Research Paper

A study on how to couple thermo-hydro-mechanical behaviour of unsaturated soils: Physical equations, numerical implementation and examples

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A B S T R A C T

This paper describes a thermo-hydro-mechanical framework suitable for modelling the behaviour of unsaturated soils. In particular, this paper focuses on bentonite clay subjected to a thermo-hydro-mechanical load, as in the case of nuclear waste engineering barriers. The paper gives a theoretical derivation of the full set of coupled balance equations governing the material behaviour as well as an extended physical interpretation. Finally, a finite element discretisation of the equations and number of simulations verifying their implementation into a custom finite element code is provided. Some aspects of the formulation are also validated against experimental data.
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1. Introduction

In some engineering applications the understanding of unsaturated soil behaviour becomes inevitably important and necessary for an effective design. A pronounced example is the case of bentonite which is the material of choice for engineering barriers due to its very low permeability, relative resistance to chemicals and swelling behaviour upon wetting. For instance, bentonite is used as barriers for nuclear waste disposal sites where safety specifications are especially strict [1,2]. Ideally, barriers should be nearly impermeable, self-healing (so the influence of cracks and initial imperfections is minimised) and possess properties such that the surrounding environment remains unaffected by radioactive waste materials for a very long time, typically tens of thousands of years. A suitable barrier material design requires prediction of complex behaviour under high temperature gradient, hydraulic processes and development of gas pressure. The design also requires prediction of the self-healing properties obtained due to swelling upon wetting and high pressure state in the material. Nonetheless, the developed swelling pressure should not be too high, as that could adversely affect the containers for the nuclear material. Finally, the material is also affected by

radioactivity and chemical reactions, though these factors are not included in this study.

A significant body of research accumulated for these sealing materials (e.g. [3,4]), which generally agree that the modelling should consider the fully coupled (chemo)-thermo-hydro-mechanical behaviour of bentonite. This paper presents a physical framework which can be extended to include chemical effects and radioactivity effects. The framework is general and suitable for unsaturated soils and geomaterials. It can also be used for porous materials, as each constitutive equation can be easily replaced by another formulation more suitable for given application.

Experience gained in different scientific disciplines [3,5–8] suggests that the finite element method is one of the best methods to numerically solve such a coupled system of equations. This study presents in details the coupled physical formulation, finite element discretisation and implementation of the thermo-hydro-mechanical equations governing the behaviour of porous geomaterials. This paper also discusses Barcelona Basic Model (BBM) [9] and its thermo-mechanical extension [10].

Finally, this paper provides verification and validation against analytical solutions, well-established THM code (CODE_BRIGHT [11]) results, and experimental data. The numerical results are satisfactory from the point of view of matching theoretical solutions and approaching real physical behaviour.

Despite focusing on bentonite behaviour, the described physical framework is general and may be used for simulation of THM

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Nomenclature

Roman

A	auxiliary term
A_o	amplitude, Θ
$\boldsymbol{A}$	Jacobian matrix
B	auxiliary term
$\boldsymbol{b}$	body force vector, $M\,L^{-2}\,T^{-2}$
c	volumetric heat capacity, $M\,L^{-1}\,T^{-2}\,\Theta^{-1}$
c_k^i	specific heat capacity of component k in phase i, $L^2\,T^{-2}\,\Theta^{-1}$
C	auxiliary term
D	auxiliary term
D_{atm}	molecular diffusivity of water vapour in air, $L^2\,T^{-1}$
$\boldsymbol{D}^e$	elastic stiffness matrix
D_{vT}	molecular diffusivity due to temperature, $M\,L^{-1}\,T^{-1}\,\Theta^{-1}$
D_{vw}	molecular diffusivity due to moisture, $M\,L^{-2}\,T^{-1}$
E	Young's modulus, $M\,L^{-1}\,T^{-2}$
E_{Tk}^i	thermodynamic state function of component k in phase i
e	Euler's number or Napier's constant
F	yield function
f_{Tv}	thermal enhancement factor
$\boldsymbol{f}_u$	external forces vector, $M\,L^{-1}\,T^{-2}$
G	shear modulus, $M\,L^{-1}\,T^{-2}$
g	earth gravity acceleration, $L\,T^{-2}$
g_α, g_n, g_m	van Genuchten curve fitting parameters
H	Henry's volumetric coefficient of solubility
H_c	Henry's constant, $M\,L^{-1}\,T^{-2}$
h_g	gas pressure head, L
$\widehat{\boldsymbol{h}}_g$	nodal gas pressure head, L
h_w	water pressure head, L
$\widehat{\boldsymbol{h}}_w$	Nodal water pressure head, L
$\overline{\boldsymbol{j}}_k^i$	non-advective flux of component k, $M\,L^{-2}\,T^{-1}$
K	material bulk modulus, $M\,L^{-1}\,T^{-2}$
k	BBM parameter
K^g	gas phase hydraulic conductivity, $L\,T^{-1}$
K_{dry}^g	gas phase dry hydraulic conductivity, $L\,T^{-1}$
k_{dry}^g	gas phase dry intrinsic permeability, L^{-2}
K^l	liquid phase hydraulic conductivity, $L\,T^{-1}$
K_{sat}^l	liquid phase saturated hydraulic conductivity, $L\,T^{-1}$
k_{ref}^l	liquid phase reference permeability, L^{-2}
k_{sat}^l	liquid phase saturated intrinsic permeability, L^{-2}
l	length, L
L	latent heat of water vaporization, $L^2\,T^{-2}$
$\boldsymbol{M}_{ij}, \boldsymbol{K}_{ij}, \boldsymbol{f}_i$	terms being defined in [Appendix B](#)
$\boldsymbol{M}$	material stiffness matrix
M	slope of critical state line
M_a	molar mass of dry air, $M\,mol^{-1}$
M_w	molar mass of vapour, $M\,mol^{-1}$
$\boldsymbol{m}$	auxiliary vector, $\{1, 1, 1, 0, 0, 0\}$
$\boldsymbol{N}_a$	basis function
$\boldsymbol{N}_b$	shape function
$\boldsymbol{n}$	normal vector
n	porosity
n_{ref}	reference porosity
P_{atm}	atmospheric pressure, $M\,L^{-1}\,T^{-2}$
P_g	total gas pressure, $M\,L^{-1}\,T^{-2}$
P_l	liquid pressure, $M\,L^{-1}\,T^{-2}$
P_v	vapour partial pressure, $M\,L^{-1}\,T^{-2}$
p_o	isotropic preconsolidation pressure, $M\,L^{-1}\,T^{-2}$
p	mean net pressure, $M\,L^{-1}\,T^{-2}$
p_{ref}^o	reference mean pressure, $M\,L^{-1}\,T^{-2}$
p_o^*	saturated isotropic preconsolidation pressure at reference temperature, $M\,L^{-1}\,T^{-2}$

p_{oi}^*	saturated isotropic preconsolidation at the beginning of loading step i, $M\,L^{-1}\,T^{-2}$
p_{oT}^*	saturated isotropic preconsolidation pressure at temperature T, $M\,L^{-1}\,T^{-2}$
p^c	reference pressure in BBM
p_w	water pressure, $M\,L^{-1}\,T^{-2}$
p_{wo}	reference water pressure, $M\,L^{-1}\,T^{-2}$
Q	plastic potential function
Q_k^i	sink/source term of component k, $M\,L^{-3}\,T^{-1}$
$\boldsymbol{q}$	Darcy velocity, $L\,T^{-1}$
$\widehat{\boldsymbol{q}}$	boundary flux vector
q	deviatoric stress, $M\,L^{-1}\,T^{-2}$
$\boldsymbol{q}_h$	total heat flux, $M\,T^{-3}$
q_{inf}	infiltration rate, $L\,T^{-1}$
$\boldsymbol{q}^T$	conductive heat flux, $M\,T^{-3}$
$\boldsymbol{R}$	residuals matrix
R	universal gas constant, $M\,L^2\,T^{-2}\,\Theta^{-1}mol^{-1}$
RH	relative humidity
r	BBM parameter
S	degree of saturation
S_{dry}^g	gas degree of saturation at completely dry system
S_{res}^g	gas degree of saturation at the residual state
S_{abs}^l	absorbed portion of degree of saturation
S_{res}^l	degree of saturation at the residual state
S_{sat}^l	degree of saturation at full saturation
s	suction, $M\,L^{-1}\,T^{-2}$
T	absolute temperature, Θ
T_o	reference absolute temperature, Θ
T_{ref}	temperature equals to 273.16 K, Θ
$\widehat{\boldsymbol{T}}$	Nodal temperature, Θ
$\overline{T}$	average temperature, Θ
$\boldsymbol{t}$	boundary traction vector, $M\,L^{-2}\,T^{-2}$
t	time, T
$\mathrm{tr}()$	trace operator
$\widehat{\boldsymbol{u}}$	Nodal displacements, L
$\boldsymbol{u}$	solid matrix displacement vector, L
υ	specific volume
$\boldsymbol{v}^i$	velocity of phase i, $L\,T^{-1}$
v_v	Mass flow factor
$\boldsymbol{X}$	storage for system unknowns
z	vertical position, L

Greek

α	BBM non-associate plasticity coefficient
α_o, α_2	elastic thermal strain parameters
α_1, α_3	parameters control thermal effects on preconsolidation pressure
α_κ	parameter controls κ value
$\alpha_{\kappa s1}, \alpha_{\kappa s2}$	parameters control κ_s value
α_{swell}	material hydraulic parameter
β_{sp}	coefficient of solid particles compressibility, $M^{-1}\,L\,T^2$
β_{sT}	coefficient of volumetric thermal expansion of solid particles, Θ^{-1}
β_{wp}	coefficient of water compressibility, $M^{-1}\,L\,T^2$
β_{wT}	coefficient of volumetric thermal expansion of water, Θ^{-1}
β	BBM parameter, $M^{-1}\,L\,T^2$
Δ	increment
$\boldsymbol{\varepsilon}$	strain vector
$\dot{\varepsilon}_e$	total elastic strain rate vector
$\dot{\varepsilon}_e^s$	elastic strain rate due to suction
$\dot{\boldsymbol{\varepsilon}}_e^\sigma$	elastic strain rate due to net stress vector
$\dot{\varepsilon}_e^T$	elastic strain rate due to temperature
$\dot{\boldsymbol{\varepsilon}}_p$	plastic strain rate vector