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A thermodynamically based thermo-mechanical model for fine-grained soils

Un modèle thermomécanique thermodynamiquement consistant pour sols fins

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ABSTRACT: During the heat transfer process of thermo-active structures with the ground, the soil is often exposed to both mechanical and thermally-induced stresses. Since the behaviour and stability of these structures are directly dependent on the thermo-mechanical behaviour of the soils, it is essential to use a constitutive model in numerical analyses that accurately accounts for the thermo-mechanical behaviour. In this paper, a thermo-mechanical model based on thermodynamics principles is developed within the hyper-plasticity framework. The model is consistent with critical state soil mechanics concepts and accounts for thermal softening as the major mechanism of thermal effects in fine-grained soils. The performance of the model is compared to experimental data, which shows a good consistency between the simulation and data.

RÉSUMÉ: Pendant dans le processus de transfert de chaleur des structures thermoactives, le sol est souvent exposé à des contraintes mécaniques et thermo-induites. Le comportement et la stabilité de ces structures dépendant directement du comportement thermomécanique des sols mêmes, il est essentiel d'implémenter, dans les analyses numériques, un modèle constitutif qui prend en compte de manière précise le comportement thermomécanique des sols. Dans cet article, un modèle thermomécanique basé sur les principes de la thermodynamique est développé à travers le cadre de l'hyper-plasticité. Le modele est compatible avec les concepts de la mécanique de l'état critique, et prend en compte l'adoucissement thermique comme mécanisme principal des effets thermiques sur les sols fins. Les performances du modele sont comparées à des données expérimentales, montrant une bonne cohérence entre simulations et données.

Keywords: Dissipation; Hyper-plasticity; Thermodynamics; Thermo-mechanical model

1 INTRODUCTION

A wide range of geo-structures impose temperature changes and thermally induced loads, as well as mechanical loads, onto soil. Energy piles, thermal retaining walls, high voltage cables and underground radioactive waste barriers are only a few examples of these kinds of structures (Brandl, 2006). The thermo-mechanical behaviour of soils has attracted attention, since it has been shown that changes in temperature affect the mechanical behaviour of soils (Hueckel et al., 2009; Sultan et al., 2002; Uchaipichat & Khalili, 2009; Zhou & Ng, 2016), and consequently might influence the

safety of the structure. As a result, there is a need for a constitutive model that can predict the thermo-mechanical behaviour of soils.

Throughout literature, a number of thermo-mechanical models can be found which are mostly developed based on variants of plasticity theory (e.g. Cui et al., 2000; Hueckel & Baldi, 1991; Mašín & Khalili, 2012; Zhou & Ng, 2015). Although these models may give fairly accurate predictions, the satisfaction of thermodynamics principals has been neglected. As a result, certain phenomena may not be well captured and/or predicted and other phenomena may be spuriously shown. In this study, a thermo-mechanical constitutive model is developed using a thermodynamics approach named hyper-plasticity, which was first developed by Collins & Houlsby (1997).

The hyper-plasticity framework is based on generalised thermodynamics, in which internal variables are utilised to capture the past history of the material. The formulations are derived from the first and second laws of thermodynamics (also known as energy conservation and admissible thermodynamic processes, respectively), in which certain restrictions are imposed on the derived formulations and the material's mechanical behaviour is enforced to automatically obey thermodynamics laws (Houlsby & Puzrin, 2007). The constitutive behaviour is defined by specifying two scalar potential functions. The first potential, which is a property of the first law of thermodynamics, is the internal energy of the material and can be transformed into other forms of energy potential, such as the Helmholtz free energy, Gibbs energy and enthalpy, by the Legendre transform. The second potential is the dissipation function that satisfies the second law of thermodynamics and is defined through the rate of change of internal variables (and must be a non-negative value) (Houlsby & Puzrin, 2007).

The rate-independent hyperplasticity approach, detailed in Houlsby & Puzrin (2007) and Puzrin (2012), is followed here and the well-known thermal softening mechanism for fine grained soils is embedded into the potential functions to capture the thermo-mechanical behaviour of soils. In the first part of the paper, the formulation is explained. This is followed by verification of the model with data available in literature.

2 FORMULATION

2.1 Energy potential function

A Gibbs-type function is proposed for the free energy potential function. The function is defined by two stress invariants (p, q; mean effective stress and deviatoric stress, respectively), internal variables (which here are only the volumetric and deviatoric plastic strains; $\varepsilon_v^p, \varepsilon_q^p$) and absolute temperature (θ). This form of energy potential leads to a "decoupled" behaviour of materials in which elastic and plastic behaviours are independent of each other (Collins & Houlsby, 1997). The Gibbs free energy potential function is defined as:

$$g\left(p, q, \varepsilon_v^p, \varepsilon_q^p, \theta\right) = g_1(p, q) - p\varepsilon_v^p - q\varepsilon_q^p - 3\varrho p(\theta - \theta_0) \quad (1)$$

ϱ is the linear thermal expansion coefficient of the soil mass (saturated soil-water mass) and the term $3\varrho p(\theta - \theta_0)$ provides the effect of temperature on the elasticity of the soil (thermo-elasticity). $g_1(p, q)$ is the Gibbs free energy potential function, previously proposed by Einav & Puzrin (2004) for geo-materials in which the elasticity of the material under isothermal conditions is derived based on it:

$$g_1(p,q) = -\frac{p^{2-n} - (2-n)pp_0^{1-n}}{\overline{K}(2-n)(1-n)p_r^{1-n}} - \frac{q^2}{6\overline{G}p_r^{1-n}p^n} + \frac{q_0(2qp_0 - nq_0p)}{6\overline{G}p_r^{1-n}p_0^{1+n}} \quad (2)$$

where p_r is the reference pressure (1 kPa); p_0 and q_0 are the initial values of the mean effective and deviatoric stresses, respectively; $\overline{K}$, $\overline{G}$ and n are material constants. Following the hyper-plasticity approach, the total strain $(\varepsilon_v^T, \varepsilon_q^T)$, consisting of elastic $(\varepsilon_v^e, \varepsilon_q^e)$, thermo-elastic (ε_v^θ), and thermo-plastic components $(\varepsilon_v^p, \varepsilon_q^p)$, can be determined by differentiating the Gibbs free energy potential with respect to the true stress components (p, q), while other components act as passive variables:

$$\varepsilon_v^T = -\frac{\partial g}{\partial p} = -\frac{\partial g_1}{\partial p} + 3\varrho(\theta - \theta_0)$$
$$+$$
$$\varepsilon_v^p = \varepsilon_v^e + \varepsilon_v^\theta + \varepsilon_v^p \ ; \quad (3)$$
$$\varepsilon_q^T = -\frac{\partial g}{\partial q} = -\frac{\partial g_1}{\partial q} + \varepsilon_q^p = \varepsilon_q^e + \varepsilon_q^p$$

Other important variables that can be extracted from the free energy potential are the generalised stresses, which are defined as the derivative of the energy potential with respect to the internal variables (Houlsby & Puzrin, 2007). In this model, as mentioned before, the internal variables are only the plastic strains, $\varepsilon_v^p, \varepsilon_q^p$. Thus, the generalised stresses are:

$$\bar{\chi}_p = -\frac{\partial g}{\partial \varepsilon_v^p} = p; \ \ \bar{\chi}_q = -\frac{\partial g}{\partial \varepsilon_q^p} = q \quad (4)$$

2.2 Dissipation

In order to determine the thermo-plasticity of the model, a definition of an appropriate dissipation function is required, which here is defined as:

$$d = C(\dot{\varepsilon}_v^p + \beta\dot{\varepsilon}_q^p) + \sqrt{A^2(\dot{\varepsilon}_v^p + \beta\dot{\varepsilon}_q^p)^2 + B^2(\dot{\varepsilon}_q^p)^2} \quad (5)$$

where $\dot{\varepsilon}_v^p$ and $\dot{\varepsilon}_q^p$ are plastic volumetric and deviatoric strain rates, respectively; and β represents the level of anisotropy by inclining the yield surface with respect to the p-axis.

A, B and C are functions, defined by stress components (p and p_c) that define the shape and size of the yield function:

$$A = (1-\gamma)p + \frac{\gamma}{2}p_{cT} \ ; \ \ C = \frac{\gamma}{2}p_{cT} \quad (6)$$
$$B = M\left((1-\alpha)p + \frac{\alpha\gamma}{2}p_{cT}\right)$$
$$p_{cT} = p_r e^{\left(\frac{\varepsilon_v^p}{\lambda-\kappa}\right)} e^{-\mu(\theta-\theta_0)} \quad (7)$$

where α and γ are parameters that affect the shape of the yield surface; M is the stress ratio at the critical state; μ is the coefficient of thermal softening, firstly presented by Cui et al. (2000); and λ and κ are the slopes of the normal compression (NCL) and unloading lines in void ratio, e, versus $\ln p$ space, respectively. p_{cT} is the apparent pre-consolidation pressure that hardens isotropically with plastic volume strain (through the term $e^{\varepsilon_v^p/(\lambda-\kappa)}$), while it softens with an increase in temperature (through the term $e^{-\mu(\theta-\theta_0)}$).

The yield function (surface) is defined by dissipative stresses determined by derivation of the dissipation potential function with respect to the rate of internal variables. The dissipative stresses are:

$$\chi_p = \frac{\partial d}{\partial \dot{\varepsilon}_v^p} = C + \frac{A^2(\dot{\varepsilon}_v^p + \beta\dot{\varepsilon}_q^p)}{\sqrt{A^2(\dot{\varepsilon}_v^p + \beta\dot{\varepsilon}_q^p)^2 + B^2(\dot{\varepsilon}_q^p)^2}} \quad (8)$$
$$\chi_q = \frac{\partial d}{\partial \dot{\varepsilon}_q^p} = \beta C +$$

$$\frac{B^2\dot{\varepsilon}_q^p + \beta A^2(\dot{\varepsilon}_v^p + \beta\dot{\varepsilon}_q^p)}{\sqrt{A^2(\dot{\varepsilon}_v^p + \beta\dot{\varepsilon}_q^p)^2 + B^2(\dot{\varepsilon}_q^p)^2}}$$

Any combination of these dissipative stresses resulting in a zero value represents an expression for the yield function (for rate-independent materials). By some algebraic substitution, the yield function can be derived as:

$$y = B^2(\chi_p - C)^2 + A^2(\chi_q - \beta\chi_p)^2 - A^2 B^2 = 0 \tag{9}$$

As can be seen, the yield function is defined in dissipative stress space (χ_p, χ_q), rather than in conventional stress space (p, q). The yield function may be transferred to true stress space, as shown below, by Ziegler's hypothesis (Ziegler, 1977).

The flow of plastic strain increments are always normal to the yield surface in dissipative stress space (i.e. the flow rule is always associated in dissipative stress space). This can be mathematically shown as:

$$\dot{\varepsilon}_v^p = \Lambda\frac{\partial y}{\partial\chi_p} = 2\Lambda\big(B^2(\chi_p - C) - \beta A^2(\chi_q - \beta\chi_p)\big) \tag{10}$$

$$\dot{\varepsilon}_q^p = \Lambda\frac{\partial y}{\partial\chi_q} = 2\Lambda\left(A^2(\chi_q - \beta\chi_p)\right)$$

where Λ is the plastic multiplier defining the plastic strain increment magnitude.

One of the useful assumptions implemented into hyper-plasticity theory is Ziegler's orthogonality postulation, also known as the maximum entropy assumption (Ziegler, 1977). This hypothesis is used to link the generalised stress (Equation (4)), to the dissipative stress (Equation (8)). According to this hypothesis, the generalised stress is equal to the dissipative stress:

$$\chi = \bar{\chi} \rightarrow \begin{Bmatrix} \chi_p \\ \chi_q \end{Bmatrix} = \begin{Bmatrix} p \\ q \end{Bmatrix} \tag{11}$$

This outcome results in the definition of both the yield (y) and plastic flow in conventional stress space, by substituting the dissipative stresses with generalised stresses (which here are the true stresses with no shift stresses). As a result, the yield surface and plastic flow in the true stress space become:

$$y = B^2(p - C)^2 + A^2(q - \beta p)^2 - A^2 B^2$$
$$\frac{\partial y}{\partial\chi_p} = 2\big(B^2(p - C) - \beta A^2(q - \beta p)\big)$$
$$\frac{\partial y}{\partial\chi_q} = 2A^2(q - \beta p) \tag{12}$$

An important conclusion is that the temperature dependency of the dissipation function results in temperature dependency of both the yield surface and plastic flow rule.

2.3 Isotropic hardening

In the model, the apparent pre-consolidation pressure p_{cT} is the isotropic hardening component of the model which hardens by plastic volumetric strain increments (similar to the Modified Cam Clay model), while it softens by an increase in temperature (Equation (7)). By differentiating the above equation, the isotropic hardening is derived:

$$\dot{p}_{cT} = \left(\frac{\dot{\varepsilon}_v^p}{\lambda - \kappa} - \mu\dot{\theta}\right)p_{cT}; \quad \dot{\varepsilon}_v^p = \Lambda\frac{\partial y}{\partial\chi_p} \tag{13}$$

3 MODEL PERFORMANCE

The model is defined by 10 parameters, of which λ, κ and M are similar to parameters used in the Cam Clay model: λ and κ are the negative slopes of the normal compression and swelling

lines in e-ln$p$ space, respectively, and M is the stress ratio at the critical state condition in q-p space. μ is the coefficient of thermal softening, which can be determined from the pre-consolidation pressure of isotropic compression tests at different temperatures. Depending on a clay's mineralogy, its value varies from 0.001 to 0.004 (Zhou & Ng, 2015). The constants α and γ, which are parameters affecting the shape of the yield surface, can be determined by trial and error. Note that, by assigning a value of 1.0 for both α and γ, the elliptical shape of the yield surface in the Modified Cam Clay model can be retrieved. The shape of the yield surface in $q - p - \theta$ space, for the isotropic state ($\beta = 0$), is illustrated in Figure 1. As can be seen, as the temperature increases the yield surface shrinks, representing thermal softening.

$\bar{K}, \bar{G}$ and n are material constants related to elastic properties. $\bar{G}$ is attributed to the initial shear modulus of the soil and can be determined as the tangential value to the shear stress-shear strain curve in the elastic region (at the beginning of loading). By assuming an appropriate value of Poisson's ratio, $\bar{K}$ can be determined from $\bar{G}$ and parameter n can be assumed to be 0.5.

The model's performance is validated by comparing simulations with experimental data reported by Uchaipichat & Khalili (2009). In their study, the shear behaviour of a fully saturated silty soil was investigated under drained conditions, at three temperatures (25, 40 and 60 °C) and for three mean effective stresses (50, 100 and 150 kPa). Prior to shearing, all the samples were isotropically loaded to 200 kPa and unloaded to 50 kPa at a constant temperature of 25 °C. As a result, all samples had an initial pre-consolidation pressure of 200 kPa. The samples were then heated and sheared under drained conditions until failure.

The parameters utilised for the predictions are reported in Table 1, which were collected From Uchaipichat & Khalili (2009) and Zhou & Ng (2015). The experimental data and model predictions are presented in Figures 2 and 3.
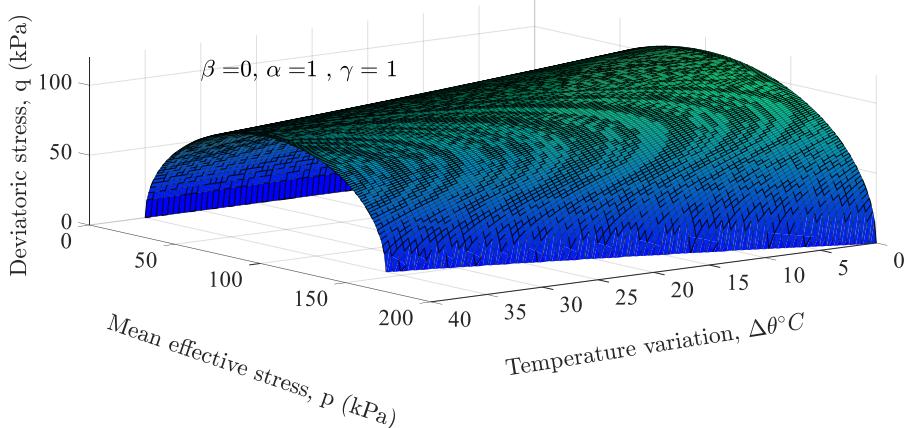

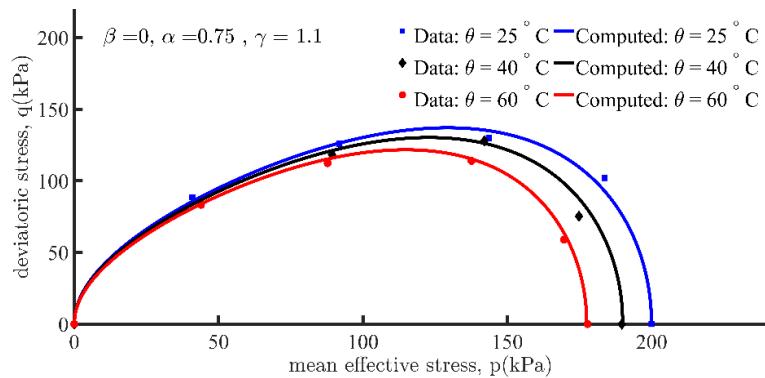*Figure 1: Yield surface at different temperatures*

Figure 2: Comparison of yield surfaces at different temperatures predicted by model with experimental data
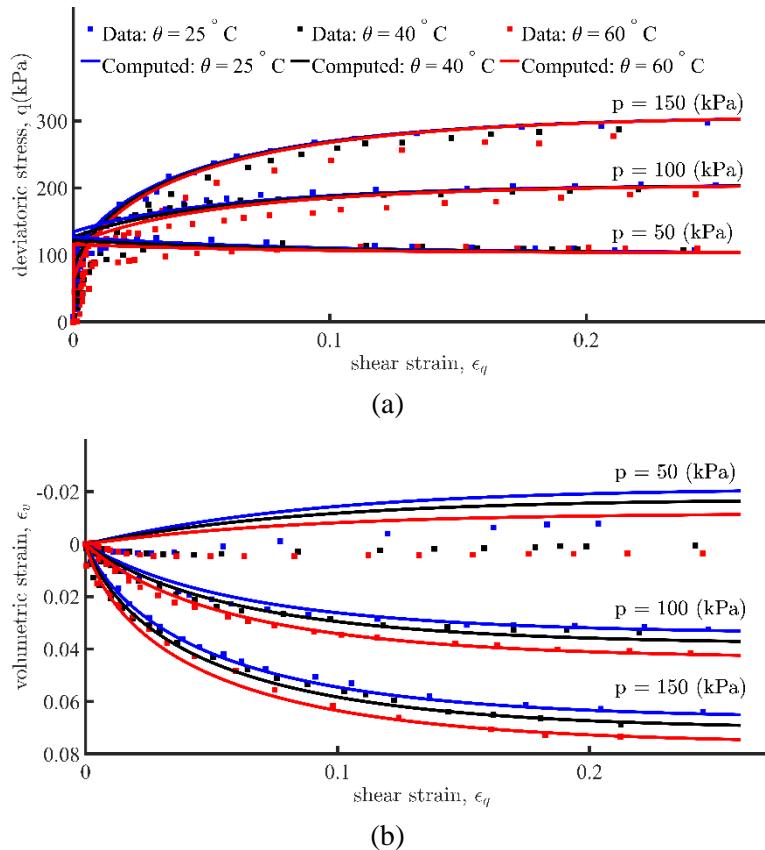

(a)

(b)

Figure 3: Comparison of model's performance with experimental data at different temperatures and initial mean effective stresses; (a): shear stress vs. shear strain; (b): volumetric strain vs. shear strain

Figure 2 shows the yield surface of the soil at different temperatures, starting with the initial surface corresponding to a pre-consolidation of 200 kPa at 25°C. From the laboratory data, it is obvious that as the temperature increases, the yield surface shrinks in size and the pre-consolidation pressure decreases. The proposed model is capable of capturing both the shape of the yield surface and the yield surface shrinkage.

Table 1: Summary of model parameters

M	λ	κ	μ
1.22	0.09	0.01	0.0034

ϱ	α	γ	$\bar{K}$
$3.4×10^{-5}$	0.75	1.1	$9×10^4$

$\bar{G}$	n
10^5	0.5

In Figures 3(a) and 3(b), the shear stress versus shear strain and volumetric strain versus shear strain curves, respectively, are shown. The model's predictions are in good agreement with the experimental data, especially for lightly over-consolidated states sheared at mean effective stresses of 150 and 100 kPa. Another feature of the model is that the shear strength of all samples sheared at identical mean effective stress reach the same ultimate value (critical state), regardless of temperature effects, in agreement with the experimental data.

4 DISCUSSION

In this paper, the development of a single two-parameter yield surface thermo-mechanical constitutive model has been explained by defining only free energy and dissipation potential functions. Although the formulation without considering temperature effects is similar to the works of Collins & Hilder (2002) and Coombs & Crouch (2011), the two potentials of the current model are defined in a way that leads to a simpler formulation without the necessity of introducing shift stresses. In their work the hardening rules are linked to shift stresses by defining extra terms (defined by internal variables) in the free energy function, while, in this study, these features are incorporated into the dissipation function which simplifies the formulation.

Another feature of this model is that the temperature-dependent non-associated flow rule (Equation (12)) is automatically derived by defining the dissipation potential. This is in contrast to conventional plasticity theory in which a non-associated flow rule requires the specification of a plastic potential function.

Similar to a single yield surface in conventional plasticity theory, an abrupt change in stress path (for undrained tests) and stress-strain curves occurs when the behaviour of the material changes from purely elastic to elasto-plastic (i.e. from inside to on the yield surface). A smooth transition can be achieved by introducing an inner surface inside the yield surface, similar to the work of Coombs et al. (2013) which will form a later investigation.

5 CONCLUSIONS

A new constitutive model based on thermo-dynamics principles has been developed to consider temperature effects on the mechanical behaviour of fine-grained soils. The thermo-mechanical aspects of the model are embedded through the addition of thermal elastic expansion and a thermal softening mechanism into the formulation of the free energy and dissipation potentials, respectively. The model is used to simulate the drained shear behaviour of a silty soil. The results indicate the ability of the model to capture the vital role of temperature effects on the shear behaviour of the soil and its performance is in good agreement with laboratory data.

6 ACKNOWLEDGMENTS

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