Introduction of a thermodynamically hyperelastic model for peat

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ABSTRACT: Peat is a complex geomaterial having extremely high water content, low shear strength and undergoes large deformations under loading. Based on the volume fraction concept, this paper presents a basic hyperelastic biphasic material model for saturated amorphous (fully decomposed) peat. It has been a common practice to study hydraulic (volumetric) and mechanical (deviatoric) processes separately, although this division is artificial and disregards the complete stress-deformation response of a soil. The present study presents a hyperelastic model implemented within a thermodynamically consistent approach of coupled hydraulic and mechanical processes, thereby eliminating associated artificial separation errors. This phenomenological material model has been implemented in *ABAQUS* using the user subroutine UMAT. In order to adequately capture the complex geomechanical behaviour of peat, future work should include the addition of viscoelasticity, creep, structural anisotropy and (when extending to larger strains) plasticity to the basic hyperelastic model presented.

1 INTRODUCTION

Peat is composed of the remains of dead plant vegetation that has accumulated under waterlogged conditions. Depending on its degree of humification, peat can occur as fibrous (least decomposed) to amorphous (completely decomposed) material. Peat deposits have been considered as geotechnically problematic on account of their low shear strength and very high compressibility (O'Kelly & Pichan 2013). At present, predictions of the geotechnical behaviour of peat for design practice are mostly based on constitutive theories developed for fine-grained mineral soils. Some specific models have been developed for soft clay and peat, such as isotache models (den Haan 1996) for simulating the one-dimensional (1D) creep behaviour of amorphous peat and the two-level microstructure rheological model (Berry & Poskitt 1972) for 1D consolidation of fibrous peat. In the early studies of constitutive modelling of soft soils, only 1D consolidation/compression conditions were considered (Zhang & O'Kelly 2013). Many conventional models (e.g. the C_α/C_c concept after Mesri & Castro (1987)) for the constitutive modelling of peat do not consider the material's micro-mechanism assumptions of consolidation/compression. Using computer-aided techniques, general models for three-dimensional (3D) analysis can be directly developed and applied in design practice. Constitutive laws developed from routine curve-fit modelling approaches in soil mechanics are not in the differential form. Hence it is not convenient to directly extend such relations from 1D to 3D. Also, such constitutive laws may violate some axioms. For instance, with Drucker's Stability postulation (Drucker 1951), a frictional material with associated flow is not frictional at all and dissipates no work plastically. Furthermore, the stored plastic work in the modified Cam-clay model is ignored in the energy equation, which is not consistent with the yield function and flow rule. The artificial separation between hydraulic (volumetric) and mechanical (deviatoric) behaviour is also not realistic for soils.

This paper introduces a thermodynamical framework of (nonlinear) hyperelastic modelling for peat. The thermodynamical approach has been used previously in a geotechnical context for sands (Zhao 2011) and clays (Collins & Kelly 2002), but not for peat or other highly organic soil materials. This phenomenologically model is a coupled mechanical and hydraulic model developed in 3D form and obeys the thermodynamic laws. Using the thermodynamical approach, micro-mechanical assumptions can be taken into consideration.

2 VOLUME FRACTION CONCEPT

The peat material is assumed a biphasic material composed of a porous organic solid structure (solid matrix) that is fully saturated with pore water. Note, in practice, peat is often not fully saturated, even below the standing groundwater table, on account of biogas generated from the humification process (O'Kelly & Pichan 2014). In the model, the peat's solid matrix and pore water are considered to be intrinsically immiscible and incompressible. Some researchers (e.g. Boylan, Jennings, & Long (2008)) claim the likely compressibility of the organic solids. The possible error introduced by this incompressibility assumption is trivial as the solid volume fraction of peat is small on account of its extreme high water content, ranging from a few hundred per cent of dry mass to greater than 2000% (Hobbs 1986). In considering similarities between the high water content and porous structure of peat materials with those of some bio-tissues, this research adopts a hyperelastic biomechanical model developed for articular cartilage (Nagel & Kelly 2012) in modelling peat. Additionally, in geotechnical engineering, Houlsby & Puzrin (2006) claim that a hyperelastic model is preferred in modelling the elastic behaviour of soils citing the following reasons:

1. The hyperelastic model has the simplest form, requiring only the definition of a scalar function for its complete specification, as compared with elastic and hypoelastic models which require second- and fourth-order tensor functions respectively.

2. With regards to the Laws of Thermodynamics, it is quite possible to specify an elastic or hypoelastic material into a hyperelastic model. However, for a closed cycle of stress or strain (i.e. work done is zero), such material creates or destroys energy in each cycle, contradicting the First Law of Thermodynamics. Also, for some elastic and hypoelastic materials, a closed cycle of stress does not necessarily result in a closed cycle of strain, contradicting the notion of elasticity.

In the present paper, the hyperelastic model with coupled hydraulic and mechanical processes is proposed for amorphous peat. From initial work, the basic isotropic material model is introduced upon which more complex behaviour (e.g. structural anisotropy, creep etc.) can be added at a later stage.

In order to utilize the constitutive laws of continuum mechanics, the porous structure of the peat is considered as 'smeared' over the solid and fluid phases. The underlying microstructure is averaged onto a macroscopic description since the exact pore geometry is generally unknown, local contact conditions between phases are complicated and one is usually not interested in fluid flow in every single pore. The considered domain is defined by the solid constituent. The solid and fluid constituents simultaneously presents in every point. The volume fraction concept (de Boer 2005) is used and assumes that the porous solid always models a control space and only the fluid contained in the pores can leave the control space. Using elements of the Theory of Mixtures restricted by the volume fraction concept, the porous media is modelled with a macroscopic body, where neither a geometrical interpretation of the poro-structure nor the exact location of the individual components of the body (in the present case, organic solids and pore water) is considered.

We proceed from the fact that the porous structure of the saturated material occupying the control space of the porous solid B_S, with the boundary ∂B_S in the $actual\ placement$, consists of constituents α, with real volumes v^α; where the index α denotes the solid (S) and pore water (F) constituents. The boundary ∂B_S is a material surface for the solid phase and a non-material surface for the pore water phase. The concept of volume fractions can be formulated as:

$$\varphi^\alpha(x,t) = \frac{dv^\alpha}{dv} \tag{1}$$

where x is the position vector of the actual placement and t the corresponding time. The volume fractions φ^α in Eq.1 satisfy the volume fraction condition for the two constituents φ^S and φ^F as:

$$\varphi^S + \varphi^F = 1 \tag{2}$$

where φ^F is the porosity. The relationship between the real density $\rho^{\alpha R}(x,t)$ and partial density $\rho^\alpha(x,t)$ (i.e. mass of the α constituent divided by its actual volume and control volume respectively) can be obtained as:

$$\rho^\alpha(x,t) = \varphi^\alpha(x,t)\rho^{\alpha R}(x,t) \tag{3}$$

Based on the volume fraction concept, all geometric and physical quantities (e.g. motion, deformation and stress) are defined in the entire control space, and thus they can be interpreted as the statistical average values of the real quantities.

3 PRINCIPLES OF THERMODYNAMICS

The constitutive framework introduced in this paper obeys the First and Second Laws of Thermodynamics. The First Law of Thermodynamics (conservation of energy principle) states that energy can neither be created nor destroyed during a process; it can only be transformed from one state to another. The second law clarifies the direction of energy transfer and makes a statement on the reversibility of processes. From the laws of thermodynamics, the balance principles (i.e. balance of mass, balance of momentum and moment of momentum, and balance of energy) have to be satisfied for each constituent

φ^α in consideration of all interactions with external agencies.

Houlsby & Puzrin (2006) stated that constitutive models which violate thermodynamics cannot be used with any confidence in describing material behaviour unless under some rather particular and well-defined conditions. The main advantage of embedding constitutive models in a thermodynamical framework is that they cannot produce thermodynamically unreasonable results. The framework makes considerable use of potential functions that are closely related to variational and extremum principles (Houlsby & Puzrin 2006). The thermodynamical approach also allows a number of competing models to be cast within a single framework, and so enables them to be more readily compared.

4 ISOTROPIC HYPERELASTIC MODEL

For saturated soils, the total mixture stress is equal to the sum of the total solid stress and the total pore water stress. It is generally accepted that the principle of effective stress, originally developed for mineral soils, also applies to peat materials. This was experimentally confirmed for fibrous and amorphous *Sphagnum* peat material by Zhang & O'Kelly (2014). Based on the principle of effective stress and considering the volume factions φ^S and φ^F, the total stress of constituent α can be decomposed as:

$$\begin{aligned}\boldsymbol{\sigma} &= \boldsymbol{\sigma}_S + \boldsymbol{\sigma}_F \\ &= \boldsymbol{\sigma}_S^E - p\varphi_S \boldsymbol{I} - p\varphi_F \boldsymbol{I} \\ &= \boldsymbol{\sigma}_S^E - p\boldsymbol{I}\end{aligned} \tag{4}$$

where p is the pore water pressure, $\boldsymbol{I}$ is the second-order unit tensor, and $\boldsymbol{\sigma}_S^E$ is the effective stress acting in the soil skeleton for which we provide a hyperelastic model.

In hyperelasticity, Cauchy stress can be derived from a Helmholtz free-energy function $\psi(\boldsymbol{C})$ by:

$$\boldsymbol{\sigma} = \frac{2}{J}\boldsymbol{F}\frac{\partial\psi(\boldsymbol{C})}{\partial\boldsymbol{C}}\boldsymbol{F}^T \tag{5}$$

where the deformation gradient $\boldsymbol{F}$ has been used to define the right Cauchy-Green tensor $\boldsymbol{C} = \boldsymbol{F}^T\boldsymbol{F}$, $\boldsymbol{F}^T$ is the transpose of $\boldsymbol{F}$, with the volume ratio $J = det\boldsymbol{F}$.

Due to its porous nature, the solid matrix is compressible in its bulk properties with respect to the mixture, although the solid phase and the pore fluid are modelled as intrinsically incompressible. For constitutive modelling of the solid matrix of peat, this paper proposes a hyperelastic model incorporating a Neo-Hookean material law, originally developed for bio-tissues (Nagel & Kelly 2012). As the Cauchy stress is not work conjugate to any convenient deformation measure, the second Piola-Kirchhoff stress is adopted as the stress measure. The relation between the Cauchy stress $\boldsymbol{\sigma}$ and the second Piola-Kirchhoff stress $\boldsymbol{T}$ is given by:

$$\boldsymbol{T} = \boldsymbol{F}^{-1}J\boldsymbol{\sigma}\boldsymbol{F}^{-T} \tag{6}$$

where $\boldsymbol{F}^{-1}$ is the inverse of the deformation gradient and $\boldsymbol{F}^{-T}$ is its transpose. Thus the second Piola-Kirchhoff stress can be derived from the Helmholtz free-energy function as:

$$\boldsymbol{T} = 2\frac{\partial\psi(\boldsymbol{C})}{\partial\boldsymbol{C}} \tag{7}$$

Any isotropic tensor function can be expressed in terms of the principal invariants of its argument. The free Helmholtz energy density function can therefore be written as:

$$\psi = \psi(I_1(\boldsymbol{C}), I_2(\boldsymbol{C}), I_3(\boldsymbol{C})) \tag{8}$$

where the principal invariants of the right Cauchy Green tensor are given by:

$$\begin{aligned}I_1(\boldsymbol{C}) &= \boldsymbol{C} : \boldsymbol{I} \\ I_2(\boldsymbol{C}) &= \frac{1}{2}[(\boldsymbol{C} : \boldsymbol{I})^2 - \boldsymbol{C}\boldsymbol{C} : \boldsymbol{I}] \\ I_3(\boldsymbol{C}) &= det\boldsymbol{C} = J^2\end{aligned} \tag{9}$$

Applying the chain rule of partial differentiation to Eq. 7 gives:

$$\boldsymbol{T} = 2\sum_{i=1}^{3}\frac{\partial\psi}{\partial I_i}\frac{\partial I_i}{\partial\boldsymbol{C}} \tag{10}$$

To reduce the number of material parameters (in this instance, the threestress invariants) and limit model complexity, a formulation independent of the second invariant was chosen. The partial derivatives of I_1 and I_3 with respect to $\boldsymbol{C}$ are given by:

$$\frac{\partial I_1}{\partial\boldsymbol{C}} = \boldsymbol{I} \qquad and \qquad \frac{\partial I_3}{\partial\boldsymbol{C}} = (det\boldsymbol{C})\boldsymbol{C}^{-1} \tag{11}$$

so that, from Eq. 10, we get:

$$\boldsymbol{T} = 2\frac{\partial\psi}{\partial I_1}\boldsymbol{I} + 2\frac{\partial\psi}{\partial I_3}I_3\boldsymbol{C}^{-1} \tag{12}$$

With respect to the Neo-Hookean material model developed for cartilage (Nagel & Kelly 2012), and proposed in this paper for modelling amorphous peat material, the coupled hydraulic and mechanical strain energy function, ψ_{iso}, can be expressed in terms of the principal invariants I_1 and I_3 of the right Cauchy-Green tensor as:

$$\psi_{iso} = C_{10}(I_1 - lnI_3 - 3) + D_2(lnI_3)^2 \tag{13}$$

where C_{10} and D_2 are material parameters. C_{10} couples the mechanical and hydraulic behaviours whereas D_2 only considers hydraulic behaviour. At small strains, these parameters are related to the linear-elastic Young's modulus, E, and Poisson's ratio, ν, by:

$$C_{10} = \frac{E}{4(1+\nu)}; \qquad D_2 = \frac{C_{10}\nu}{2(1-2\nu)} \tag{14}$$

5 NUMERICAL IMPLEMENTATION

The material model presented above has been implemented using the commercial software *ABAQUS*. Pre-processing of the model is performed in *ABAQUS* CAE, with the coupled hydraulic and mechanical material model coded as a UMAT user material subroutine in $Fortran$. A total Lagrangian description for a mixed $u - p$ formulation (where u is the solid matrix deformation and p is the pore water pressure) has been implemented.

At the time of writing this paper, the coded hyperelastic model is being validated against data from triaxial compression tests on amorphous peat (Zhang & O'Kelly 2014), using an axisymmetric model in simulating the test conditions (Fig. 1). An all-around confining pressure σ_3 is applied to simulate the effective confining pressure. The top surface of the test specimen is loaded axially via a rigid platen having zero contact friction. The deviator stress is obtained from the reaction force generated between the platen and the top of the specimen.

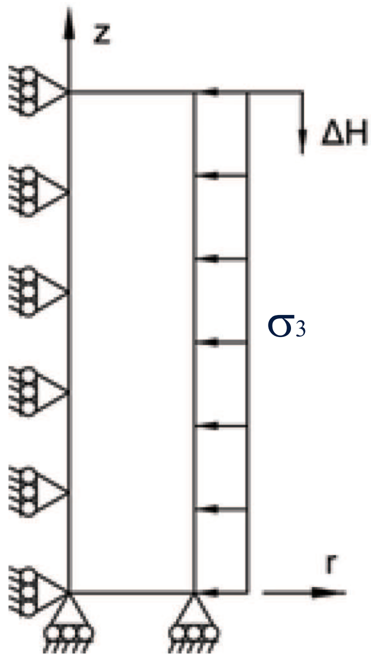

Figure 1: Triaxial Compression

6 CONCLUSIONS AND RECOMMENDATIONS

Peat soils are complex geomaterials having extremely high water content (void ratio), low shear strength, undergoing large deformations under loading. Fibrous peat has significant structural anisotropy and its constituent organic solids are themselves compressible. Under such circumstances, it is difficult to build a constitutive model that adequately capture all of these significant features.

As a starting point towards a new approach for modelling peat, this paper has presented a thermodynamically consistent hyperelastic model adopted from the biomechanical field, drawing analogies between the properties and behaviour of peat and some bio-tissues. Due to the complexity of the nature of peat, further features (e.g. viscoelasticity, creep, structural anisotropy and plasticity when extending to larger strains) should be added to the isotropic hyperelastic model presented in the paper.

It is worth noting that the application of the hyperelastic model, like any elastic form, is strictly only valid within the material's 'elastic region'. However, in the case of peat, it is particularly difficult to separate the viscoelastic and elastic responses for peat in compression and to define the extent of the elastic region. This can lead to under/over-estimations of the elastic parameter values determined from experimental data for numerical simulations. Although outside the scope of this paper, fundamental studies of the micro-mechanisms of peat consolidation/compression are necessary in order to gain a better understanding of the physical meaning of the parameters used in elastic/plastic models for peat. Since the hyperelastic model does not consider soil hardening during compression, deformation paths towards failure cannot be approached. In order to simulate stress paths towards failure, (more) realistic formulations of yield functions, flow rules and hardening rules should be developed specifically for peat.

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