Research Paper

An alternative coupled thermo-hydro-mechanical finite element formulation for fully saturated soils

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ABSTRACT

Accounting for interaction of the soil's constituents due to temperature change in the design of geo-thermal infrastructure requires numerical algorithms capable of reproducing the coupled thermo-hydro-mechanical (THM) behaviour of soils. This paper proposes a fully coupled and robust THM formulation for fully saturated soils, developed and implemented into a bespoke finite element code. The flexibility of the proposed formulation allows the effect of some coupling components, which are often ignored in existing formulations, to be examined. It is further demonstrated that the proposed formulation recovers accurately thermally induced excess pore water pressures observed in undrained heating tests.

1. Introduction

Significant temperature effects have been exposed in a range of geotechnical engineering problems, such as oil & gas pipelines, pavements, buried power cables, ground energy storage, and the storage of high-level radioactive waste [20]. They are also important in ground-atmosphere interaction [8]. To investigate the thermal behaviour of soils, extensive laboratory and field experimental studies have been carried out (e.g. [12,16,13,19]). It is observed that temperature changes result in the variation of stress equilibrium in the ground, as well as pore fluid flow. These problems, where *mechanical, hydraulic and thermal systems in soils interact with each other, with the independent solution of any one system being impossible without simultaneous solution of the others*, are defined as coupled THM problems, while the interaction between the systems is referred to as the THM coupling [34]. Further work has been carried out on THM-Chemical (i.e. THMC) coupling, with example references being those of Rutqvist et al. [29] or Seetharam et al. [30]. Despite being of interest to the modelling of some phenomena, such as chemical dissolution of dissolvable materials in soils, the present paper focuses only on the THM coupling.

To solve a coupled problem, it is necessary to first develop the coupled equations based on the governing law of each physical system [35]. A number of studies have been carried out to model the coupled THM behaviour of soils, and the most extensively used numerical tool has been the finite element (FE) method.

Aboustit et al. [1,2] adopted a general variation principle to develop the governing field equations for the problem of thermo-elastic consolidation. The mechanical behaviour was modelled based on the force equilibrium of the solid-fluid mixture, while the hydraulic and thermal behaviour were taken into account using the laws of volume and energy conservation, respectively. To achieve a symmetric stiffness matrix in the FE code, Aboustit et al. [1] simply assumed the same coupling term to represent the mutual effects between the mechanical and thermal systems. It is also noted that heat advection, as well as the thermal effect on pore fluid flow, were not considered. Following this pioneering work, various approaches have been proposed for modelling the coupled THM behaviour of porous media. One commonly used approach is to first formulate the mass or volume balance equations, the momentum balance equations and the energy balance equations for each phase (e.g. solid, fluid, etc.) of a porous medium (e.g. [24]). Then the coupled THM formulation for the mixture is derived by combining the governing equations for each phase (e.g. [25,22]). Another approach takes account of the behaviour of each coupling system in the soil, thus resulting in the mechanical, hydraulic and thermal governing equations for the solid-fluid mixture (e.g. [21,10,33,18]). The difference between these two approaches is that in the first the governing equations are derived for each phase and then combined, while in the second each of the governing equations is derived for the complete mixture. It should be noted that both approaches can lead to the same governing equations. However, it is also noted that, even when the same approach is followed, the adoption of different assumptions during the derivation procedure may result in differences in the final

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coupled THM FE formulation. For example, different time-marching schemes can be used to approximate a variation over the time step in the solution process.

The new THM FE formulation for saturated soils proposed in this paper adopts the second of the above two theoretical approaches, consolidates and extends the work in the literature detailing its full derivation with clearly stated and justified assumptions. The implementation platform for the new formulation is the authors' FE software ICFEP [27,28], developed specifically for geotechnical engineering analysis. As such, it enables access to source code, which is essential for numerical developments of this type. ICFEP is already capable of performing coupled hydro-mechanical (HM) simulations (consolidation and seepage) in both fully and partially saturated soils. For THM coupling a new equation governing the heat transfer is introduced, which is also able to account for the effect of pore fluid flow and stress-strain behaviour on heat transfer. Furthermore, the existing HM coupled formulation in ICFEP is further modified to account for thermal effects on pore fluid flow and thermal deformation of soils. The adopted development approach of considering each coupling system individually ensures that any of the three systems can be disabled if they are not active in the analysis, thus reducing the full THM formulation straightforwardly to HM, TM or TH coupling. The paper further discusses the performance of the new formulation in comparison with those found in the literature. Lastly, a fully coupled THM FE analysis is performed to model the thermally induced excess pore water pressures in an undrained triaxial heating test. The results demonstrate the ability of the new formulation to predict excess pore water pressure generation due to temperature changes, without resorting to soil thermo-plastic constitutive modelling. The presented formulation adopts a tension positive sign convention, while displacement, pore fluid pressure and temperature are adopted as nodal degrees of freedom.

2. Development and implementation of a coupled THM formulation

2.1. Mechanical equation

If only the mechanical behaviour of soils is considered, the FE formulation can be developed based on the soil constitutive behaviour, expressed as:

$$\{\Delta\sigma\} = [D]\{\Delta\varepsilon\} \tag{1}$$

where $\{\Delta\sigma\}$ and $\{\Delta\varepsilon\}$ are the incremental total stress and strain vectors, respectively, and [D] is the constitutive matrix. With the FE formulation derived from Eq. (1), only the extreme soil conditions, i.e. fully drained or fully undrained, can be simulated. If soil behaviour is somewhere between these two extremes, the principle of effective stress is adopted to formulate the mechanical governing equations for fully saturated soils in an isothermal HM coupled analysis [27]. Therefore, Eq. (1) becomes:

$$\{\Delta\sigma\} = [D']\{\Delta\varepsilon\} + \{\Delta\sigma_f\} \tag{2}$$

where [D'] is the effective constitutive matrix, $\{\Delta\sigma_f\}^T = \{\Delta p_f\ \Delta p_f\ \Delta p_f\ 0\ 0\ 0\}$ and Δp_f is the change in pore fluid pressure. In a coupled THM problem, the effect of temperature change on the mechanical behaviour of soils is generally characterised by a thermally induced volumetric change, namely thermal expansion/contraction. To formulate the mechanical governing equation that accounts for thermal behaviour, two assumptions are introduced:

(1) The temperature of the soil particles, T_s, is assumed to be equal to the temperature of the pore fluid, T_f. Therefore, only the overall temperature of the soil, T, is adopted here, which implies an instantaneous temperature equilibrium between soil particles and pore fluid;

(2) If soil grains are in mineral-to-mineral contact and the temperature is changed, the thermal elastic strain of the soil particles, $\Delta\varepsilon_{T,p}$, is assumed equal to the thermal elastic strain of the soil skeleton, $\Delta\varepsilon_{T,s}$. This assumption agrees with the observations of Campanella and Mitchell [12]. Given this equality, in the remainder of the paper the symbol $\Delta\varepsilon_T$ is used instead of $\Delta\varepsilon_{T,p}$ or $\Delta\varepsilon_{T,s}$ to represent the effect of temperature on the solid part of the porous medium. Conversely, the incremental thermal strain of the pore fluid is defined independently as $\Delta\varepsilon_{T,f}$.

Under non-isothermal conditions, the incremental total strain $\{\Delta\varepsilon\}$ can be expressed as the sum of the incremental strain due to stress change (mechanical strain), $\{\Delta\varepsilon_\sigma\}$, and the incremental strain due to temperature change (thermal strain), $\{\Delta\varepsilon_T\}$:

$$\{\Delta\varepsilon\} = \{\Delta\varepsilon_\sigma\} + \{\Delta\varepsilon_T\} \tag{3}$$

where $\{\Delta\varepsilon_T\}^T = \{\alpha_T\Delta T\ \alpha_T\Delta T\ \alpha_T\Delta T\ 0\ 0\ 0\}$ and α_T is the linear thermal expansion coefficient of the soil skeleton. Substituting Eq. (3) into Eq. (2) leads to:

$$\{\Delta\sigma\} = [D']\{\Delta\varepsilon\} + \{\Delta\sigma_f\} - [D']\{m_T\}(\Delta T) \tag{4}$$

where $\{m_T\}^T = \{\alpha_T\ \alpha_T\ \alpha_T\ 0\ 0\ 0\}$. The last two terms on the right-hand side of Eq. (4) illustrate the change in total stresses induced by the variation in pore fluid pressure and temperature, which represent the coupled effects of the hydraulic and thermal systems on the mechanical system. Applying the principle of minimum potential energy, and minimising the potential energy with respect to the incremental nodal displacements $\{\Delta d\}_{nG}$, results in a finite element equation associated with force equilibrium for a coupled THM problem of fully saturated soils:

$$[K_G]\{\Delta d\}_{nG} + [L_G]\{\Delta p_f\}_{nG} - [M_G]\{\Delta T\}_{nG} = \{\Delta R_G\} \tag{5}$$

The matrices in Eq. (5) are defined in the Appendix, where $[K_G]$ represents soil mechanical behaviour, $[L_G]$ is the HM coupling term for pore fluid effect on mechanical response and $[M_G]$ is the TM coupling term for temperature effect on the mechanical response.

2.2. Hydraulic equation

Under isothermal conditions, the governing equations for pore fluid flow through the soil skeleton can be established by combining the continuity equation with Darcy's law (e.g. [27]). For a soil saturated with a compressible pore fluid, the continuity equation can be formulated based on the volume conservation of the pore fluid, which implies that the net volume of the pore fluid flowing into and out of a compressible element of fully saturated soil is equivalent to the total volumetric change of the soil skeleton, such that:

$$\nabla \cdot \{v_f\} - \frac{n}{K_f}\frac{\partial p_f}{\partial t} - Q^f = -\frac{\partial \varepsilon_v}{\partial t} \tag{6}$$

where $\{v_f\}$ represents the vector of the seepage velocity, $\nabla\cdot$ is the symbol of divergence defined as $\nabla \cdot \Theta = \partial\Theta/\partial x + \partial\Theta/\partial y + \partial\Theta/\partial z$, n is porosity, K_f is the bulk modulus of the pore fluid, Q^f represents any pore fluid sources and/or sinks, ε_v is the volumetric strain of the soil skeleton, and t is time. The seepage velocity $\{v_f\}$ in Eq. (6) is considered to be governed by the generalised Darcy's law, expressed as:

$$\{v_f\} = [k_f]\left(\frac{\{\nabla p_f\}}{\gamma_f} - \{i_G\}\right) \quad (7)$$

where $[k_f]$ is the permeability matrix, or hydraulic conductivity, of the soil, p_f is the pore fluid pressure, $\{\nabla p_f\}$ represents the gradient of pore fluid pressure, the vector $\{i_G\}^T = \{i_{Gx}\ i_{Gy}\ i_{Gz}\}$ is the unit vector parallel, but in the opposite direction, to gravity, γ_f is the specific weight of the pore fluid.

Under non-isothermal conditions, however, the changes in volume of the pore fluid due to the temperature change need to be taken into account, as often its coefficient of thermal expansion is different from that of the soil particles (or the soil skeleton, as per earlier assumption). The difference in the two thermal expansion coefficients can generate a volume of pore fluid flowing into or out of the soil element when there is a temperature change. If no flow can enter or leave the soil element, a variation in the pore fluid pressure is induced. Adopting the principle of volume conservation, the equation of continuity for a compressible pore fluid can be extended from Eq. (6) as:

$$\nabla \cdot \{v_f\} - \frac{n}{K_f}\frac{\partial p_f}{\partial t} - 3n\alpha_{Tf}\frac{\partial T}{\partial t} - Q^f = -\left[\frac{\partial \varepsilon_v}{\partial t} - 3(1-n)\alpha_T\frac{\partial T}{\partial t}\right] \quad (8)$$

where α_{Tf} is the thermal expansion coefficient of the pore fluid. It should be noted that the effect of buoyancy is not taken into account here.

Clearly, the first term on the left-hand side of Eq. (8) is related to the flow of pore fluid into and out of the soil element, the second term denotes the changes in the volume of the pore fluid due to its compressibility, while the third term expresses the thermal expansion/contraction of the pore fluid. On the right-hand side of Eq. (8), the first term is the total volumetric strain, while the second term reflects the changes in pore space available for the pore fluid within the porous medium due to the thermal expansion/contraction of the soil skeleton. Eq. (8) can be further rearranged as:

$$\nabla \cdot \{v_f\} - \frac{n}{K_f}\frac{\partial p_f}{\partial t} - 3n(\alpha_{Tf} - \alpha_T)\frac{\partial T}{\partial t} - Q^f = -\frac{\partial(\varepsilon_v - \varepsilon_{vT})}{\partial t} \quad (9)$$

where $\Delta\varepsilon_{vT} = 3\alpha_T\Delta T$. It should be noted that when the undrained heating behaviour of soils is modelled by employing Eq. (9) with a very low soil permeability and a relatively small time-step, the difference in thermal expansion coefficients between the soil skeleton and the pore fluid leads to an increase in pore fluid pressure. It should also be noted that applying the principle of mass conservation (the expression for which is shown in the next section) instead of volume conservation, leads to the same formulation as Eq. (6) for the isothermal case, and Eq. (9) for the non-isothermal case. The same hydraulic formulation was also obtained by Lewis and Schrefler [22], who followed the approach which combines the mass balance equation for the solid phase with the mass balance equation for the fluid phase.

Transfer of pore liquid as well as pore moisture under temperature gradients was observed in experiments on porous materials [26,11]. For partially saturated soils the effect of temperature gradients on pore liquid flow can be significant; however, for fully saturated soils, the fluid flow due to a temperature gradient is negligible [26]. Therefore, Eq. (7) is adopted here to model the seepage velocity under non-isothermal conditions. Substituting Eq. (7) into Eq. (9) and applying the principle of virtual work as well as the divergence theorem, the finite element equation governing the pore fluid flow under non-isothermal conditions can be assembled in terms of global matrices as [35,27]:

$$[L_G]^T\left(\frac{\{\Delta d\}_{nG}}{\Delta t}\right) - [\Phi_G]\{p_f\}_{nG} - [S_G]\left(\frac{\{\Delta p_f\}_{nG}}{\Delta t}\right) - [Z_G]\left(\frac{\{T\}_{nG}}{\Delta t}\right)$$
$$= -[n_G] + Q^f \quad (10)$$

Details of the matrices in Eq. (10) are given in the Appendix, where $[L_G]$ and $[Z_G]$ represent the influence of stress-strain and temperature changes on the hydraulic behaviour respectively, and $[\Phi_G]$ and $[S_G]$ are the permeability and compressibility matrices of the pore fluid. To solve this time-dependent equation, a time marching scheme is adopted here, which assumes that for the time interval $[t_1, t]$, where t_1 is the initial time and t is the current time,

$$\int_{t_1}^{t}[\Phi_G]\{p_f\}_{nG}dt = [\Phi_G][(\{p_f\}_{nG})_1 + \beta_1\{\Delta p_f\}_{nG}]\Delta t \quad (11)$$

where β_1 is the time marching parameter for pore fluid flow, and $(\{p_f\}_{nG})_1$ is the initial pore fluid pressure at the given time interval. To ensure the stability of the marching process, the value of β_1 should be between 0.5 and 1.0 [9], while the time-step should be chosen carefully to guarantee accuracy (i.e. not excessively large) and to avoid spatial oscillations (i.e. not excessively small), as highlighted in Cui et al. [15]. Substituting Eq. (11) into Eq. (10) yields:

$$[L_G]^T\{\Delta d\}_{nG} + (-\beta_1\Delta t[\Phi_G] - [S_G])\{\Delta p_f\}_{nG} - [Z_G]\{\Delta T\}_{nG}$$
$$= \{-[n_G] + Q^f + [\Phi_G](\{p_f\}_{nG})_1\}\Delta t \quad (12)$$

2.3. Thermal equation

Heat transfer in soils generally involves three modes [17]: diffusion, advection and radiation. To obtain the equations governing heat transfer for THM coupled problems, the following assumptions have been made:

(1) The effect of radiation is assumed negligible [23] and is therefore not taken into account;
(2) Following the assumption adopted for the mechanical equation, that the volumetric strain of particles and solid skeleton due to changes in temperature are identical (i.e. $\Delta\varepsilon_{T,p} = \Delta\varepsilon_{T,s} = \Delta\varepsilon_T$), thermal volumetric changes of the solid part in a free draining, mechanically unrestrained soil element do not change the void ratio. Indeed, conceptually, it is argued that when the particles thermally expand, volumes of both the soil skeleton and the voids change proportionally, resulting in a constant void ratio, such that: $\Delta e = \frac{V_{v0}+\Delta V_{v,T}}{V_{s0}+\Delta V_{s,T}} - \frac{V_{v0}}{V_{s0}} = \frac{V_{v0}+3\alpha_T\cdot V_{v0}}{V_{s0}+3\alpha_T\cdot V_{s0}} - \frac{V_{v0}}{V_{s0}} = 0$, where V_{v0} and V_{s0} are the initial volumes of the voids and the soil skeleton, respectively, and $\Delta V_{v,T}$ and $\Delta V_{s,T}$ are the corresponding incremental volumes due to the temperature change. Therefore, in this formulation, only the mechanical volumetric change, which is induced by the change in effective stresses, can affect the void ratio of the porous medium. It should be noted that under undrained heating conditions the change in the void ratio could indeed be caused by changes in pore fluid pressure due to the differential thermal expansion of the pore fluid and the soil skeleton, as discussed in the previous section.

The equation governing ground heat transfer is formulated based on the law of energy conservation [31,32]:

$$\frac{\partial(\Phi_T dV)}{\partial t} + \nabla \cdot Q_T dV - Q^T dV = 0 \quad (13)$$

where Φ_T is the heat content of the soil per unit volume, Q_T is the heat flux per unit volume, which includes heat diffusion and heat advection, Q^T represents any heat source and/or sink, and dV is an infinitesimal volume of the soil. The heat content term, Φ_T, is defined proportionally to soil phases, hence for fully saturated soils:

$$\Phi_T = [n\rho_f C_{pf} + (1-n)\rho_s C_{ps}](T - T_r) \quad (14)$$

where C_{pf} is the specific heat capacity of the pore fluid and therefore associated with the pore space (i.e. porosity, n) and C_{ps} is the specific heat capacity of soil particles, hence associated with the remaining volume (i.e. $1 - n$), ρ_f and ρ_s are the densities of the pore fluid and soil particles respectively, and T_r is a reference temperature. The heat flux Q_T is written as the sum of heat diffusion q_d and heat advection q_c, where

$$q_d = -[k_T]\{\nabla T\} \tag{15}$$

$$q_c = \rho_f C_{pf}\{v_f\}(T - T_r) \tag{16}$$

and $[k_T]$ is the thermal conductivity matrix. Substituting Eqs. (14)–(16) into Eq. (13) gives:

$$\frac{\partial\{[n\rho_f C_{pf} + (1-n)\rho_s C_{ps}](T - T_r)dV\}}{\partial t}$$
$$+ \{\nabla \cdot [\rho_f C_{pf}\{v_f\}(T - T_r)] - \nabla \cdot ([k_T]\{\nabla T\}) - Q^T\}dV = 0 \tag{17}$$

The first term on the left-hand side of Eq. (17) can be expanded to give:

$$\frac{\partial\{[n\rho_f C_{pf} + (1-n)\rho_s C_{ps}](T - T_r)dV\}}{\partial t}$$
$$= \underbrace{[n\rho_f C_{pf} + (1-n)\rho_s C_{ps}]dV\frac{\partial T}{\partial t}}_{(1)} + \underbrace{\frac{\partial[(1-n)\rho_s C_{ps}dV]}{\partial t}(T - T_r)}_{(2)}$$
$$+ \underbrace{\frac{\partial[n\rho_f C_{pf}dV]}{\partial t}(T - T_r)}_{(3)} \tag{18}$$

where terms (2) and (3) in Eq. (18) represent the influence of deformation of the soil on heat transfer. In effect, these two terms denote the influence of changes in the heat capacity of the porous medium, resulting from variations in porosity which arise from mechanical deformation. Naturally, the overall impact of this part of the formulation is essentially controlled by the difference in heat capacity of the fluid and solid phases of the medium. The second term on the left-hand side of Eq. (17), which represents the advective heat transfer, can be derived as:

$$\nabla \cdot [\rho_f C_{pf}\{v_f\}(T - T_r)]dV$$
$$= \underbrace{\rho_f C_{pf}\{v_f\}^T\{\nabla T\}dV}_{(1)} + \underbrace{C_{pf}(T - T_r)\nabla \cdot (\rho_f\{v_f\})dV}_{(2)} \tag{19}$$

Applying the principle of mass conservation for the pore fluid (omitting the source term) and soil particles, gives [22,32]:

$$\frac{\partial(n\rho_f dV)}{\partial t} + [\nabla \cdot (\rho_f\{v_f\})]dV = 0 \tag{20}$$

$$\frac{\partial[(1-n)\rho_s dV]}{\partial t} + [\nabla \cdot (\rho_s\{v_s\})]dV = 0 \tag{21}$$

where $\{v_s\}$ is the velocity of the soil particles. Clearly, using Eq. (20), it is possible to establish that term (3) in Eq. (18) and term (2) in Eq. (19) are equal in magnitude but have opposite signs. Therefore, eliminating those terms from Eq. (17) and neglecting the advective heat flux in the solid phase (the second term in Eq. (21)), Eq. (17), which governs heat transfer, can be expressed as:

$$[n\rho_f C_{pf} + (1-n)\rho_s C_{ps}]\frac{\partial T}{\partial t} + \rho_f C_{pf}\{v_f\}^T\{\nabla T\} - \nabla \cdot ([k_T]\{\nabla T\}) - Q^T = 0 \tag{22}$$

It is noted that Eq. (22) reproduces that proposed by Lewis and Schrefler [22] and in a fully coupled THM FE analysis it may adequately illustrate the coupled behaviour of soils. However, when a coupled thermo-mechanical (TM) FE analysis (e.g. an undrained analysis, typical of low permeability clays, where the two-phase nature of the soil is ignored and only the behaviour of the mixture

is considered) is carried out, cancelling the two terms which are equal in magnitude from Eq. (17) leads to the absence of TM coupling in the heat transfer equation. Therefore, the formulation proposed here retains all the terms in Eq. (17). Introducing the void ratio, e, as a soil property that is measured in experiments, $n = e/(1 + e)$, and noting that $dV = (1 + e)dV_s$, where dV_s is the infinitesimal volume of the soil particles, into Eq. (17) yields:

$$\frac{\partial\{[e\rho_f C_{pf} + \rho_s C_{ps}](T - T_r)dV_s\}}{\partial t}$$
$$+ \{\nabla \cdot [\rho_f C_{pf}\{v_f\}(T - T_r)] - \nabla \cdot ([k_T]\{\nabla T\}) - Q^T\}(1 + e)dV_s = 0 \tag{23}$$

Under isothermal conditions, dV_s is generally assumed to be constant in a simulation, regardless of the change in effective stresses. Under non-isothermal conditions, however, based on the assumptions presented earlier, dV_s is temperature dependent and can be written as:

$$dV_s = (1 + \varepsilon_{vT})dV_{s0} \tag{24}$$

where dV_{s0} is the initial volume of the soil particles. It is noted that dV_{s0} is assumed to be constant here, which is different from Thomas et al. [32] who assume that dV_s is constant in a coupled THM problem. Substituting Eq. (24) into Eq. (23) and eliminating dV_{s0} leads to:

$$\frac{\partial\{[e\rho_f C_{pf} + \rho_s C_{ps}](T - T_r)(1 + \varepsilon_{vT})\}}{\partial t}\frac{1}{(1 + e)(1 + \varepsilon_{vT})}$$
$$+ \nabla \cdot [\rho_f C_{pf}\{v_f\}(T - T_r)] - \nabla \cdot ([k_T]\{\nabla T\}) = Q^T \tag{25}$$

Noting that variables in Eq. (25) are e, T, ε_{vT}, ρ_f and ρ_s, and $\{v_f\}$, the first term on the left-hand side of Eq. (25) can be further derived as:

$$\frac{\partial\{[e\rho_f C_{pf} + \rho_s C_{ps}](T - T_r)(1 + \varepsilon_{vT})\}}{\partial t}\frac{1}{(1 + e)(1 + \varepsilon_{vT})}$$
$$= \underbrace{[n\rho_f C_{pf} + (1-n)\rho_s C_{ps}]\frac{\partial T}{\partial t}}_{(1)} + \underbrace{\rho_f C_{pf}(T - T_r)\frac{1}{1 + e}\frac{\partial e}{\partial t}}_{(2)}$$
$$+ \underbrace{[n\rho_f C_{pf} + (1-n)\rho_s C_{ps}]\frac{(T - T_r)}{1 + \varepsilon_{vT}}\frac{\partial \varepsilon_{vT}}{\partial t}}_{(3)}$$
$$+ \underbrace{\left[nC_{pf}(T - T_r)\frac{\partial \rho_f}{\partial t} + (1-n)C_{ps}(T - T_r)\frac{\partial \rho_s}{\partial t}\right]}_{(4)} \tag{26}$$

In this equation, term (2) denotes the influence of the mechanical deformation, through the variation of void ratio, on the simulated heat transfer. Clearly, the contribution of this term could potentially be significant in applications where considerable stress changes are expected, such as in the design of thermo-active structures. If the material density is assumed to be temperature dependent, substituting $\rho = \rho_0/(1 + \varepsilon_{vT})$ for the pore fluid and solid phases, into Eq. (26) leads to the elimination of terms (3) and (4) from Eq. (26), resulting in

$$\frac{\partial\{[e\rho_f C_{pf} + \rho_s C_{ps}](T - T_r)(1 + \varepsilon_{vT})\}}{\partial t}\frac{1}{(1 + e)(1 + \varepsilon_{vT})}$$
$$= \underbrace{[n\rho_f C_{pf} + (1-n)\rho_s C_{ps}]\frac{\partial T}{\partial t}}_{(1)} + \underbrace{\rho_f C_{pf}(T - T_r)\frac{1}{1 + e}\frac{\partial e}{\partial t}}_{(2)} \tag{27}$$

However, if this is done, then a variable material density should also be applied to the development of the mechanical and hydraulic equations and be updated during the iteration of each increment to ensure the consistency of this approach. As far as the authors are aware, this complication has not been fully taken into account in any of the existing published THM formulations using

the finite element method. Therefore, constant densities are assumed in the formulation proposed here so that comparisons can be made with results from the literature. As a result, Eq. (26) becomes:

$$\frac{\partial\{[e\rho_f C_{pf} + \rho_s C_{ps}](T - T_r)(1 + \varepsilon_{vT})\}}{\partial t} \frac{1}{(1+e)(1+\varepsilon_{vT})}$$

$$= [n\rho_f C_{pf} + (1-n)\rho_s C_{ps}]\frac{\partial T}{\partial t} + \rho_f C_{pf}(T - T_r)\frac{1}{1+e}\frac{\partial e}{\partial t}$$

$$+ [n\rho_f C_{pf} + (1-n)\rho_s C_{ps}]\frac{(T - T_r)}{1 + \varepsilon_{v\theta}}\frac{\partial \varepsilon_{vT}}{\partial t} \qquad (28)$$

Since the changes in void ratio are assumed to be only a result of the mechanical strain, it is possible to establish the following relationship in a small displacement analysis:

$$\frac{1}{1 + e_0}\frac{\partial e}{\partial t} = \frac{\partial(\varepsilon_v - \varepsilon_{vT})}{\partial t} \qquad (29)$$

where e_0 is the initial void ratio of the soil. If the fluid density is assumed not to change ($\nabla \cdot \rho_f = 0$), the second term on the left-hand side of Eq. (25) can be derived as:

$$\nabla \cdot [\rho_f C_f\{v_f\}(T - T_r)] = \rho_f C_{pf}\{v_f\}^T\{\nabla T\} + \rho_f C_{pf}(T - T_r)\nabla \cdot \{v_f\} \qquad (30)$$

Substituting Eqs. (7), (28)–(30) into Eq. (25) and following a procedure similar to that for the hydraulic FE formulation, gives the following finite element equations associated with heat transfer:

$$[Y_G]\frac{\{\Delta d\}_{nG}}{\Delta t} - [\Omega_G]\{p_f\}_{nG} + [X_G]\frac{\{\Delta T\}_{nG}}{\Delta t} + [\Gamma_G]\{T\}_{nG} = -[n_G^T] + Q^T \qquad (31)$$

where the matrices are defined in the Appendix, with $[Y_G]$ representing the mechanical effect on thermal response, $[\Omega_G]$ the hydraulic effect on thermal response, $[X_G]$ the thermal expansion and $[\Gamma_G]$ defining both conduction and advection capacities. To solve Eq. (31) the same time marching scheme, as that adopted for solving the FE equations governing the pore fluid flow, has been used here, resulting in:

$$[Y_G]\{\Delta d\}_{nG} - \beta_2\Delta t[\Omega_G]\{\Delta p_f\}_{nG} + ([X_G] + \alpha_1\Delta t[\Gamma_G])\{\Delta T\}_{nG}$$

$$= \{-[n_G^T] + Q^T + [\Omega_G](\{p_f\}_{nG})_1 - [\Gamma_G](\{T\}_{nG})_1\}\Delta t \qquad (32)$$

where β_2 and α_1 are time marching parameters for heat transfer. Note that the same concerns on the adequate selection of the time-step previously raised for the solution of the hydraulic equation apply to the solution of the thermal equation (Eq. (32)). Indeed, Cui et al. [15] demonstrates that for problems involving heat flux, the minimum time-step required to prevent the occurrence of spatial oscillations is highly affected by the chosen discretisation, the applied boundary conditions and by the relative weight of advection on the overall rate of heat transfer. Assembling Eqs. (5), (12) and (32) gives the fully coupled THM formulation in the incremental matrix form as:

$$\begin{bmatrix} [K_G] & [L_G] & -[M_G] \\ [L_G]^T & -\beta_1\Delta t[\Phi_G] - [S_G] & -[Z_G] \\ [Y_G] & -\beta_2\Delta t[\Omega_G] & \alpha_a\Delta t[\Gamma_G] + [X_G] \end{bmatrix} \begin{Bmatrix} \{\Delta d\}_{nG} \\ \{\Delta p_f\}_{nG} \\ \{\Delta T\}_{nG} \end{Bmatrix} = \begin{Bmatrix} \{\Delta R_G\} \\ \{\Delta F_G\} \\ \{\Delta H_G\} \end{Bmatrix} \qquad (33)$$

2.4. Boundary conditions

To adequately model a coupled THM problem with the FE method, appropriate mechanical, hydraulic and thermal boundary conditions (BC) are required. Details of the mechanical and hydrau-

lic BC for geotechnical engineering can be found in Potts and Zdravković [27], while the thermal BC, which are commonly used and have also been implemented into ICFEP, involve: (i) Prescribed temperature; (ii) Prescribed heat flux; (iii) Heat source and sink; (iv) Natural heat loss BC which enables heat flux exchange between a body and its surrounding fluid due to temperature difference between the two (for example between the ground and the atmosphere).

In particular, a new coupled thermo-hydraulic BC has been developed and implemented into ICFEP to balance the change in energy associated with the flow of pore fluid through the boundary in a coupled THM or TH analysis [14].

It should be noted that both the natural heat loss BC and the coupled thermo-hydraulic BC are non-linear, as the variables employed by these two BC can vary over an increment of the analysis.

3. Validation and application

To demonstrate the performance of the newly developed and implemented THM formulation, a series of benchmark analyses have been performed and some are discussed here. In the first instance ICFEP predictions are compared against analytical solutions and numerical studies found in the literature. Subsequently, a comparison is made against laboratory experimental results.

3.1. Thermo-elastic consolidation of a soil column

The 1D thermo-elastic consolidation analysis of a fully saturated column of soil was first presented by Aboustit et al. [1,2], and was subsequently used as a benchmark by Noorishad et al. [24], Lewis et al. [21], Lewis and Schrefler [22], and Gatmiri and Delage [18] for checking their FE formulations. Consequently, this example is also analysed using ICFEP.

To ensure the consistency between material properties adopted in the literature and those used in ICFEP, a plane strain analysis of 1D isothermal elastic consolidation was first performed, for which an analytical solution [7] is available. The adopted FE mesh is shown in Fig. 1, employing 8-noded quadrilateral elements, with both displacement and pore pressure degrees of freedom at all element nodes. The adopted material properties are shown in Table 1.

A vertical surface pressure of 1 Pa was applied at the top boundary of the soil column at the start of the analysis and displacement boundary conditions as shown in the figure were prescribed to ensure 1D vertical deformation of the column. The prescribed hydraulic boundary conditions allowed for drainage only through the top boundary and the initial pore water pressure is hydrostatic from this boundary. Two sets of time-steps (see Table 2) were investigated and $\beta_1 = 0.875$ was adopted for both sets as the time marching parameter in Eq. (11). Set I was the same as in Aboustit et al. [1,2] and Lewis et al. [21] and it resulted in spatial oscillations in the pore pressure at the beginning of the analysis (both in the above references and in the ICFEP analysis). The authors' earlier studies have shown that these oscillations are induced by an excessively small time-step. In this respect, Cui et al. [15] derived the minimum time-step that ensures non-oscillatory results:

$$\Delta t_{min} = \frac{\gamma_f h^2(1 + v)(1 - 2v)}{16\beta_1 k_f(1 - v)} \qquad (34)$$

where h is a measure of element size. Substituting the values given for the parameters in Table 1 and with $h = 0.2$ m, gives a minimum time step of 0.056 s. Clearly, the initial time step of 0.01 s in the first analysis violates this constraint and explains the observed oscillations.

Fig. 2 shows the evolution of the column surface settlement with time, due to the applied pressure, for both analyses. Analytical
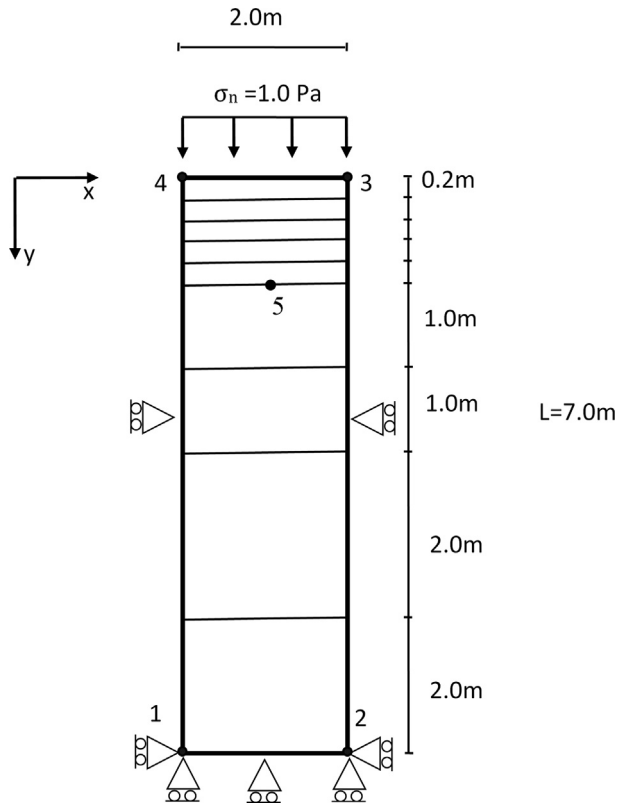
Fig. 1. Finite element mesh for a 1D thermo-elastic consolidation.

Table 1
Material properties.

Young's modulus, E (Pa)	6.0×10^3
Poisson ratio, v (–)	0.4
Permeability, k_f (m/s)	3.92×10^{-5}
Initial void ratio, e_0 (–)	0.25
$\rho_s C_{ps}$, $\rho_f C_{pf}$ (kJ/(m^3 K))	167.2
Conductivity k_T (kJ/(m s K))	0.836
Thermal expansion coefficient α_T (m/(m K))	3.0×10^{-7}

Table 2
Time-step parameters for column analysis.

Set I		Set II	
Increment	Time-step (s)	Increment	Time-step (s)
1–10	0.01	1–10	1
11–20	0.1	11–5000	10
21–30	10		
31–40	100		
41–60	1000		

solutions from Biot [7] are also plotted. It is noted that both analyses produce very close transient and steady state results, with the second one matching the analytical solutions exactly. The latter result is then compared in Fig. 3 to those shown in the literature. A very good match is evident with the results of Lewis et al. [21] and Noorishad et al. [24], while the formulation of Gatmiri and Delage [18] differs significantly from all others.

The subsequent exercise is a non-isothermal consolidation analysis, which uses the same 2D mesh in Fig. 1, but with an additional temperature degree of freedom at all element nodes. The material parameters are listed in Table 1 and the initial temperature of the soil column is 0 °C. The mechanical and hydraulic boundary conditions stayed unchanged, while a constant temperature of 50 °C and a vertical surface pressure of 1 Pa are prescribed
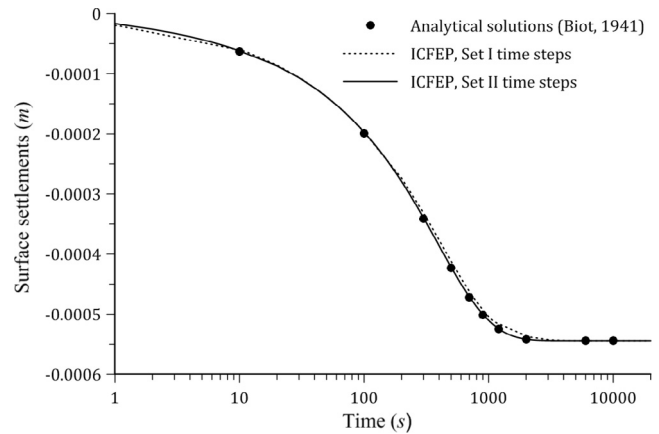

Fig. 2. Surface settlements versus time for 1D isothermal consolidation (HM) analysis with ICFEP.
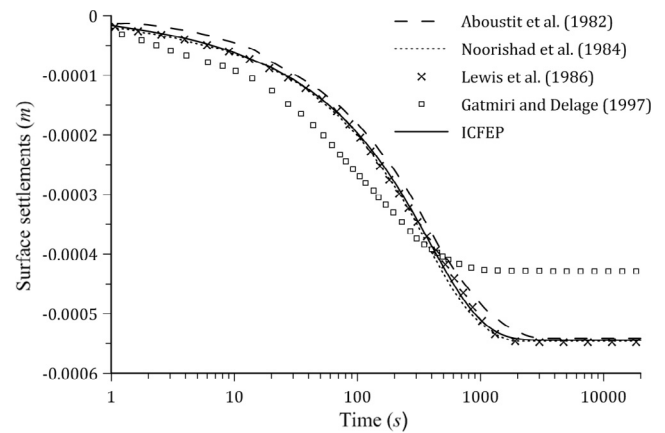

Fig. 3. Comparison between ICFEP solutions and those in the literature for 1D isothermal consolidation (HM) analysis.

at the top surface. No heat flow is prescribed at any of the other boundaries (i.e. insulated boundary). Both time-step sets in Table 2 were attempted and Fig. 4 shows that the biggest difference between the two results is in the predicted maximum settlement. Further inspection showed that the Set I analysis missed the peak settlements due to a large time-step $\Delta t = 1000$ s between increments 41 (t = 1000 s) and 42 (t = 2000 s). Additionally, oscillations in the nodal temperature distribution along the soil column were observed in this analysis, as the initial time step is lower than the minimum one established by Cui et al. [15]. Therefore, the results from the new THM formulation (as implemented in ICFEP) with the Set II time steps are compared to those from the same references used in the HM analysis. It should be noted that Lewis et al. [21] adopted a Petrov-Galerkin FE method and upwinding techniques to avoid oscillations as the effect of advection is taken into account here. The authors have recently implemented the Petrov-Galerkin FE method into ICFEP for highly advective flows. However, their previous work [14] has shown that even the conventional Galerkin FE method can accurately simulate this problem, depending on the magnitude of the maximum Péclet number. This parameter is used to represent the ratio between the advective and conductive heat fluxes, which in this analysis is 0.002 and therefore below the critical value of 2.0 established by Cui et al. [14]. Consequently, the Galerkin FE method is adopted here in the THM analysis of the soil column.

Fig. 5 compares the prediction of the variation in both temperature and excess pore fluid pressure at a depth of 1 m (point 5 in the mesh, see Fig. 1) from the new THM formulation against the
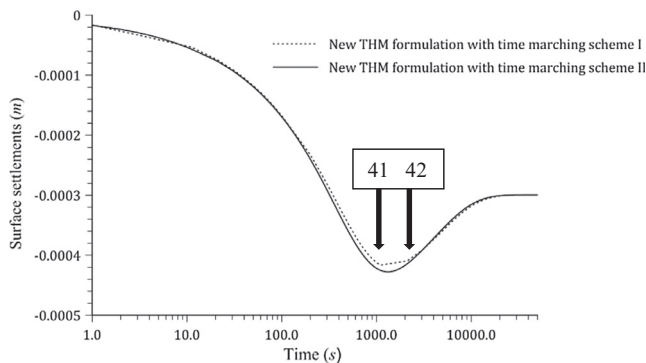
Fig. 4. Surface settlements versus time for 1D non-isothermal consolidation analysis with different time-step sizes (THM).

available data from Lewis et al. [21]. Good matches can be found for both temperature and pore fluid pressure. The slight difference in the temperature variation at the initial stage of the analysis is due to the different time marching schemes adopted for heat transfer in the two analyses (i.e. Set I by Lewis et al. [21] and Set II by the authors).

Fig. 6 compares the prediction of the surface settlement with time from the new THM formulation against those shown in the literature. The solid line result is from the analysis with the new THM formulation (as implemented in ICFEP) in which $\alpha_T = \alpha_{T,f}$, as adopted in the analyses from the literature. As noted by Lewis et al. [21], there was probably a printing error in the results of Aboustit et al. [2] which has been corrected in Fig. 6 and shows very good agreement with the ICFEP results, although there are limited discrete results for the former publication. Also, the same
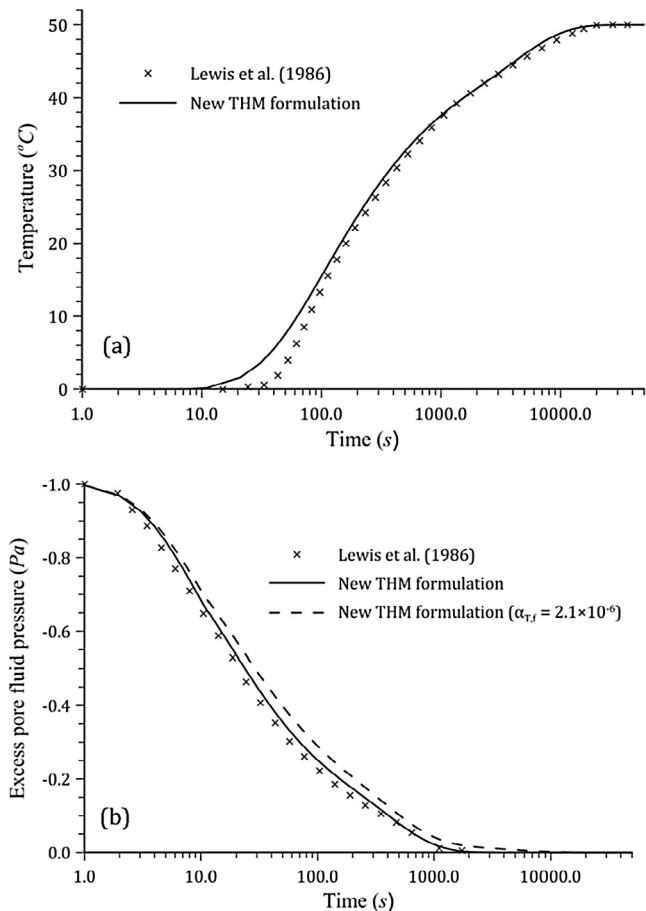

Fig. 5. Variation in (a) temperature, and (b) excess pore fluid pressure at point 5.

steady-state was achieved by Lewis et al. [21], Noorishad et al. [24] and the current work. The difference in the peak settlement between the prediction of the new formulation and that given by Lewis et al. [21] is mainly due to the fact that the latter formulation assumes no coupling effect of temperature on the hydro-mechanical response. In terms of the THM governing Eq. (33) this is equivalent to the coupling matrix $[Z_G]$ being equal to zero. In the new formulation, however, this is not the case and the $[Z_G]$ matrix depends on the magnitudes of α_T and $\alpha_{T,f}$. A further example of the level of difference in predicted maximum settlements from the new THM formulation is presented by the dashed line, from an analysis with different thermal expansion coefficients ($\alpha_T = 3 \times 10^{-7}$ as in Table 1, and $\alpha_{T,f} = 2.1 \times 10^{-6}$). Although differences in excess pore fluid pressure (see Fig. 5(b)) and maximum settlement (see Fig. 6) between the two analyses with the new THM formulation may not be seen as significant (10% on average for both) for this validation exercise, they could be substantial in a complex boundary value problem. Unfortunately, it is difficult to assess the reasons for differences between the results from the new THM formulation and those from Noorishad et al. [24] or Gatmiri and Delage [18], due to limited information on their numerical formulations given in the literature.

3.2. Undrained heating test

The next validation exercise involved application of the fully coupled THM formulation proposed in this paper in the analysis of a triaxial undrained heating test reported by Abuel-Naga et al. [3]. The particular interest here is the development of thermally-induced excess pore water pressures. A fully saturated Soft Bangkok clay was used in the test with an initial temperature of 25 °C. The specimen was isotropically consolidated under isothermal conditions to 200 kPa, followed by an unloading which resulted in an overconsolidation ratio (OCR) of 4.0. Subsequently, the sample was heated under undrained conditions to 90 °C with increments of 10 °C, and the thermally induced pore water pressure was measured after each temperature increment. Laboratory tests of the thermo-mechanical response of Soft Bangkok clay have shown that overconsolidated samples tend to behave elastically [4,5], and consequently such an assumption is adopted here.

A single element axi-symmetric fully coupled THM analysis was carried out with the present THM formulation. The relevant properties of Soft Bangkok clay (K, n_o and α_T) were obtained from data provided by Abuel-Naga et al. [6,4], whereas the thermal expansion coefficient of water ($\alpha_{T,f}$) was adopted from Abuel-Naga et al. [3]
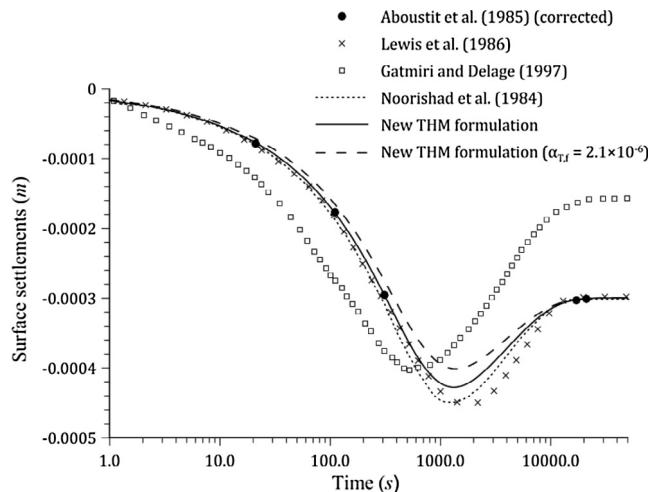

Fig. 6. Comparison in displacement between solutions from the new THM formulation and those in the literature, for 1D non-isothermal consolidation analysis.

Table 3
Material properties for the analysis under undrained heating conditions.

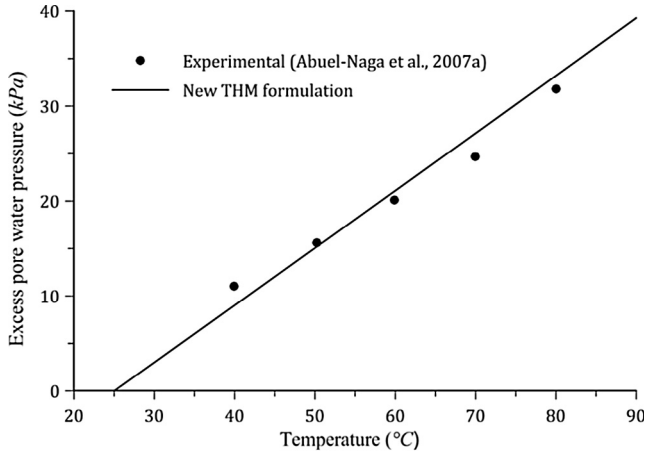|	
Bulk modulus of soil, K (MPa)	1.98
Initial porosity, n_0 (–)	0.634
Linear thermal expansion coefficient of soil skeleton, α_T (°C^{-1})	1.0×10^{-5}
Linear thermal expansion coefficient of pore fluid, $\alpha_{T,f}$ (°C^{-1})	1.7×10^{-4}
Bulk modulus of water, K_f (MPa)	2200

Fig. 7. Comparison between numerical and experimental results for undrained heating test.

which represents an average value within the temperature range. All key material properties are summarised in Table 3. All boundaries of the finite element were modelled as impermeable so that an undrained condition was enforced. A total temperature increase of 65 °C was applied to all element nodes with an incremental temperature of 1 °C. A value of 0.8 was adopted for all time-marching parameters and the time-step was chosen arbitrarily as 1.0 s. The changes in pore fluid pressure were monitored in the analysis and plotted in Fig. 7 against the experimental results. Considering the inevitable experimental scatter, the agreement between the two is excellent. It is the coupling matrix $[Z_G]$ in the proposed formulation that enables the prediction of excess pore water pressures in an undrained heating test, without resorting to a constitutive model specially developed to simulate such an effect.

4. Conclusions

This paper presents a complete finite element formulation accounting for fully coupled thermo-hydro-mechanical behaviour of saturated soils. While the formulation is independent and based on a set of clearly stated assumptions, the final equations are similar to, but differ in some important aspects from those in the literature. The following are the key characteristics of the proposed formulation:

(1) The formulation is fully coupled and all terms, including the cross-coupling terms, are independently defined.
(2) Full derivation of the coupled THM formulation identifies cross-coupling terms which can be cancelled out in the heat transfer equation. This has been exploited by others in the literature. However, the proposed formulation shows that this results in an error in a thermo-mechanical analysis. Consequently, it retains all the terms.
(3) The difference in the thermal expansion coefficient between the pore water and the soil skeleton is explicitly accounted for. This enables simulation of undrained heating which results in the generation of excess pore water pressures without having to use a specially developed thermo-plastic

constitutive model to simulate this effect. Comparison of predictions using this facility against experimental results shows excellent agreement.

Appendix A

$$[K_G] = \sum_{i=1}^{N} \left(\int_{Vol} [B]^T [D'][B] dVol \right)_i$$

$$[L_G] = \sum_{i=1}^{N} \left(\int_{Vol} [B]^T \{m\}[N_p] dVol \right)_i$$

$$[M_G^T] = \sum_{i=1}^{N} \left(\int_{Vol} [B]^T [D']\{m_T\}[N_T] dVol \right)_i$$

$$\{\Delta R_G\} = \sum_{i=1}^{N} \left[\left(\int_{Vol} [N]^T \{\Delta F\} dVol \right)_i + \left(\int_{Srf} [N]^T \{\Delta T\} dSrf \right)_i \right]$$

$$[\Phi_G] = \sum_{i=1}^{N} \left(\int_{Vol} \frac{[E_p]^T [k_f][E_p]}{\gamma_f} dVol \right)_i$$

$$[S_G] = \sum_{i=1}^{N} \left(\int_{Vol} \frac{n}{K_f} [N_p]^T [N_p] dVol \right)_i$$

$$[Z_G] = \sum_{i=1}^{N} \left(\int_{Vol} 3[n(\alpha_{T,f} - \alpha_T) + \alpha_T][N_p]^T [N_T] dVol \right)_i$$

$$[n_G] = \sum_{i=1}^{N} \left(\int_{Vol} [E_p]^T [k_f]\{i_G\} dVol \right)_i$$

$$[Y_G] = \sum_{i=1}^{N} \left(\int_{Vol} \rho_f C_{pf}(T - T_r) \left(\frac{1+e_0}{1+e} \right) [N_T]^T \{m\}^T [B] dVol \right)_i$$

$$[X_G] = \sum_{i=1}^{N} \left(\int_{Vol} \left\{ [n\rho_f C_{pf} + (1-n)\rho_s C_{ps}] \left[1 + \frac{3\alpha_T(T - T_r)}{1+\varepsilon_{vT}} \right] [N_T]^T [N_T] \right. \right.$$
$$\left. \left. - \rho_f C_{pf}(T - T_r) \left(\frac{1+e_0}{1+e} \right) 3\alpha_T [N_T]^T [N_T] \right\} dVol \right)_i$$

$$[\Omega_G] = \sum_{i=1}^{N} \left(\int_{Vol} \frac{\rho_f C_{pf}(T - T_r)[E_T]^T [k_f][E_p]}{\gamma_f} dVol \right)_i$$

$$[\Gamma_G] = \sum_{i=1}^{N} \left(\int_{Vol} ([E_T]^T [k_T][E_T] + \rho_f C_{pf}[N_T]^T \{v_f\}^T [E_T]) dVol \right)_i$$

$$[n_G^T] = \sum_{i=1}^{N} \left(\int_{Vol} \rho_f C_{pf}(T - T_r)[E_T]^T [k_f]\{i_G\} dVol \right)_i$$

$$\{\Delta F_G\} = \{-[n_G] + Q^f + [\Phi_G](\{p_f\}_{nG})_1\}\Delta t$$

$$\{\Delta H_G\} = \{-[n_G^T] + Q^T + [\Omega_G](\{p_f\}_{nG})_1 - [\Gamma_G](\{T\}_{nG})_1\}\Delta t$$

$$[E_p] = \left[\frac{\partial N_P}{\partial x}, \frac{\partial N_P}{\partial y}, \frac{\partial N_P}{\partial z} \right]^T$$

$$[E_T] = \left[\frac{\partial N_T}{\partial x}, \frac{\partial N_T}{\partial y}, \frac{\partial N_T}{\partial z} \right]^T$$

$$\{m\}^T = \{1 \quad 1 \quad 1 \quad 0 \quad 0 \quad 0\}$$

where [B] is a matrix which contains only spatial derivatives of the shape functions, [N] is the matrix of displacement interpolation functions (or shape functions), [N$_P$] is the matrix of pore fluid pressure interpolation functions, [N$_T$] is the matrix of temperature interpolation functions.

List of symbols for derivation of the coupled THM formulation

[B]	Matrix containing derivatives of the displacement interpolation functions
C_{pf}	Specific heat capacity of the pore fluid
C_{ps}	Specific heat capacity of the soil particle
[D]	Constitutive matrix
[D′]	Effective constitutive matrix
[E$_P$]	Matrix containing derivatives of the pore fluid pressure interpolation functions
[E$_T$]	Matrix containing derivatives of the temperature interpolation functions
e	Void ratio
K_f	Bulk modulus of the pore fluid
[k_f]	Permeability matrix
[k_T]	Conductivity matrix
[N]	Matrix of displacement interpolation functions
[N$_P$]	Matrix of pore fluid pressure interpolation functions
[N$_T$]	Matrix of temperature interpolation functions
n	Porosity
p_f	Pore fluid pressure
Q^f	Pore fluid sources and/or sinks
Q^T	Heat sources and/or sinks
q_d	Heat diffusion
q_c	Heat convection
T_s	Temperature of the soil particle
T_f	Temperature of the pore fluid
T	Temperature of the soil
T_r	Reference temperature
t	Time
V_v	Volume of the voids
V_s	Volume of the soil skeleton
dV	Volume of the soil
v_f	Seepage velocity
α_1	Time marching parameter
α_T	Thermal expansion coefficient of the soil
α_{Tf}	Thermal expansion coefficient of the pore fluid
β_1, β_2	Time marching parameter
γ_f	Specific weight of the pore fluid
ε	Total strain
$\varepsilon_{T,p}$	Thermal strain of the soil particle
$\varepsilon_{T,s}$	Thermal strain of the soil skeleton
ε_T	Thermal strain of the soil
ε_σ	Mechanical strain of the soil
ε_v	Volumetric strain of the soil skeleton
ε_{vT}	Thermal volumetric strain of the soil
ρ_f	Densities of the pore fluid
ρ_s	Densities of the soil particle

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