Numerical Implementation of an Equilibrium Thermodynamics-based Thermo-Hydro-Mechanical model for clay soils

Mohammadhossein Sojoudi, Biao Li
Department of Building, Civil & Environmental Engineering, Concordia University, Montreal, Quebec, Canada

ABSTRACT
Describing the material behavior based on the fundamentals of thermodynamics theory has been one of the recommended methods in constitutive modeling. However, due to the rate of dependency on deformation behaviors of clay soils, for decades the use of thermodynamics theory in constitutive modeling has been always under hesitation. In this paper, we have extended the Equilibrium Thermodynamics theory to account for the thermo-hydro-mechanical behavior of clay soils. The fundamental of energy dissipation function and momentum balance has been used to develop the proposed model. Dehydration behavior is considered in the framework based on the use of the laws of thermodynamics. Thermo-mechanical modeling is utilized to carry out constitutive modeling on temperature-controlled triaxial tests under the drained stress path condition. Different thermal conditions are simulated to demonstrate the impacts of stress and thermal histories on stress-strain relations.

RÉSUMÉ
Décrire le comportement des matériaux sur la base des principes fondamentaux de la théorie thermodynamique a été l'une des méthodes recommandées dans la modélisation constitutive. Cependant, en raison du taux de dépendance aux comportements de déformation des sols argileux, pendant des décennies, l'utilisation de la théorie thermodynamique dans la modélisation constitutive a toujours été hésitante. Dans cet article, nous avons étendu la théorie de la thermodynamique d'équilibre pour rendre compte du comportement thermo-hydro-mécanique des sols argileux. Les principes fondamentaux de la fonction de dissipation d'énergie et de l'équilibre de quantité de mouvement ont été utilisés pour développer le modèle proposé. Le comportement de déshydratation est considéré dans le cadre basé sur l'utilisation des lois de la thermodynamique. La modélisation thermomécanique est utilisée pour effectuer une modélisation constitutive sur des essais triaxiaux à température contrôlée dans la condition de chemin de contrainte drainé. Différentes conditions thermiques sont simulées pour démontrer les impacts des contraintes et des historiques thermiques sur les relations contrainte-déformation.

1. INTRODUCTION

The accurate description of thermo-hydro-mechanical (THM) behavior of geomaterials is one of the complex and necessary topics in geotechnical engineering. In the THM behavior, each part has an interaction with the other part which makes the overall behavior very complex. The schematic view of such interaction has been shown in Fig.1. As an example of this interaction, changing the temperature causes mechanical strain, simultaneously mechanical strain changes the void ratio and accordingly this change has direct effect on hydraulic pressure and so on.

The THM numerical modelling has been widely used in projects with temperature variation including nuclear waste disposal projects, thermal energy storage, geothermal energy extraction and oil and gas reservoir engineering projects (Nowak et al. 2011, Hudson et al. 2005, Wang and Kolditz.2007). However, the effect of bounding water and dehydration strain is not considered in most of the previous research. When clay soil is heated, the bonding between water and the surface of clay minerals is weakened in which some of bound water transforms into free water under certain temperature and pressure conditions. This transformation of water composes a deformation in the soil skeleton and produces dehydration strain (Li and Wong 2017, Vidal and Dubacq.2009). This strain naturally develops on a microscopic scale which causes difficulties for an appropriate understanding of dehydration behavior. Quantitative description of dehydration strain in clay soils draws considerable attention from geotechnical and geological communities (Li and Wong 2017, Zymnis et al 2019).

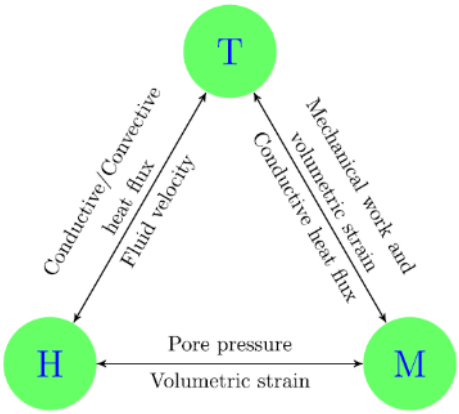

Fig 1. Schematic interaction of THM. (Neaupane et al. 1999)

During the past decades, two approaches have been widely used by researchers for describing THM behavior. Plasticity-based and thermodynamic-based approaches. The thermodynamics-based model is an approach that describes the soil behaviors based on the fundamental laws of thermodynamics and free energy functions (Darabi et al. 2012; Zhang 2017). In this type of approach, constitutive models are proposed based on the free energy and dissipation functions, thus they are always complying with the fundamental law of thermodynamics. On the other hand, In the plasticity based-approached, the model is proposing based on yield function and flow rule (Ghasemzadeh et al. 2017 and Xiong et al. 2017). The main drawback with the plasticity-based model is related to the disability of these models to obey all fundamental laws of thermodynamics. In Fig. 2. the comparison of the plasticity-based model and the thermomechanics-based model has been presented.

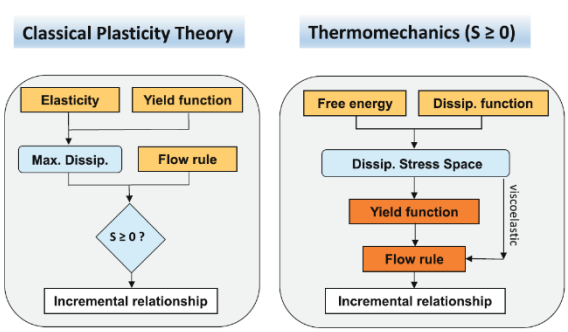

Fig.2 Schematic comparison of plasticity theory and thermodynamics-based theory. (Jacquey and Lieb 2021,)

The main objective of this research is to present a constitutive model to describe the thermo-hydro mechanical and dehydration strain behavior of clay materials based on the thermodynamics theory.

2. THERMO-HYDRAULIC BEHAVIOR

In this study the thermohydraulic behavior of clay materials is described based on the water pressure potential function. This can be defined according to the volume work done by the pore pressure. To describe the governing equation of fluid pressure and porosity, the mass balance equation for the soil particles, free water and bound water can be written as:

$$\frac{\partial(n_s\rho_s)}{\partial t} + \nabla\cdot(n_s\rho_s v_s) = 0 \qquad [1]$$

$$\frac{\partial(n_f\rho_f)}{\partial t} + \nabla\cdot(n_f\rho_f v_f) + \rho_b n_b \alpha_{bf}\frac{\partial T}{\partial t} = 0 \qquad [2]$$

$$\frac{\partial(n_b\rho_b)}{\partial t} + \nabla\cdot(n_b\rho_b v_s) - \rho_b n_b \alpha_{bf}\frac{\partial T}{\partial t} = 0 \qquad [3]$$

Where n_s, n_f and n_b are the volume fractions of the soild, free water and bounding water phases. v_s and v_f are soil particles and free water velocity; T is the temperature and α_{bf} is the mass of free water converted from per unit mass of bound water per unit rise in temperature.

The volume fraction of phases can be written according to the soil porosity n and degree of saturation of free water s_f and bound water s_b,

$$n_f + n_b = n, \quad s_f + s_b = 1 \qquad [4]$$

$$n_s + n_f + n_b = 1, \qquad [5]$$

$$n_s = 1 - n$$

$$n_f = s_f n, \qquad [6]$$

$$n_b = s_b n$$

Accordingly, based on the Darcy's law, the momentum conservation equation of the fluid phase can be expressed in terms of fluid and solid velocity.

$$q = s_f n(v_f - v_s) = \frac{-k}{\gamma_f}\cdot(\nabla p^f - \rho_f g) \qquad [7]$$

Where q is the volumetric flow rate per unite of surface area and k is the the hydraulic conductivity matrix, which is function of both pressure and temperature and γ_f is the unit weight of water.

Substituting Eq. (7) into Eq. (2) and summation of Eq (2) and (3) yields,

$$\frac{\partial(s_f n\rho_f)}{\partial t} + \nabla\cdot(\rho_f q) + \nabla\cdot(\rho_f s_f n\, v_s) + \frac{\partial(s_b n\rho_b)}{\partial t} + \nabla\cdot(s_b n\rho_b v_s) = 0 \quad [8]$$

The mass conservation of Eq1 and 8 can be rewritten by applying the Lagrangian derivation with respect to a moving solid,

$$(1-n)\cdot\frac{D_s\rho_s}{D_t} - \rho_s\frac{D_s n}{D_t} + \rho_s(1-n)\nabla\cdot v_s = 0 \quad [9]$$

$$s_f n\frac{D_f\rho_f}{D_t} + \rho_f s_f\frac{D_s n}{D_t} + n\rho_f\frac{D_s s_f}{D_t} + \rho_f\nabla\cdot q + \rho_f s_f n\nabla\cdot v_s + s_b n\frac{D_b\rho_b}{D_t} + \rho_b s_b\frac{D_s n}{D_t} + n\rho_b\frac{D_s s_b}{D_t} + \rho_b s_b n\nabla\cdot v_s = 0 \quad [10]$$

By using Eq 9 and assuming the incompressibility of solid grains the evolution of the porosity with respect to the solid deformation velocity can be described as,

$$\cdot\frac{D_s\rho_s}{D_t} = 0 \Rightarrow \frac{D_s n}{D_t} = (1-n)\nabla\cdot v_s \quad [11]$$

The variation of free water and bound water density over variation of time can be expressed in terms of pressure and temperature respectively.

$$\frac{D_f\rho_f}{D_t} = \left(\frac{1}{k_f}\frac{D_f p^f}{D_t} - \beta_f\frac{D_f T}{D_t}\right) \quad [12]$$

$$\frac{D_b\rho_b}{D_t} = \left(\frac{1}{k_b}\frac{D_b\overline{\sigma}}{D_t} - \beta_b\frac{D_b T}{D_t}\right) \quad [13]$$

Where p^f is the pore water pressure; $\frac{1}{k_f}$ and $\frac{1}{k_b}$ are the inverse of the fluid bulk and bounding water bulk modulus; β_f and β_b are the free water and bound water volumetric thermal expansion coefficient.

Substituting Eq 11,12 and 13 into Eq 10, and by expressing the gradient of soil velocity in terms of rate of stress tensor and considering($\nabla v_s = \dot{\varepsilon}$) the following governing equation obtains as,

$$\frac{s_f n}{k_f}\frac{\partial p^f}{\partial t} + s_b n\cdot\dot{\varepsilon}_{kk}^{Deh} + n(\rho_f - \rho_b)\frac{\partial s_f}{\partial t} - (s_f n\beta_f + s_b n\beta_b)\frac{\partial T}{\partial t} + (\rho_f s_f + \rho_b s_b)\dot{\varepsilon} + \rho_f\nabla q = 0 \quad [14]$$

Total strain can be decomposed into elastic, viscoplastic, thermal strain and dehydration,

$$\varepsilon = \varepsilon^e + \varepsilon^T + \varepsilon^{Deh} \quad [15]$$

Thermal strain can be expressed in terms of deformation induced by temperature variation as,

$$\dot{\varepsilon}^T = \frac{1}{3}\beta_T\frac{\partial T}{\partial t} \quad [16]$$

$$\beta_T = (1-n)\beta_s + nS_f\beta_f + nS_b\beta_b \quad [17]$$

Rate of dehydration strain can be expressed based on the work of Zymnis et al. (2019), in terms of variation of volume fraction of bounding water over the variation of time.

$$n_b = s_b n \quad [18]$$

$$\frac{\partial}{\partial t}n_b = \dot{\varepsilon}_{kk}^{Deh} = \frac{\partial n_b}{\partial s_b}\cdot\frac{\partial s_b}{\partial t} + \frac{\partial n_b}{\partial n}\cdot\frac{\partial n}{\partial t} = -n\frac{\partial s_f}{\partial t} + s_b(1-n)\dot{\varepsilon} \quad [19]$$

In this study we used the Bishop effective stress equation in terms of total stress, pore water pressure and bounding water pressure as follow,

$$\sigma' = \sigma + s_f p^f \mathrm{I} \quad [20]$$

Where I is an identity matrix, σ is the total stress and σ' is the effective stress. The linear momentum balance equation of the whole system in terms of Bishop effective stress can be expressed as,

$$\nabla.\sigma' - \nabla s_f p^f + \rho b = 0 \quad [21]$$

Where *b* is the body force.

Describing the energy balance equation for three phases material yield the following equation,

$$(\rho c)_{eff}\frac{\partial T}{\partial t} + a\nabla T + L_f\xi\frac{\partial S_f}{\partial t} = -\nabla \mathrm{q}^{\alpha} \quad [22]$$

where q^{α} is the conductive heat flux and L_f is the latent heat of fusion.

$$(\rho c)_{eff} = (1-n)\rho_s c_s + nS_f \rho_f c_f + nS_b \rho_b c_b \quad [23]$$

The c_s, c_f and c_b are the respective specific heat capacities for each phase.

According to the foundamentals of soil mechanics the following equation can be written for the degree of saturation of bound water,

$$S_b = \frac{(1-n)w_b G_s}{n} \quad [24]$$

Where w_b is the bound water content and G_s is the specific gravity measured at room temperature.

Accordingly by using the chain derivation, the time variation of S_b can be writen as,

$$\frac{\partial S_b}{\partial t} = \frac{\partial S_b}{\partial n}\frac{\partial n}{\partial t} + \frac{\partial S_b}{\partial w_b}\frac{\partial w_b}{\partial t} \quad [25]$$

Where by using Eq 23 the following can be achieved,

$$\frac{\partial S_b}{\partial n} = \frac{-w_b G_s}{n^2} \quad [26]$$

$$\frac{\partial S_b}{\partial w_b} = \frac{(1-n)G_s}{n} \quad [27]$$

Zymnis et al. 2019, proposed an experimantal relation for temperature variation of bound water conent

$$\frac{\partial w_b}{\partial T} = -\alpha_{bf} w_b \quad [28]$$

based on, the variation of bound water content over time can be expressed as follow,

$$\frac{\partial w_b}{\partial t} = \frac{\partial w_b}{\partial T}\frac{\partial T}{\partial t} = -\alpha_{bf} w_b \frac{\partial T}{\partial t} \quad [29]$$

Substituting Eq 11, 25, 26 and 27 into Eq 24 yields,

$$\frac{\partial S_b}{\partial t} = \frac{w_b G_s (n-1)}{n^2}\dot{\varepsilon} + \frac{w_b \alpha_{bf} G_s (n-1)}{n}\frac{\partial T}{\partial t} \quad [30]$$

Where by using Eq 4 the variation of degree of flud saturation over time can be expressed as,

$$\frac{\partial S_f}{\partial t} = \frac{w_b G_s (1-n)}{n^2}\dot{\varepsilon} + \frac{w_b \alpha_{bf} G_s (1-n)}{n}\frac{\partial T}{\partial t} \quad [31]$$

$$w_b = \frac{(1 - G_s \frac{\rho_f}{\rho_s})}{G_s(\frac{\rho_f}{\rho_b} - 1)} \quad [32]$$

According to Eq 30 the dehydration strain can be rewrite as,

$$\dot{\varepsilon}_{kk}^{Deh} = \frac{(w_b G_s - nS_b)(n-1)}{n}\dot{\varepsilon} + w_b \alpha_{bf} G_s (n-1)\frac{\partial T}{\partial t} \quad [33]$$

$$d\sigma' = E(d\varepsilon - d\varepsilon^{Deh} - d\varepsilon^{T}) \quad [34]$$

The elastic bulk modulus and shear modulus of the soil is given as,

$$K = \frac{P}{\gamma} \quad [35]$$

$$G = \frac{3K(1-2\nu)}{2(1+\nu)} \quad [36]$$

3. MODEL VALIDATION

To investigate the ability of the proposed model in describing the thermo-mechanical behavior of clay soils, some published test data on Kaolin clay have been used to validate the performance of numerical model in simulation.

3.1 Determination of material parameters

In the proposed model, three mechanical parameters υ, m, γ; eight thermo-dehydration parameters α_{bf}, β_s, β_f, β_b, L_f, C_s, C_f, C_b; one hydraulic parameter k and four mass and volume parameters *n*, ρ_s, ρ_f, ρ_b are required to describe the thermo-poro-mechanical behavior of a clay soil.

A common drained shear stress test at the saturated state of the soil can be used for determining the Poisson's ratio (υ) and the slope of the critical state line (m). The parameter γ indicate the slopes of swelling lines in $\ln \nu - \ln p$ plane.

The value of α_{bf} determined by using the following equation that is proposed by Zymnis et al:

$$\alpha_{bf} = -\frac{G_s}{(1 - G_s \frac{\rho_{fw}}{\rho_s})}\frac{1}{M_s}\frac{\partial M_w}{\partial T} \quad [37]$$

where G_S is the specific gravity at room temperature, ρ_f and ρ_s are the densities of free water and oven-dried solid minerals respectively, M_s is the mass of solid and $\frac{\partial M_w}{\partial T}$ is the change of mass of water with temperature.

The value of β_s, β_f and β_b can be obtained by carrying out thermal consolidation tests.

3.2 kaolin clay

Cekerevac and Laloui (2003) conducted a series of drained triaxial compression tests on kaolin clay under different OCRs and temperatures. In the test, the samples are isotropically consolidated to a stress of 600 kPa at room temperature firstly, and then unloaded to achieve different OCRs. Under a drained condition, the temperature of the sample is increased slowly to obtain 22°C and 90°C, respectively. Figures 3- 6 has shown the comparison of measured results and the model. As displayed in the Figures the model predictions have a proper correspondence with the test results. The decrease in the volumetric strain and failure of stress due to the increase of overconsolidation ratio are simulated accurately. The thermal hardening phenomenon during temperature variations is another aspect that is appropriately predicted by the model. Model parameters are listed in table 1.

Table 1. Model parameters

			Kaolin clay
Mechanical	υ	(-)	0.3
	m	(-)	0.85
	γ	(-)	0.001
	σ'	(MPa)	0.6
Thermo-Dehydration	α_{bf}	($^{\circ}C^{-1}$)	0.0357
	β_b	($^{\circ}C^{-1}$)	-5e-5
	L_f	KJ/Kg	334
	c_s	J/Kg/K	800
Hydraulic	c_f	J/Kg/K	4190
	c_b	J/Kg/K	3000
Mass and Volume	k	m/s	-1e-8
	n	(-)	0.44
	ρ_s	Kg/m^3	2650
	ρ_f	Kg/m^3	1000
	ρ_b	Kg/m^3	1250

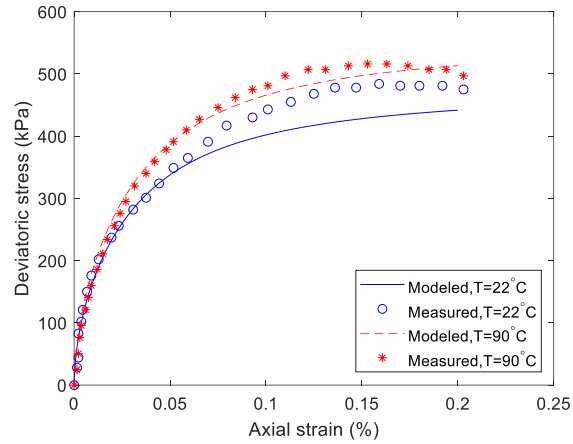

Figure 3. Comparison of modeled results and test data for drained triaxial compression test on OCR=1.2 kaolin clay: (measured data is from Cekerevac and Laloui 2003).

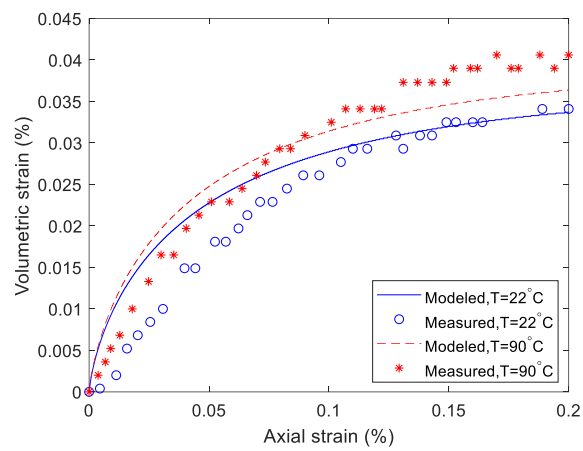

Figure 4. Comparison of modeled results and test data for drained triaxial compression test on OCR=1.2 kaolin clay: (measured data is from Cekerevac and Laloui 2003).

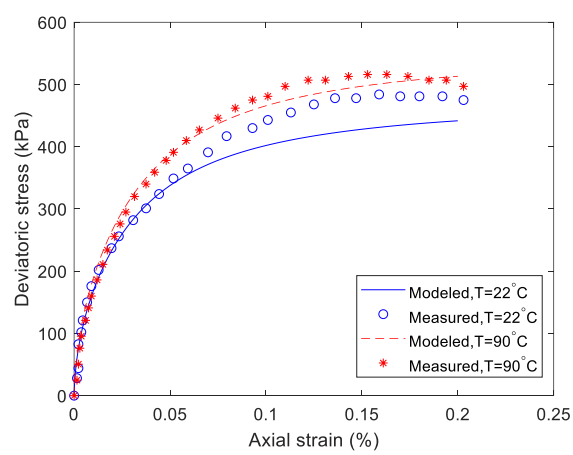

Figure 5. Comparison of modeled results and test data for drained triaxial compression test on OCR=1.5 kaolin clay: (measured data is from Cekerevac and Laloui 2003).

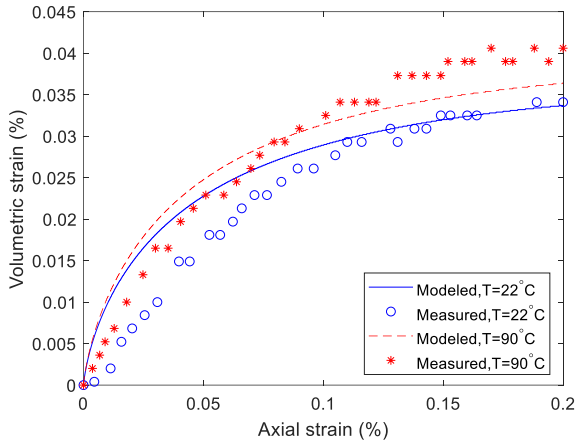

Figure 6. Comparison of modeled results and test data for drained triaxial compression test on OCR=1.5 kaolin clay: (measured data is from Cekerevac and Laloui 2003).

4. CONCLUSIONS

In this paper, a thermodynamic-based model for describing the thermo-hydro-mechanical behavior of clayey material was developed. The proposed model employed the mass balance, momentum balance and energy balance equations for simulating hydraulic -dehydration-induced strain under thermo-mechanical loading.

The effect of dehydration strain and bounding water on a total strain of the soil has been considered in the model by using a novel and simple methods. A comparison between model predictions and experimental data for kaolin clay soils is presented and a reasonable result is achieved.

5. REFRENCES

Bekele, Y.W., Kyokawa, H., Kvarving, A.M., Kvamsdal, T. and Nordal, S., 2017. Isogeometric analysis of THM coupled processes in ground freezing. Computers and Geotechnics, 88, pp.129-145.

Cacace, M. and Jacquey, A.B., 2017. Flexible parallel implicit modelling of coupled thermal–hydraulic–mechanical processes in fractured rocks. Solid Earth, 8(5), pp.921-941.

Darabi, M. K., Al-Rub, R. K. A., Masad, E. A., & Little, D. N. (2012). Thermodynamic-based model for coupling temperature-dependent viscoelastic, viscoplastic, and viscodamage constitutive behavior of asphalt mixtures. International Journal for Numerical and Analytical Methods in Geomechanics, 36(7), 817-854.

Ghasemzadeh, H., Sojoudi, M.H., Amiri, S.G. and Karami, M.H., 2017. Elastoplastic model for hydro-mechanical behavior of unsaturated soils. Soils and Foundations, 57(3), pp.371-383.

Houlsby, G.T. and Puzrin, A.M., 2000. A thermomechanical framework for constitutive models for rate-independent dissipative materials. International journal of Plasticity, 16(9), pp.1017-1047.

Houlsby, G.T. and Puzrin, A.M., 2007. Principles of hyperplasticity: an approach to plasticity theory based on thermodynamic principles. Springer Science & Business Media.

Jacquey, A.B. and Cacace, M., 2020. Multiphysics modeling of a brittle-ductile lithosphere: 2. Semi-brittle, semi-ductile deformation and damage rheology. Journal of Geophysical Research: Solid Earth, 125(1), p.e2019JB018475.

Jacquey, A.B. and Regenauer-Lieb, K., 2021. Thermomechanics for geological, civil engineering and geodynamic applications: Rate-dependent critical state line models. Rock Mechanics and Rock Engineering, 54(10), pp.5355-5373.

Jacquey, A.B., Regenauer-Lieb, K. and Cacace, M., 2021. Thermomechanics for geological, civil engineering and geodynamic applications: numerical implementation and application to the Bentheim sandstone. Rock Mechanics and Rock Engineering, 54(10), pp.5337-5354.

Hudson, J. A., Stephansson, O., & Andersson, J. (2005). Guidance on numerical modelling of thermo-hydro-mechanical coupled processes for performance assessment of radioactive waste repositories. International Journal of Rock Mechanics and Mining Sciences, 42(5-6), 850-870.

Laloui, L., & Cekerevac, C. (2003). Thermo-plasticity of clays: an isotropic yield mechanism. Computers and Geotechnics, 30(8), 649-660.

Li, B. and Wong, R.C., 2017. A mechanistic model for anisotropic thermal strain behavior of soft mudrocks. Engineering Geology, 228, pp.146-157.

Neaupane, K. M., Yamabe, T., & Yoshinaka, R. (1999). Simulation of a fully coupled thermo–hydro–mechanical system in freezing and thawing rock. International Journal of Rock Mechanics and Mining Sciences, 36(5), 563-580.

Nowak, T., Kunz, H., Dixon, D., Wang, W., Görke, U. J., & Kolditz, O. (2011). Coupled 3-D thermo-hydro-mechanical analysis of geotechnological in situ tests. International Journal of Rock Mechanics and Mining Sciences, 48(1), 1-15.

Sojoudi, M. H., and Biao Li.,2020 "Thermodynamic-based model for the thermo-poro-elastoplastic behavior of saturated clay." Geovirtual conference,2020.

Vidal, O., & Dubacq, B. (2009). Thermodynamic modelling of clay dehydration, stability and compositional evolution with temperature, pressure and H2O activity. Geochimica et Cosmochimica Acta, 73(21), 6544-6564.

Wang, W., & Kolditz, O. (2007). Object-oriented finite element analysis of thermo-hydro-mechanical (THM) problems in porous media. International Journal for Numerical Methods in Engineering, 69(1), 162-201.

Xiong, Y.L., Ye, G.L., Zhu, H.H., Zhang, S. and Zhang, F., 2017. A unified thermo-elasto-viscoplastic model for soft rock. International Journal of Rock Mechanics and Mining Sciences, 93, pp.1-12.

Zhang, Z., 2017. A thermodynamics-based theory for thethermo-poro-mechanical modeling of saturated clay. International Journal of Plasticity, 92, pp.164-185.

Zymnis, D. M., Whittle, A. J., & Cheng, X. (2019). Simulation of long-term thermo-mechanical response of clay using an advanced constitutive model. Acta Geotechnica, 14(2), 295-311.