Simulation of long-term thermo-mechanical response of clay using an advanced constitutive model

Despina M. Zymnis\textsuperscript{1} · Andrew J. Whittle\textsuperscript{2} · Xiaohui Cheng\textsuperscript{3}

Received: 29 May 2018 / Accepted: 8 October 2018 / Published online: 31 October 2018
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Abstract
There is extensive data to show that heating and cooling produces irrecoverable deformations in clays under fully drained conditions. The effects are most pronounced for normally and lightly overconsolidated clays that undergo significant compression. Most constitutive models have key limitations for predicting the thermo-mechanical response of clays through long-term (seasonal) cycles of heating and cooling. The Tsinghua ThermoSoil model (TTS; Zhang and Cheng in Int J Numer Anal Methods Geomech 41(4):527–554, 2017) presents a novel theoretical framework for simulating the coupled thermo-mechanical response of clays. The model uses a double-entropy approach to capture effects of energy dissipation at the microscopic particulate contact level on continuum behavior. This paper proposes a simple procedure for calibrating input parameters and illustrates this process using recent laboratory data for Geneva Clay (Di Donna and Laloui in Eng Geol 190:65–76, 2015). We then investigate capabilities of the TTS model in simulating familiar aspects of thermal consolidation of clays as well as the long-term, progressive accumulation of strains associated with seasonal heating and cooling processes for shallow geothermal systems installed in clays. The model predicts the existence of a long-term steady-state condition where there is no further accumulation of strain. This state depends on the consolidation stress and stress history but is independent of the imposed range of temperature, $T_{\text{cyc}}$. However, the value of $T_{\text{cyc}}$ does affect the rate of accumulation of strain with thermal cycles. Simulations for normally consolidated Geneva Clay find steady-state strain conditions ranged from 2.0 to 3.7% accumulating within $N = 10$–50 thermal cycles.

Keywords Constitutive modeling · Cyclic thermal loading · Irrecoverable deformations · Long-term response · Thermo-mechanical response

List of symbol

| Lower case | Description |
|---|---|
| $a$ | TTS model input constant that controls rate effects |
| $c$ | TTS model input constant related to cohesion |
| $c'$ | TTS model input constant related to the critical state friction angle |
| $e$ | Void ratio |
| $h$ | TTS model input constant that controls hysteretic strains |
| $m_1$ | TTS model input constant that controls elastic strain evolution |
| $m_2$ | TTS model input constant that controls elastic strain evolution and location of reload curve |
| $m_3$ | TTS model input constant that controls the contribution of volumetric and deviatoric strains on granular temperature production |
| $m_4$ | TTS model input constant that controls the rate of granular temperature production |
| $m_5$ | TTS model input constant that controls the amount of thermal volumetric strains produced due to heating and cooling |
| $p$ | Mean total stress |
| $p'$ | Mean effective stress |
| $q$ | Shear stress |
| $w$ | Water content |
1 Introduction

The thermo-mechanical response of clays has been studied in the context of applications including nuclear waste disposal (e.g., [15–20]), energy foundations (e.g., [32, 33]) and seasonal ground heat storage (e.g., [49]). Laboratory measurements show that temperature changes can significantly alter the properties of clays and induce permanent deformations [1, 3, 6, 8, 24]. These effects become more pronounced when cyclic heating and cooling is imposed (e.g., due to the continuous operation of ground source heat pumps) and can generate significant long-term settlements [6, 13, 26]. Zymnis and Whittle [50] have shown that cyclic thermal loading induced by borehole heat exchangers can lead to thermal volumetric strains, and hence, the study of cyclic thermal loading is crucial when designing shallow geothermal installations.

Existing thermo-elastic constitutive models (e.g., [4, 43]) cannot describe irreversible thermal strains. More advanced thermo-elastoplastic constitutive models are macroscopic, usually based on an extension of the Cam-Clay model to account for temperature (e.g., [24, 25, 31]) and can describe thermal response reasonable well. However, their validity beyond experimental results is questionable since the physical processes at the microscale are not accounted for. Furthermore, most constitutive models have key limitations for predicting the thermo-mechanical response of clays through long-term (seasonal) cycles of heating and cooling. For example, in the model proposed by [25], all of the irreversible strain takes place during the first heating and cooling cycle and the model is incapable of describing accumulation of irreversible thermal strain thereafter. Di Donna and Laloui [13] extend the ACMEG-T model [31] to account for irreversible strain accumulation, using ‘the cyclic plastic radius’ that makes the model much more complex, without basing the soil response on physical processes. The Tsinghua ThermoSoil model (TTS; [48]) associates the accumulation of volumetric strain during continuous cycles of heating and cooling with the exchange between bound (i.e., adsorbed on clay particles) and free water. The underlying basis for TTS is supported by recent molecular simulations presented by [5], who relate macroscopic thermo-mechanical response of clay to water
adsorption at the nanoscale. The TTS model is the first constitutive model capable of describing macroscopic thermo-mechanical clay while accounting for physical processes at the microscale.

The current paper has implemented the TTS model to study 1-D settlements due to seasonal cycles of heating and cooling. The paper begins with a review of the main concepts of the TTS model formulation and clarifies the simplifications assumed for the current application. One key aspect of the TTS model relates to the thermal effects on the conversion of ‘bound water’ (i.e., water adsorbed onto the surface of clay particles, e.g., [11, 34, 39, 41]) to free water. The paper proposes simple and effective calibration techniques for TTS parameters related to thermo-mechanical effects and illustrates this methodology using recent laboratory data for Geneva Clay [13]. The paper concludes with an in-depth evaluation of the TTS model, with an emphasis on the simulation of clay response to long-term cyclic heating and cooling.

2 Tsinghua ThermoSoil (TTS) model formulation

The TTS model is based on non-equilibrium thermodynamic theory [21] in order to provide a more fundamental physical basis for characterizing the complex (transient and steady state) behavior of geomaterials, based on the framework of Granular Solid Hydrodynamics (GSH; [28]). The current application considers the thermo-mechanical behavior of clays and can be contrasted with prior models based on classical elasto-thermoplasticity (e.g., [9, 25, 31]). The TTS model does not use a yield function, flow rules or other constraints of classical plasticity, but is able to describe many key empirical observations of clay behavior, including virgin consolidation of normally consolidated clay and hysteretic stress–strain response in unloading and reloading. The current implementation of the TTS model makes the following assumptions:

1. Soil is fully saturated (for isothermal conditions, deformation and shear strength are controlled by effective stresses) and is composed of a mixture of solid and liquid phases (Fig. 1).
2. All three phases are continuous in space and have the same temperature.
3. There is no phase change in water for the temperature range considered (i.e., no solidification or vaporization).

The liquid phase is divided into free water, which fully fills the macroscopic pores and whose migration is described by Darcy’s Law; and bound water, which is fully adsorbed by the soil particles and fills the microscopic pore space (for sands, the specific surface area is small, SSA ~ 0.03 m²/g, while for clay particles SSA can range from 10 to 270 m²/g, with the highest values for smectites). The total porosity, φ, and dry density of solid particles, ρ_d, are then given by:

\[ \phi = \phi_{fw} + \phi_{bw} \]  
\[ \rho_d = G_s\rho_{fw}(1 - \phi) \]

where \(G_s\) is the specific gravity of soil, and \(\rho_{fw}\) is the density of free water.

The thermal response of clays is often linked to physicochemical clay–water interactions, based on the mass transfer of bound water from a solid state to a fluid state [23]. At elevated temperatures, part of the bound water is converted to free water, which in turn produces irreversible reorganization of the clay particles and thermal irreversible strains. Zhang and Cheng [48] have proposed an exponential decay function relating changes in bound water content, \(w_{bw}\), to temperature, \(T\):

\[ w_{bw} = w_{bw,20} \exp[-a_{bw}(T - 20)], \quad T[^{\circ}C] \]

where \(w_{bw,20}\) is the bound water content at 20°C and \(a_{bw}\) is a characteristic material property:

\[ a_{bw} = -\frac{1}{w_{bw}} \frac{\partial w_{bw}}{\partial T} \]

Zymnis et al. [51] performed a series of experiments that study this process through measurements of temperature dependence in the specific gravity of the solid particles. Three clays of widely differing mineralogy were tested: (1) Kaolinite, with a specific surface area, SSA = 14 m²/g; (2) illite-rich, Boston Blue Clay (BBC Series IV) with SSA = 49 m²/g; and (3) smectite-rich, Eugene Island (El-GOM) clay sourced from the Gulf of Mexico, with SSA = 267 m²/g. The laboratory experiments confirm that the specific gravity of clays decreases with temperature consistent with the conversion of bound water to free water. Figure 2 presents the estimated change of bound water content with temperature for all three clays, by assuming a mass density of bound water \(\rho_{bw}(T) = 1.07\rho_{fw}(T)\), based on pycnometer measurements reported in the literature [2, 10, 36, 38, 40] and assuming that the adsorbed water layer adjacent to clay minerals has a thickness of about three water molecules as reported by several authors (e.g., [14, 37, 44–46]). The bound water content at 20°C estimated for El-GOM clay is \(w_{bw,20} = 24%\) which is considerably higher than that for BBC (\(w_{bw,20} = 5%\)) and Kaolinite (\(w_{bw,20} = 1%\)). For a temperature increase of 20°C, the bound water content of El-GOM clay decreases by ~ 4%, while reductions in BBC and Kaolinite are ~ 1.2% and ~ 0.3%, respectively.
In the current formulation, we use the following evolution of bound water porosity:

$$\dot{\phi}_{bw} = -\phi_{bw} \left( 2\beta - \frac{\beta_w}{1 - \beta_w \Delta T} \right) \dot{T}$$  \hspace{1cm} (4)$$

where $\beta_w$ is the thermal expansion coefficient of water ($\beta_{w,vol} = 3.4 \times 10^{-4}/^\circ C$). We assume that bound water porosity is not affected by changes in total volumetric strain (i.e., deformations of the soil skeleton only change the free water porosity).

The TTS model accounts for interactions between the continuum (macro-level) and micro-level (i.e., particle or granular level) behavior through a double-entropy formulation. The total entropy is used to describe macroscopic phenomena (irreversible deformations), while the granular entropy represents microscopic phenomena (sliding, rolling and collision of particles, which results in a change in their kinetic energy and elastic potential energy, as shown in Fig. 3). It is assumed that once external loading is applied, there is a simultaneous increase in both total and granular entropies and granular entropy is subsequently converted to total entropy at a rate, $\dot{I}_g [J/m^3s]$. The energy generation at the microscopic scale is the source of plastic deformation for granular solids and is attenuated by heat generation at the macro-level. Jiang and Liu [29] proposed that energy generation at the microscopic level is similar to molecular motion and can be described through a granular entropy density and its conjugate variable, granular temperature, $T_g [\text{s}^{-2}]$. The evolution of granular temperature is given by:

$$\dot{T}_g = \frac{1}{\rho_d} \left[ m_2 m_4 (\dot{e}_v)^2 + m_2 m_3 m_4 (\dot{e}_{ij})^2 + \frac{m_5 \sigma'_{oc3} \dot{\phi}_{bw} T^2}{(1 - \phi)} - m_4 T_g \right]$$  \hspace{1cm} (5)$$

where $\dot{e}_v = e_{kk}$ is the volumetric strain and $e_{ij} = \sqrt{e_{ij} e_{ij}}$, $e_{ij} = e_{ij} - e_{kk} \delta_{ij}/3$ is the second invariant of the deviatoric strain rate tensor, $\sigma'_{oc3}$ is the mean effective stress and $m_2$, $m_3$, $m_4$, $m_5$ are input constants (migration coefficients) for the TTS model.

External loading, either as a strain rate, $\dot{e}_{ij}$ or temperature rate, $\dot{T}$, increases the granular temperature, $T_g$ (first
three terms of Eq. 5). The current simplified version of the TTS model assumes \( m_3 = 1 \) and represents the case where volumetric and shear components contribute equally to the evolution of granular temperature. The third term of the right-hand side of Eq. 5 reflects the irrecoverable particulate level movement induced by the conversion of bound to free water to simulate the irreversible volumetric deformation caused by changes in temperature (cf., Eqs. 3a and 3b).

It is assumed that \( m_5 = 0 \) for \( \dot{T} \leq 0 \), since cooling does not produce irreversible thermal strain, as confirmed in experimental tests (e.g., [3]). The fourth term (i.e., \( m_4 T_g \)) is a damping component, while \( m_4 \) controls the time lag required for \( T_g \) to reach steady-state conditions.

The total strain rate \( \dot{\varepsilon}_{ij} \) is the sum of elastic strain rate, \( \dot{\varepsilon}_{ij}^e \), and ‘irrecoverable’ strain rate, \( \dot{\varepsilon}_{ij}^D \), as shown below:

\[
\dot{\varepsilon}_{ij} = \dot{\varepsilon}_{ij}^e - \dot{\varepsilon}_{ij}^D
\]

Figure 4a illustrates the prediction of cyclic strain accumulation due to mechanical loading and unloading (cf., Eq. 6c). The shear strain rate is linked to the current granular temperature and elastic shear strain. In order to avoid overestimation of strain accumulation (large ratcheting strains, as shown in Fig. 4a), [47] introduced a ‘hysteretic’ strain, \( \dot{\varepsilon}_{ij}^h \), as an additional state variable in the TTS model formulation, such that each cycle of loading produces smaller net irrecoverable strain (Fig. 4b). The evolution of irrecoverable strain rate, \( \dot{\varepsilon}_{ij}^D \), is expressed as a function of granular temperature \( T_g \) and the elastic and hysteretic strains:

\[
\dot{\varepsilon}_{ij}^D = 3 m_1 \left( T_g \right)^a \left( \varepsilon_{ij}^e - \varepsilon_{ij}^h \right)
\]

\[
\dot{\varepsilon}_{ij}^D = \left(T_g\right)^a \left( \varepsilon_{ij}^e - \varepsilon_{ij}^h \right)
\]

where the migration coefficient \( m_1 = m_{1,0}[1 + L_T(T - T_0)] \) (we are assuming \( m_{1,0} = 1 \)), \( T_0 \) is a reference temperature, \( L_T \) is an input constant that describes the dependence

![Image](image1.png)

**Fig. 3** Double-entropy concept assumed in TTS model (after [47])

![Image](image2.png)

**Fig. 4** Effect of hysteretic strain on strain accumulation due to cyclic loading and unloading (after [48])
of parameter $m_4$ on temperature and $a$ is a parameter that controls rate dependence (‘Appendix A’ shows that $a = 0.5$ produces rate independent virgin consolidation states).

The evolution of the volumetric and deviatoric components of hysteretic strain assumed in the current implementation is:

$$
\varepsilon_v^h = \varepsilon_v^D - \frac{\frac{1}{3} \varepsilon_v^D \varepsilon_v + \varepsilon_v^D}{H^{0.5} \left[ \frac{1}{3} \left( \varepsilon_v^h \right)^2 + \left( \varepsilon_v^h \right)^2 \right]^{0.75}} \varepsilon_v^h
$$

(7a)

$$
\varepsilon_s^h = \varepsilon_s^D - \frac{\frac{1}{3} \varepsilon_s^D \varepsilon_s + \varepsilon_s^D}{H^{0.5} \left[ \frac{1}{3} \left( \varepsilon_s^h \right)^2 + \left( \varepsilon_s^h \right)^2 \right]^{0.75}} \varepsilon_s^h
$$

(7b)

where parameter $h$ is an input constant.

Since the evolution of irrecoverable strain rate depends on granular temperature, $T_g$, it becomes apparent that the application of external loading will increase the granular temperature and will also produce irrecoverable strain (cf., Eqs. 5, 6b and 6c). Figure 5 illustrates TTS simulations of the time-varying response of mean effective stress to a step change in applied volumetric strain (for Geneva Clay) for an element undergoing hydrostatic compression. Higher values of $m_4$ produce rapid convergence to steady-state conditions (for $m_4 = 1000$ kg/m$^3$s, the stress reaches its constant value in 5 s, while for $m_4 = 100$ kg/m$^3$s, the stress equilibrates in 30 s). The current application focuses on steady-state conditions, and hence, we assume a large value of $m_4 = 6 \times 10^4$ kg/m$^3$s.

The TTS model assumes that reversible energy processes result in locked-in elasticity in the system that can be expressed by an elastic potential energy function. The effective stress state is expressed as the derivative of the elastic potential energy density function, $\omega_e$:

$$
\sigma_i^j = \frac{\partial \omega_e}{\partial \epsilon_i^j}
$$

(8)

This definition is common to all ‘hyperelastic’ models of soil behavior (e.g., [22]). Zhang and Cheng [48] propose an expression for $\omega_e$ that limits the range of possible stress states (reflecting limits on cohesive and frictional shear strength components) and includes thermal elastic strains of the solid minerals:

$$
\omega_e = \frac{2}{5} B (\varepsilon_v + c)^{1.5} (\varepsilon_s + c')^{1.5} + 0.8 B (\varepsilon_v + c)^{1.5} + 1.5 B \xi (\varepsilon_v + c')^{1.5}
$$

(9)

By combining Eqs. 8 and 9, the mean effective stress and deviatoric stress can be expressed by:

$$
p' = K_e (\varepsilon_v + c)^{0.5} (\varepsilon_s + c')
$$

$$
q = \sqrt{6} B \xi (\varepsilon_v + c')^{1.5}
$$

(10)

(11)

It is subsequently shown that $B_0$ and $B_1$ can be related to the location and slope of the virgin consolidation line, respectively; $c$ is linked to cohesion of soils ($c = 0$ for sands; here we assume a nominal value, $c = 0.01$ for reconstituted clays); $\xi$ is related to the size of the state boundary surface (i.e., limit on possible effective stress states that is linked to maximum allowable ratios of shear to normal stress) and affects the peak internal friction and the in situ coefficient of earth pressure at rest $K_0 (= \sigma_v^T/\sigma_v)$ and $c'$ controls the critical state friction angle.

Zhang and Cheng [48] derive the state boundary surface, also referred to as the Ultimate Stress State Surface (USSS) from the singularity condition of the Hessian matrix, det $\omega_{ij} = 0$. [42] presents an in-depth study of the shear response of the TTS model in relation to critical state soil mechanics and shows that the slope, $M$, of the critical state line (CSL) is simulated by the TTS model and can be derived as (see Appendix B):

$$
M = \frac{\sigma_T}{
\frac{\sigma_T}{\sqrt{6} \xi (\varepsilon_v + c')^{1.5}}}
$$

(12)

Table 1 summarizes the state variables used in the TTS model, which comprise the bound and free water porosity, $\varphi_{bw}$ and $\varphi_{fw}$, the temperature, $T$, the granular temperature,
3 Cyclic thermal tests on Geneva Clay

Di Donna and Laloui [13] carried out a series of drained thermal cyclic tests on samples of medium plasticity silty clay from Geneva, Switzerland \((I_\text{p} = 11–19\% \text{, } w = 22–28\%)\). As there are very few cyclic thermal tests reported in the literature (notable exceptions include data presented by [6, 26]), these tests are very useful in evaluating TTS model capabilities for representing the accumulation of long-term thermal movements induced in clay. The soil samples were collected from a site near Geneva as part of a project involving the construction of a new building and the installation of a large array of borehole heat exchangers for space heating and cooling. Table 3 shows the in situ state of stress (normally consolidated clay) and index properties for samples S3 and S4b, which are considered here. The samples are saturated and have a fines fraction \((d < 2 \mu m)\) between 38 and 45%.

Two sets of experiments were undertaken: (i) 1-D oedometric compression tests at different constant temperatures; and (ii) thermal cycles under constant vertical effective stress. Details of the laboratory procedure are provided by Di Donna and Laloui [13] and are summarized in Table 4. Figure 6 presents the oedometric test results (in the conventional void ratio \(e = \log \sigma'_v \text{, space, where } e = \phi \div (1 - \phi)\)) on sample S3 at temperature \(T = 20^0\text{C}, 40^0\text{C and 60}^0\text{C}\) for the entire duration of the test. Sample S3 was initially equilibrated at the selected temperature at a nominal vertical stress of 1 kPa (weight of top cap). Once the temperature and deformation were stable, incremental load sequences were performed, with loading steps up to 1000 kPa and unloading to 60 kPa. It is observed that all consolidation curves are parallel and so the compressibility of VCL is unaffected by temperature, thus confirming trends reported previously in the literature (e.g., [26]). Figure 6a shows that the main effect of higher temperature is to increase density (reduce void ratio) at a given effective consolidation stress (i.e., the void ratio is lower at \(40^0\text{C and 60}^0\text{C than at } 20^0\text{C at a given effective consolidation stress}\).
effective stress \((\sigma'_{v0} \approx \sigma'_p)\) at ambient temperature, \(T = 20^\circ \text{C}\), and then thermal cycles were performed in the range between 5\(^\circ\)C and 60\(^\circ\)C. Vertical displacements were recorded throughout the experiments and the heating phases were applied in steps of 10\(^\circ\)C, imposing a heating rate of 2\(^\circ\)C per hour in order to ensure drained conditions and thus provide enough time for excess pore water pressure dissipation. The cooling phases were applied in steps of 20 \(^\circ\)C and with a cooling rate of 5\(^\circ\)C/h. Thermal cycling of the OC specimen resulted in small dilative strains \((\varepsilon_v \approx -0.1\%)\) similar to prior results (e.g., [3, 8]). Assuming that the measured deformation corresponds to the thermo-elastic expansion and compression of the solid skeleton, Di Donna and Laloui [13] computed the volumetric thermal expansion coefficient of the solid skeleton equal to \(\beta_{v,vol} = 1.8 \times 10^{-5}\text{C}^{-1}\). On the other hand, cyclic heating and cooling of NC clay specimens results in larger irreversible contractive strains (with accumulated volume strain, \(\Delta\varepsilon_v \approx 0.6-0.9\%).

### 4 TTS model calibration for Geneva Clay

The following paragraphs present our proposed method for calibrating the TTS model and illustrate this process for intact specimens of Geneva Clay. Initial values of the state variables can be derived by consolidating from a reference slurry state \((\sigma'_{v0} = 0 \text{ kPa})\) with void ratio \(e = 2.0\) (porosity \(\phi = 0.5\) and bound water porosity \(\varphi_{bw} = 1\%), based on results for Kaolinite; c.f., Fig. 2) and assuming that the other state variables shown in Table 1 are initially zero at ambient temperature, \(T_0 = 20^\circ\text{C}\). The model is driven by specified rates of strain, \(\dot{\varepsilon}\), and temperature, \(T\) (Eqs. 5, 6a and 6b).

It should be noted that using the Specimen Quality Designation (SQD) method recommended by Ladd and DeGroot [30], the samples S3 and S4b are highly disturbed (Fig. 6a, 6b shows that the vertical strains measured at 20\(^\circ\)C at \(\sigma'_{v0}\) are 6.3\% and 8.7\% for S3 and S4b, respectively). These results imply that the compression index, \(C_v\),

### Table 3 In situ state of stress and identification properties of the tested soil samples (after [13])

| Test number | Material | Type | Temperature, \(T\) (\(^\circ\)C) | Vertical eff. stress, \(\sigma'_v\) (kPa) | OCR before thermal cycles |
|-------------|----------|------|-------------------------------|---------------------------------------|--------------------------|
| 1           | S3       | SO   | 20                            | 1–1000–60                              | –                        |
| 2           | S3       | TO   | 40                            | 1–1000–60                              | –                        |
| 3           | S3       | TO +(TC) | 60 (5–60)                   | 1–1000–60 (16.0)                     |                          |
| 7           | S3       | TC   | 5–60                          | 125                                   | 1.0                      |
| 10          | S4b      | TC +(SO) | 5–60                        | 125 (1000–60)                        | 1.0 (–)                  |

\(SO\) standard oedometer, \(TO\) thermal oedometer, \(TC\) thermal cycles
will be systematically underestimated. Calibration of the VCL was based on the sample S4b measurements.

4.1 Mechanical components

The main input constants that control the 1-D compression response of clays are $B_0$, $B_1$, $m_2$, $h$ and $\xi$ (Table 2). The clay was loaded from an initially slurry condition to a void ratio $e = 0.63$, unloaded to void ratio $e = 0.7$ and reloaded to $e = 0.57$ (the void ratios correspond to those reached by sample S4b during the laboratory experiments). Figure 8 presents results for normalized vertical stresses ($\sigma'_v/\sigma'_r_{\text{ref}}$, where $\sigma'_r_{\text{ref}}$ is the vertical stress calculated by the TTS model at void ratio $e = 0.63$, where unloading begins). The slope of the VCL increases as $B_1$ decreases, and $B_1 = 0.0162 \, \text{m}^3/\text{kg}$ provides a good fit to the measured data. Parameter $h$ controls the slope of the unload curve as shown in Fig. 9a, with larger unloading slopes occurring for larger $h$ (Eqs. 7a, 7b). Figure 9b shows that the reloading response depends on parameter $m_2$, with larger $m_2$ affecting the reloading branch of the test.

For a friction angle $\phi = 24^\circ$, determined by triaxial tests on Geneva Clay [12], the slope, $M$, of the critical state line is:

$$M = \frac{\sin \phi}{3 - \sin \phi} = 0.94$$

from which $c'$ can be obtained using Eq. 12:
For normally consolidated clay, $K_{0NC}$ increases with decreasing $n$ (i.e., horizontal stresses are larger for smaller $n$, while vertical stresses remain unchanged). Assuming $K_{0NC} = 0.6$ (using Eq. 15 suggested by [27]) for Geneva Clay with friction angle of $24^\circ$, $\xi = 0.1$ (Fig. 10).

$$K_{0NC} = 1 - \sin \phi$$

(15)

The TTS model predicts $K_{0OC}$ decreasing with OCR contrary to established soil behavior. This represents a notable limitation of the model that should be addressed in future research but has little effect on the model capabilities in describing accumulation of 1-D settlements under cyclic thermal loading [49].

The final part of the mechanical calibration involves setting the reference void ratio for the VCL by calibrating parameter $B_0$ (Eqs. 10, 11). Figure 11 illustrates that the reference void ratio (i.e., $e$ at a selected $\sigma'_v$) increases with $B_0$ and shows good agreement with data for Geneva Clay for $B_0 = 3.8 \times 10^{-4}$ Pa. It should be noted that all of the input constants affect the location of the VCL and hence, parameter $B_0$ must be chosen last in the calibration process.

Figure 12 presents the resulting TTS fit for Geneva Clay sample S4b using the calibrated parameters shown in Table 2. The loading steps followed are:

1–2: 1-D Consolidation from an initially slurry condition up to $\sigma'_v = 230$ kPa
2–3: 1-D Unloading to $\sigma'_v = 1$ kPa
3–4: Reloading to $\sigma'_v = 1$ MPa
4–5: Unloading to $\sigma'_v = 60$ kPa
5–6: Reloading to $\sigma'_v = 3$ MPa

Figure 12c and d presents the evolution of the strain state variables ($e_v^e$, $e_h^e$, $e_v^h$, $e_h^h$) of the TTS model during these steps. All internal strains start from zero in the slurry condition (point 1) and reach a constant value once the clay is consolidated along the VCL ($\sigma'_v \approx 1$ kPa, as shown in Fig. 12a). This condition occurs as the TTS model assumes there is a fixed amount of locked-in elasticity in the normally consolidated stress states. During unloading (steps 2–3), the volumetric (elastic and hysteretic) strains and elastic deviatoric strains decrease (Fig. 12c, d) and increase again during reloading, while the hysteretic deviatoric strains ($e_h^h$, as shown in Fig. 12d) have the opposite response. The primary state variable that changes when compressing a NC clay on the VCL is the void ratio, $e$ (and corresponding dry density, $\rho_d$). Figures 12b and 13 show

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**Fig. 12** Resulting TTS fit to Geneva Clay sample S4b and evolution of strain state variables using calibrated parameters shown in Table 2

**Fig. 13** Effect of parameter $L_e$ on temperature dependence of the VCL and comparison to Geneva Clay laboratory measurements
that the TTS model describes closely the 1-D compression behavior of natural Geneva Clay (samples S3 and S4b) measured by Di Donna and Laloui [13].

4.2 Thermal components

The input constants that control the thermal behavior of the TTS model are $a_{bf}$, $L_T$ and $m_5$. Based on index properties, it is concluded that Geneva Clay will have similar $a_{bf}$ parameter to BBC and Kaolinite and thus $a_{bf} = 0.0237 \, {\text{C}}^{-1}$ (cf., Fig. 2).

The parameter $L_T$ affects the temperature dependence of the VCL (Eq. 6b), with larger $L_T$ resulting in a more pronounced effect of temperature. Figure 13 shows that the best overall agreement is achieved for $L_T = 0.020 \, {\text{C}}$, which is used in all subsequent calculations. The measurements at $T = 40 \, {\text{C}}$ have not been used for calibration since as already discussed (cf., Fig. 6a) they do not show a monotonic response with temperature, in contrast to prior results in the literature and hence have been omitted from the figure.

Figure 14b–d illustrates the effect of selected values of $m_5$ (Eqs. 5, 6b) on predictions of thermal volumetric strains for cyclic tests at OCR = 1.0 and 16.0 (sample S3). As $m_5$ increases, the accumulation of compressive strains for NC clay and dilative strains for OC clay both increases. For Geneva Clay, using $m_5 = 0.1 \, {\text{s}}^3 \, {\text{m}}^{-2} \, {\text{C}}^{-1}$ accurately described the thermal volumetric strain induced during the first heating–cooling cycle for NC clay and results in 0.4% larger thermal strain accumulation after 4 cycles of heating–cooling compared to the laboratory measurements shown in Fig. 14b. These effects are accentuated at higher values of $m_5$. For the case of the OC clay, the TTS model generally overestimates the dilative strains (accumulated in 4 cycles) by 0.6%.

![Fig. 14 Effect of $m_5$ on simulated accumulation of thermal volumetric and comparison to Geneva Clay laboratory measurements](image-url)
It can be readily seen that the TTS model calibration proposed herein is straightforward and the parameters can be obtained from independent tests, typically performed in the laboratory.

5 Evaluation of model predictions for long-term response to cycles of heating and cooling

Figure 15 shows TTS simulations for a single cycle of heating and cooling at different initial OCRs, under constant vertical stress. The results show that the TTS model provides a reasonable estimate of thermal volumetric strains at different stress levels with a transition to dilative response in the range OCR = 2.0–4.0. Moreover, the TTS model predicts that the thermal volumetric strains are always irreversible even for OC clays, something that has been reported in some thermal tests in the literature, although prior models generally suggest elastic response for OC clays (e.g., [25, 31]). Figure 15b shows the porosity of bound water against temperature. An increase in temperature from 20°C to 60°C causes a decrease in bound water porosity \( \Delta \phi_{bw} = -0.6\% \) (\( \phi_{bw} = 1\% \) at 20°C and \( \phi_{bw} = 0.4\% \) at 60°C), while at 5°C, \( \phi_{bw} = 1.4\% \). Figure 15d presents the evolution of elastic and hysteretic volumetric strains during loading to \( \sigma'_v = 125 \) kPa and unloading to vertical stress \( \sigma'_v \) corresponding to the different OCRs. At \( \sigma'_v = 60 \) kPa, where \( \varepsilon_v = \varepsilon'_v \), the resulting thermal volumetric strains computed by the TTS model are nearly zero as shown by the OCR = 2 line (Fig. 15c). For vertical stress \( \sigma'_v > 60 \) kPa (i.e., lower OCR), the resulting thermal volumetric strains are contractive, while for \( \sigma'_v < 60 \) kPa (i.e., higher OCR), the resulting thermal volumetric strains are dilative (Fig. 15c, d).

**Fig. 15** TTS model simulation of thermal volumetric strains produced due to one heating–cooling cycle for Geneva Clay of different OCR
Figure 16 illustrates the long-term cyclic strain accumulation simulated by TTS for initial OCR’s = 1.0–8.0 for the temperature range used in laboratory tests on Geneva Clay ($T = 5^\circ C$–$60^\circ C$, $T_{ave} = 32.5^\circ C$). Continuous heating and cooling of NC clay (at vertical stress $\sigma_v' = 125$ kPa) results in long-term accumulation of contractive strain, $\varepsilon_v = 2.0\%$, while similar thermal cycles produce $\varepsilon_v = 3.66\%$ at $\sigma_v' = 1$ MPa. Continuous heating and cooling of highly overconsolidated clay (OCR = 8) results in long-term accumulation of dilative volumetric strain ($\varepsilon_v = 1.24\%$), while clays of intermediate OCR produce smaller accumulated strain (Fig. 16c). The TTS model provides a good fit to the laboratory measurements on NC Geneva Clay (Test #7 on S3 sample, as shown in Fig. 16c). The accumulation of volumetric strain reaches a limit when $\varepsilon_v^e = \varepsilon_v^h$ as shown in Fig. 16d. In fact, long-term cyclic heating and cooling induce a steady-state condition shown in Fig. 16a that depends on the mechanical calibration of the TTS model (controlled by parameters $h$ and $m_2$).

Figure 17 shows the strain accumulation for cycles of heating and cooling with $T_{cyc} = \pm 5^\circ C$ to $\pm 20^\circ C$ (and $T_{ave} = 20^\circ C$). The TTS model predicts that heating and cooling of normally consolidated Geneva Clay ultimately trend to the same maximum volumetric strain ($\varepsilon_v = 2.0\%$) independent of the imposed temperature range, while rates of strain accumulation are directly linked to the imposed cyclic range, $T_{cyc}$. For example, with $T_{cyc} = \pm 20^\circ C$, the maximum strain accumulates within 40 cycles, while for $T_{cyc} = \pm 5^\circ C$, the maximum strain develops in 150 cycles. Figures 16 and 17 demonstrate the capabilities of the TTS model to describe volumetric strain accumulation due to continuous heating and cooling. Although, there are currently no laboratory data to validate these results and the existence of a steady state is still a hypothesis, the model...
offers a useful framework to assess the long-term ground settlements due to seasonal heating and cooling of clays.

6 Summary and conclusions

The Tsinghua ThermoSoil model (TTS; [48]) presents a novel theoretical framework for simulating the coupled thermo-mechanical properties of clays. To our knowledge, it is the only model that can describe volumetric accumulation due to cyclic heating and cooling of clay, while accounting for physical processes. The model uses a double-entropy approach (following the Granular Solid Hydrodynamics framework of [29]) to capture effects of energy dissipation at the microscopic particulate contact level on continuum behavior and is capable of describing strain rate and thermal dependence in clay properties. The conversion of bound to free water represents a key concept that controls irreversible thermo-mechanical strains in the TTS model. This paper proposes simple and effective calibration techniques of the TTS model and demonstrates them using recently published cyclic thermal tests on Geneva Clay [13]. The paper illustrates the TTS model capabilities in simulating familiar aspects of thermal consolidation of clays as well as the long-term, progressive accumulation of strains associated with seasonal heating and cooling processes for shallow geothermal systems installed in clays. Although there is limited experimental data for the behavior of clay subjected to a large number of thermal cycles, the model provides a useful framework for evaluating the thermo-mechanical response of clay and suggests the existence of a long-term steady-state condition. Further laboratory studies of thermo-mechanical properties of different types of clay are needed to evaluate these TTS modeling capabilities.

Acknowledgements

The Authors are grateful for the support provided by the Low Carbon Energy University Alliance (LCEUA), which enabled three-way collaborations with colleagues at Tsinghua University and the University of Cambridge. The first Author (DMZ) also received a Robert A. Brown, Onassis Foundation, Exponent and Martin Foundation Fellowships for her Ph.D. studies.

Appendix A

The TTS model accounts for strain rate dependence through parameter $a$ shown in Eqs. 6b and 6c. Figure 18 presents hydrostatic compression of Geneva Clay, as simulated by the TTS model, assuming different strain rates.

![Figure 17](image1.png)  
**Fig. 17** TTS model simulation of thermal volumetric strains produced due to long-term cyclic heating and cooling of NC Geneva Clay with different $T_{cyc}$.

![Figure 18](image2.png)  
**Fig. 18** Effect of input constant, $a$, on rate dependence assumed in TTS model.
Using \( a = 0.5 \) results in a unique response (cf., solid lines overlap in Fig. 18), providing rate independence of the model. On the other hand, using \( a = 0.3 \) (dashed lines) results in different VCLs for different strain rates. An increase in rate of strain results in a decrease in density (increased void ratio) at a given effective consolidation stress (i.e., the void ratio is higher at \( \dot{e}_v = 0.05/\text{min} \) than at \( \dot{e}_v = 0.001/\text{min} \) at a given effective consolidation stress). The effect of strain rate is similar to the effect of temperature (cf., Fig. 6a) since they both affect the viscous deformation of soils, as reported previously in the literature (e.g., [35]).

### Appendix B

Panagiotidou [42] studied the TTS model behavior at critical state assuming undrained triaxial shearing with axial strain \( \dot{e}_v \), under isothermal conditions (i.e., \( T = 0 \)). The resulting total volumetric and deviatoric strain rates are \( \dot{e}_v = 0 \) and \( \dot{e}_s = \sqrt{2/3} \dot{e}_a \), respectively. At critical state, the soil reaches steady-state conditions with constant deformations without change in volume or stresses \( \dot{e}_v = \Delta p_f/\Delta q_f = 0 \) and so all internal state variables are constant (cf., Table 1). Therefore, since the change of elastic strain is zero, the plastic strain is equal to the total applied strain:

\[
\dot{e}_v^D = \dot{e}_s^D = 0 \quad (16a)
\]

\[
\dot{e}_s^D = \dot{e}_s = \sqrt{2/3} \dot{e}_a \quad (16b)
\]

From Eq. 5, under isothermal conditions and assuming that \( T_s = 0 \), the granular temperature at critical state becomes:

\[
T_{gsCS} = m_2(\dot{e}_s)^2 \quad (17)
\]

From Eq. 7b, given that \( \dot{e}_s^h = 0 \) and \( \dot{e}_v^D = 0 \):

\[
\dot{e}_s^h = h \quad (18)
\]

For \( \dot{e}_s^h = 0 \), it is deduced from Eq. 7a that:

\[
\dot{e}_v^h = 0 \quad (19)
\]

For \( \dot{e}_v^D = 0 \) and using Eq. 6a:

\[
\dot{e}_v^* = \dot{e}_v^h = 0 \quad (20)
\]

From Eq. 6b and assuming rate independence (i.e., \( a = 0.5 \)):

\[
\dot{e}_v^D = (T_b)^2(\dot{e}_v^* - \dot{e}_v^h) = \left[ m_2(\dot{e}_s^D)^2 \right]^a (\dot{e}_s^* - \dot{e}_s^h)
\]

\[
\therefore \dot{e}_v^* = h + \frac{1}{\sqrt{m_2}} \quad (21)
\]

The evolution of the stress components at critical state can then be calculated (cf., Eq. 11):

\[
p_f = 1.5B\dot{\varepsilon}_v^*(\dot{\varepsilon}_d^*)^{0.5}(\dot{\varepsilon}_d^*)^2 \quad (22a)
\]

\[
q_f = \sqrt{6B\dot{\varepsilon}_v^*(\dot{\varepsilon}_d^*)^{1.5}} \quad (22b)
\]

Therefore, the slope of the critical state line, \( M \), is given by the ratio of the deviatoric to the mean effective stress:

\[
M = \frac{q_f}{p_f} = \frac{\sqrt{6c'}}{1.5 \left( h + \frac{1}{\sqrt{m_2}} \right)} \quad (23)
\]

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