Computers and Geotechnics xxx (2017) xxx–xxx

Contents lists available at ScienceDirect

Computers and Geotechnics

journal homepage: www.elsevier.com/locate/compgeo

Research Paper

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

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ARTICLE INFO

Article history:
Received 16 January 2017
Received in revised form 18 July 2017
Accepted 16 August 2017
Available online xxxx

Keywords:
Finite element methods
THM coupling
Geomechanics

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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http://dx.doi.org/10.1016/j.compgeo.2017.08.011
0266-352X/© 2017 The Authors. Published by Elsevier Ltd.

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, $\{\Delta\sigma_f\}^{\mathrm{T}} = \{\Delta p_f\ \Delta p_f\ \Delta p_f\ 0\ 0\ 0\}$ 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 $\{\Delta\varepsilon_T\}^{\mathrm{T}} = \{\alpha_T\Delta T\ \alpha_T\Delta T\ \alpha_T\Delta T\ 0\ 0\ 0\}$ 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 $\{m_T\}^{\mathrm{T}} = \{\alpha_T\ \alpha_T\ \alpha_T\ 0\ 0\ 0\}$. 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:

Please cite this article in press as: Cui W et al. An alternative coupled thermo-hydro-mechanical finite element formulation for fully saturated soils. Comput Geotech (2017), http://dx.doi.org/10.1016/j.compgeo.2017.08.011