the swelling potential of MX80 bentonite as well as the parameters of the compression curve. Villar (2005) performed oedometer tests to understand the constrained swell pressure for specimens with different initial dry densities, along with the free swell and

compression curve at room temperature, as shown in Figure 6. Under constrained conditions, the bentonite will induce large stresses as it hydrates. Villar (2005) also characterized the swell pressure of bentonite under a range of initial dry densities, and for example, MX80 bentonite compacted to a dry unit weight of 1.4 Mg/m³ has a swell pressure of approximately 2 MPa.

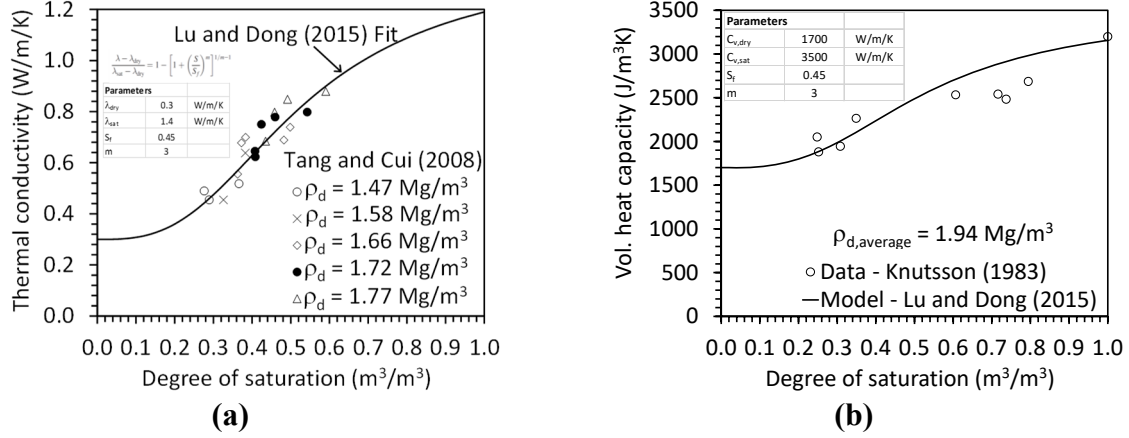


Fig. 5: Lu and Dong (2015) model: (a) Thermal conductivity of MX80 bentonite from Tang et al. (2008a); (b) Volumetric heat capacity of compacted bentonite from Knutsson (1983)

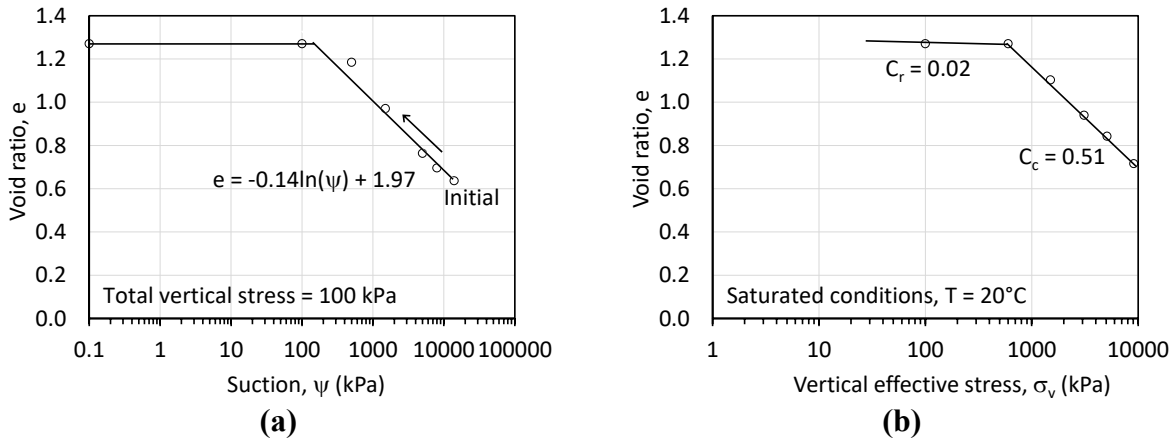


Fig. 6: Volume change of MX80 bentonite (Villar 2005): (a) Free swelling of a specimen with an initial dry density of 1.69 Mg/m³ at a suction of 14 MPa; (b) Compression curve

The final characteristic of bentonite relevant to the thermo-hydro-mechanical response is the volume change due to changes in temperature. Tang et al. (2008b) studied the drained thermal volume change of compacted MX80 bentonite having different initial mean total stresses and suction values with selected results shown in Figure 7. For some combinations of suction and total stress (i.e., low total stress together with high suction or high total stress and high suction), elastic thermal expansion occurs during heating up to 80°C. For these combinations, the average volumetric coefficient of thermal expansion is shown in Figure 7. Thermo-elastic volumetric expansion is expected if the bentonite is constrained and if heating starts prior to full hydration. However, the results in Figure 7 indicate that for some combinations of suction and total stress (i.e., low total stress and low suction), plastic thermal contraction may occur. The

latter combination is not always considered in bentonite buffers and requires an advanced thermo-elasto-plastic model for simulation (e.g., Tang and Cui 2009), but this case may be relevant when considering the thermal volume change of bentonite closer to the host rock.

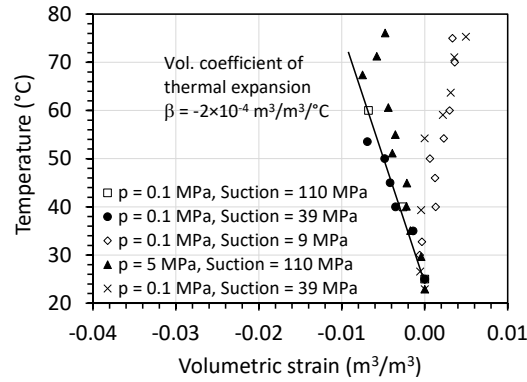


Fig. 7: Thermal volume changes of compacted MX80 measured by Tang et al. (2008b)

EFFECT OF ELEVATED TEMPERATURES ON SWRC OF MX80 BENTONITE

The SWRC of MX80 bentonite under elevated temperatures up to a maximum temperature of 60 °C have been evaluated in the literature. Dueck and Nilsson (2010) presented the SWRC of powdered MX80 bentonite under temperatures of 20 and 50 °C, while Villar (2005) presented wetting-path SWRCs of compacted MX80 bentonite in constrained conditions under temperatures of 20 and 60 °C, with results shown in Figures 8(a) and 8(b), respectively. While a reduction in water retention is observed in the powdered bentonite in Figure 8(a) that is inconsistent with the expected trends in Figure 2(b), a slight increase in water retention at high suctions is observed for the compacted bentonite with a dry density of 1.6 Mg/m³ in Figure 8(b).

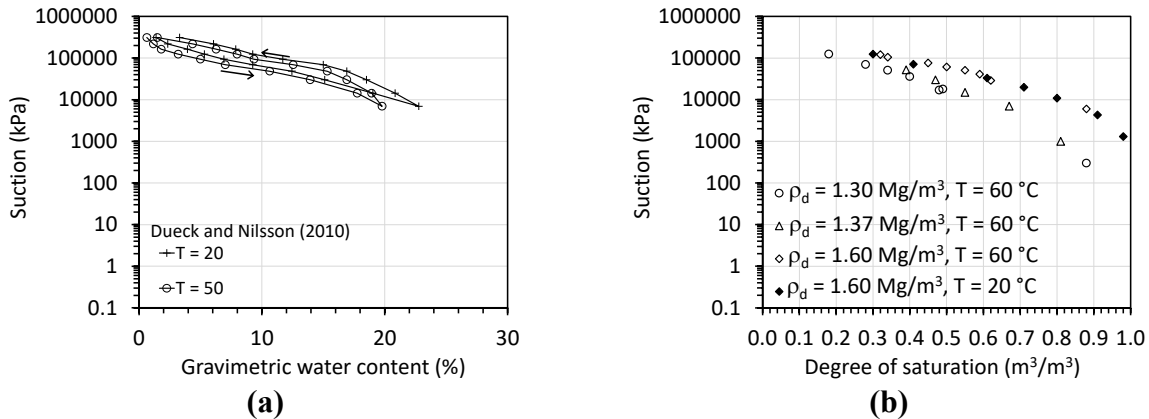


Fig. 8: Temperature effects on: (a) Hysteretic SWRC of powdered MX80 bentonite (Dueck and Nilsson 2010); (b) Wetting SWRC of compacted MX80 bentonite (Villar 2005)

The different components of the model of Lu (2016) in Figure 2(b) were modified to account for elevated temperatures in fitting the SWRC data for compacted MX80 bentonite having a dry density of 1.6 Mg/m³ ($\theta_s = 0.42$) reported by Villar (2005) in Figure 8(b). The

results of the fit are shown in Figures 9(a) and 9(b) in terms of volumetric water content and degree of saturation, respectively. It is clear from the volumetric water contents at saturation (the porosities) in Figure 9(a) that the compacted MX80 is denser than the powdered bentonite of Lu (2016) in Figure 2. Both specimens have the same values of the parameters α and n of 0.0002 kPa^{-1} and 1.6, respectively, that govern the capillary regime. These parameters are slightly smaller than those in Figure 3(b), likely as the data in Figure 8(b) were for constrained specimens. To consider temperature effects on suction in the capillary regime, the temperature-dependent value of β in the model of Grant and Salehzadeh (1996) was calculated using a model for the temperature-dependent water-soil contact angle and air-water surface tension described by Vahedifard et al. (2018) with an enthalpy of immersion per unit area of -0.516 J/m^2 at a reference temperature of 20°C (293.15 K). The suction at cavitation ψ_c represents the boundary where capillary and adsorptive forces dominate water retention, and a reduction in ψ_c from 18,000 kPa to 12,000 kPa with the increase in temperature from 20°C to 60°C was found to fit the data. However, further research is needed to predict temperature effects on ψ_c . The model of Revil and Lu (2013) indicates that the value of $\theta_{a,\max}$ should be sensitive to temperature as it is related to the thickness of the diffuse double layer and indirectly to the cation exchange capacity (CEC). Wada and Harada (1971) found that an increase in temperature of 40°C led to a 1 to 11% increase in the CEC of montmorillonite. An increase in $\theta_{a,\max}$ from 0.25 to 0.27 with the increase in temperature from 20°C to 60°C was used for fitting purposes in Figure 9 because the method of Revil and Lu (2013) to predict $\theta_{a,\max}$ from the CEC does not work for dense soils with values of θ_s less than 0.7. Both soils had the same adsorption strength m parameter of 0.4. The model of Revil and Lu (2013) also indicates that the adsorptive water content will increase uniformly with temperature over the full suction range, but Lu and Khorshidi (2015) predicted a reduction in maximum suction with increased temperature. For a change in temperature of 39°C the maximum suction was predicted to decrease from 331,739 kPa to 297,432 kPa according to the model of Lu and Khorshidi (2015). A decrease in maximum suction occurs as temperature is in the numerator of the $\psi_{\max}$ equation but in the denominator of the c equation in Figure 2(b).

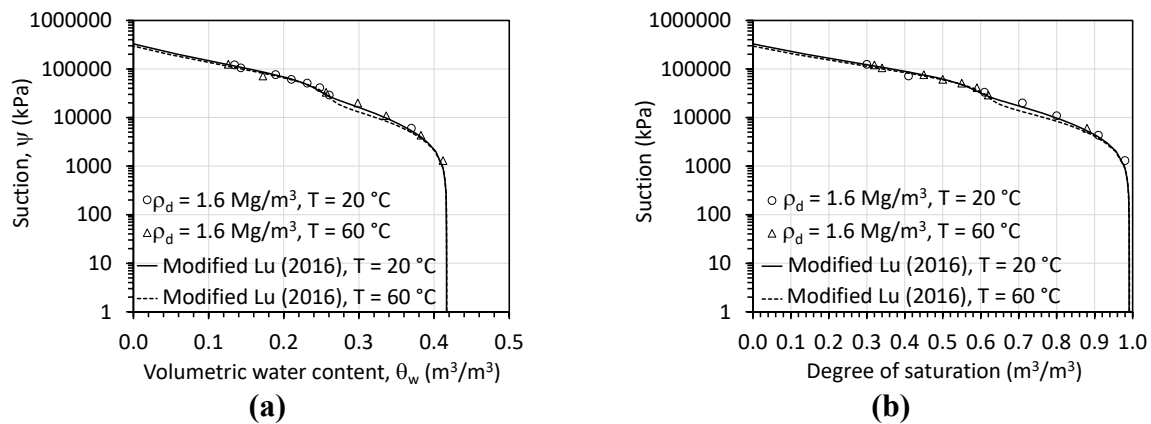


Fig. 9: Effects of temperature on MX80 bentonite from the SWRC model of Lu (2016) extended to elevated temperatures: (a) Vol. water content; (b) Degree of saturation

Overall, the incorporation of temperature effects into the SWRC model of Lu (2016) analysis indicates small effects of temperature on the SWRC for compacted MX80 bentonite, although the changes in water retention should not be discounted due to the logarithmic scale for suction. As this study was focused on the effects of temperature on constrained soils, further developments are needed to integrate the effects of swelling and thermally induced volume change into the parameters of the SWRC to capture the behavior of bentonite under unconstrained or partially constrained conditions. Nonetheless, the shift in the SWRC curves is assumed representative of the constrained condition encountered in nuclear waste repositories.

CONCLUSION

This paper presents a characterization of the coupled thermo-hydraulic properties of MX80 bentonite needed to simulate the coupled heat transfer and water flow processes in engineered barrier systems, including a discussion on the effects of temperature on the mechanisms of water retention in MX80 bentonite. A modified version of the SWRC model of Lu (2016) considering temperature effects on surface tension, wetting angle, cavitation, adsorption, and maximum suction was found to compare well with data for compacted bentonite in constrained conditions.

ACKNOWLEDGEMENTS

The author appreciates support from US Department of Energy Nuclear Energy University Program grant CFA-20-20093. The views in this paper are those of the author alone.

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