Numerical study of damage in unsaturated bentonite with θ-stock finite element code

Étude numérique d'endommagement pour les milieux poreux non saturés avec le code des éléments finis θ-stock

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ABSTRACT: A coupled thermohydromechanical damage model of Arson and Gatmiri (THHMD model) in an unsaturated quasi-brittel rock mass is briefly indicated in this paper. The model is based on the use of independent state variables (net stress, suction, and thermal stress). The approach has been mixed thermodynamic and micromechanical theories. The stress-strain thermodynamic relations have been derived from the free energy, which has been written as the sum of damaged elastic deformation energies and of residual strain potentials; moreover, the damage rigidities have been computed by applying the Principal of Equivalent Elastic Energy for each stress state variable. Damage has been assumed to have an isotropic influence on air and heat flows, through the inelastic component of volumetric strains. The influence of damage on liquid water and vapor transfers has been accounted for by introducing internal length parameters, related to specific damage-induced intrinsic conductivities. The THHMD model has been implemented in θ-Stock Finite Element code. A numerical study is conducted on the impact of the thermal loading on the response of the unsaturated bentonite.

RÉSUMÉ : un modèle d'endommagement introduit par Arson et Gatmiri (THHMD model) pour un milieu non saturé fragile est brièvement présenté dans cet article. Ce modèle est développé en utilisant des variables d'état indépendants et en combinant les approches thermodynamique et micromécanique. La relation de déformation-contrainte a été obtenue en dérivant l'énergie libre qui a été considéré comme la somme de l'énergie de déformation élastique endommagée et le potentiel de déformation résiduelle. La rigidité du milieu endommagé est calculée par le principe de l'énergie équivalant élastique (PEEE). L'influence de l'endommagement sur les flux de l'air et de la chaleur est considéré isotrope. L'impact de l'endommagement sur le transfert de l'eau et de la vapeur a été introduit en utilisant les paramètres de la longueur interne qui affecte la conductivité intrinsèque endommagée. Ce modèle a été implanté dans le code des éléments finis θ-Stock. Des études numérique et paramétrique sont menées afin de clarifier les effets du chargement sur la réponse de la bentonite non saturé.

KEYWORDS: Damage, Finite element method, Poromechanics, Thermohydromechanical coupling.

1 INTRODUCTION

Damage modeling has become a crux point in the study of the Excavation Damaged Zone (EDZ) (Martino and Chandler, 2004, Mertens and Bastiaens 2004). In the context of nuclear waste storage, cracking effects have to be accounted for in the constitutive laws of non-isothermal unsaturated porous media (Gens et al. 1998). The geological barriers, often made of quasi-brittle material like granite or clay-rock, undergo damage during the excavation phase. Hydro-mechanical interaction may occur in the neighborhood of the engineered barrier, which is generally constituted of unsaturated compacted clay.

Most of the existing damage models proposed to unsaturated porous media are formulated by means of an effective stress, defined in same way as Bishop's stress (Arson and Gatmiri 2008.a). These framework are not satisfactory to represent some aspects of the behavior of unsaturated soils, like wetting collapse (Houlsby 1997, Fredlund and Morgenstern 1977). Alternatively, the THHMD model involves independent state variables (net stress, suction and thermal stress), in order to emphasize the role of suction rigidity. Waste is a heat source which can generate traction, and thus cracks. After a brief presentation of the theoretical frame in the first part of this paper, the numerical parametric study which is inspired from a laboratory test is performed in order to determine the main parameters controlling the generation of damage in THHMD model.

2 OUTLINE OF THE MODEL

2.1 *Damage representation*

It should be mentioned that in this paper, presentation of the main concepts of damage is just for help us to deduce and adapt the deductions to the theoretical concepts of damage.
In the following, the damage variable Ω will be defined as crack density tensor expressed in a principal base:

$$\Omega_{ij} = \sum_{k=1}^{3} d^k n_i^k n_j^k \tag{1}$$

Stress and damage will be assumed to have the same principal directions. Physically, the damaged behavior of the RVE is modeled by three meso-cracks representing three main families of fissures. Each meso-crack is characterized by a direction $\mathbf{n^k}$ (normal to the crack plane) and a volumetric faraction d^k.

2.2 *Phenomenological approach*

Following the modeling approach of Gatmiri (Gatmiri and Arson 2008.b), it has been assumed that thermal and capillary phenomena are isotropic. Assuming each strain contribution may encompass an elastic (e) and an inelastic (d) part leads to:

$$d\varepsilon_{ij} = (d\varepsilon_{M\,ij}^{e} + d\varepsilon_{M\,ij}^{d}) + \frac{1}{3}(d\varepsilon_{Sv}^{e} + d\varepsilon_{Sv}^{d})\delta_{ij} + \frac{1}{3}(d\varepsilon_{Tv}^{e} + d\varepsilon_{Tv}^{d})\delta_{ij} \tag{2}$$

M, S and T subscripts refer to a thermodynamic conjugation to net stress, suction and thermal stress, respectively. The free energy breakdown used by Dragon and his coworkers (Dragon et al. 2000), for damaged dry materials, is generalized and extended to multiphase media:

$$\begin{aligned}\Psi_S(\varepsilon_{M_{ij}},\varepsilon_{Sv},\varepsilon_{Tv},\Omega_{ij}) &= \frac{1}{2}\varepsilon_{M_{ij}} : D_{eijkl}(\Omega_{ij}) : \varepsilon_M + \frac{1}{2}\varepsilon_{Sv}\beta_S(\Omega_{ij})\varepsilon_{Sv} \\ &+ \frac{1}{2}\varepsilon_{Tv}\beta_T(\Omega_{ij})\varepsilon_{Tv} - g_M\Omega_{ij}\varepsilon_{Mij} - \frac{g_S}{3}\delta_{ij}\Omega_{ji}\varepsilon_{Sv} - \frac{g_T}{3}\delta_{ij}\Omega_{ji}\varepsilon_{Tv}\end{aligned} \tag{3}$$

The first three terms are the mechanical, capillary and thermal degraded elastic energies respectively. They depend respectively on damage mechanical, capillary and thermal rigidities ($\mathbf{D_e}(\Omega_{ij})$, $\beta_s(\Omega_{ij})$ and $\beta_T(\Omega_{ij})$ respectively). The second three terms are residual strain potentials, which quantify the remaining openings due to cracks after unloading. The derivation of the free energy $\psi_S(\varepsilon_{Mij},\varepsilon_{Sv},\varepsilon_{Tv},\Omega_{ij})$, provides the whole stress/strain relations. The damage stress Y_d, conjugated to damage, writes:

$$\begin{aligned}Y_{d_{ij}} &= -\frac{1}{2}\varepsilon_{M_{mn}}\frac{\partial D_{e_{nmij}}(\Omega_{kl})}{\partial\Omega_{qp}}\varepsilon_{M_{pq}} \\ &-\frac{1}{2}\varepsilon_{Sv}\frac{\partial\beta_s(\Omega_{kl})}{\partial\Omega_{ij}}\varepsilon_{Sv} - \frac{1}{2}\varepsilon_{Tv}\frac{\partial\beta_T(\Omega_{kl})}{\partial\Omega_{ij}}\varepsilon_{Tv} \\ &+ g_M\varepsilon_{M_{ij}} + \frac{g_s}{3}\varepsilon_{Sv}\delta_{ij} + \frac{g_T}{3}\varepsilon_{Tv}\delta_{ij}\end{aligned} \tag{4}$$

The damage evolution function is assumed to depend on the tensile strains that develop the skeleton. As in many models (Dragon et al. 2000, Homand-Etienne et al. 1998, Shao et al. 2005) (among others), a very simple damage evolution function is used:

$$f_d(Y_{dij},\Omega_{ij}) = \sqrt{\frac{1}{2}Y^+_{d1_{ij}}Y^+_{d1_{ij}}} - C_0 - C_1\delta_{ij}\Omega_{ji} \tag{5}$$

C_0 is the initial damage-stress rate that is necessary to trigger damage. C_1controls the damage increase rate. The damage evolution law is computed by an associative flow rule (Arson and Gatmiri, 2010).

2.3 *Micro-mechanical approach*

The elastic components of the strain tensor are determined by computing the damaged rigidities $D_{eijkl}(\Omega)$, $\beta_S(\Omega)$ and $\beta_T(\Omega)$. Damaged Stress state variables are defined (damaged net stress, damaged suction and damaged thermal stress), by using the forth-order operator of cordebois and Sidoroff (1982) (noted $M_{ijkl}(\Omega)$):

$$M_{ijkl}(\Omega)\sigma_{lk} = (\delta-\Omega)^{-1/2}_{ik}\ \sigma_{kl}(\delta-\Omega)^{-1/2}_{lj} \tag{6}$$

The Principle of Equivalent Elastic Energy is applied on the three elastic potentials $\frac{1}{2}\varepsilon_{Mji}D_{eijkl}(\Omega)\varepsilon_{Mlk}$, $\frac{1}{2}\varepsilon_{Sv}\beta_s(\Omega)\varepsilon_{Sv}$ and $\frac{1}{2}\varepsilon_{Tv}\beta_T(\Omega)\varepsilon_{Tv}$. The final expressions of the damaged rigidities are:

$$\begin{aligned}D_{eijkl}(\Omega_q) &= M_{ijnm}(\Omega)^{-1} : D^0_{emnpq} : M_{qpkl}(\Omega)^T \\ \beta_S(\Omega) &= \frac{9\beta^0_S}{[(\delta-\Omega)^{-1}_{ij}\delta_{ji}]^2} \\ \beta_T(\Omega) &= \frac{9\beta^0_T}{[(\delta-\Omega)^{-1}_{ij}\delta_{ji}]^2}\end{aligned} \tag{7}$$

D^0_{eijkl}, β^0_s and β^0_T are the mechanical, capillary and thermal rigidities in the intact state, respectively.

2.4 *Moisture Transfer laws*

The details of the modeling of isothermal transfers in porous media may be found in (Gatmiri & Arson 2008.b).

Liquid water and vapour transfers are assumed to be diffusive. Hydraulic conductivity is modeled by a second-order permeability tensor Kw_{ij} :

$$Kw_{ij} = k_T(T)k_r(S_w)K\mathrm{int}_{ij}(n,\Omega_{pq}) \tag{8}$$

Only the intrinsic water permeability $K\mathrm{int}_{ij}(n,\Omega_{pq})$, depending on porosity n, and thus on the behavior of the solid skeleton, may be influenced by damage. A specific crack related component k2ij is introduced in order to model the influence of damage on liquid water transfer:

$$K\mathrm{int}_{ij}(n,\Omega_{rs}) = k_{w0}10^{\alpha we^{rev}}\delta_{ij} + k_{2ij}(n^{frac},\Omega_{ij}) \tag{9}$$

The intrinsic permeability related to fracturing is thus a function of the crack densities, d^k:

$$k_{2ij}\left(n^{frac},\Omega\right) = \frac{\gamma_w}{12\mu_w}\pi^{-2/3}\chi^{4/3}b^2\sum_{k=1}^{3}\left(d^k\right)^{5/3}\left(\delta_{ij}-n_in_j\right) \tag{10}$$

γ_w and μ_w are the volumetric weight and the dynamic viscosity of liquid water respectively. b is the characteristic dimension of the REV and plays the role of an internal length parameter (Arson and Gatmiri, 2010).

3 NUMERICAL RESULTS OF UNSATURATED BENTONITE

3.1 *The Simulation*

The numerical simulation has been inspired by the laboratory test of Pintado (Pintado et al. 2002) , and the simulation has been performed by damage model integrated in θ-Stock Finite Element code (Gatmiri and Arson 2008b). In the Pintado laboratory test, a thermal source is installed between two cylinder-shaped bentonite samples with diameters of 38mm and heights of 76mm which are both wrapped in isolate foam. The bottom being maintained at a constant temperature (Gatmiri et al. 2010). The calculations are performed through axial symmetry. The initial saturation degree Sw0 is equal to 0.63 like in the experiment conditions. After a heating period of one week, a relaxation period of seven weeks is observed. All of the imposed boundary conditions are given in Figure 1.

3.1.1 *Discussion and results*

Here we are interested in the effects of different Van Genuchten water retention curves introducing by A to E in Figure 3, on the variation of different parameters of damage model. Table 1 represents the parameters chosen in the five water retention curves.

Figure 4 shows the damage force for specimens A to E in different times. The strains resulting from heating and drying are thus isotropic, which leads to isotropic permeability, damage and thus isotropic damage force. That is, the reason why only the radial components of permeability, damage and damage force are represented in this paper. It can be seen that there are some values showing the height of the region with damage force getting less in comparison with the previous time; further, the magnitude of damage force in a specific height decreases in comparison with the previous time.

This is because the damage is affected by different parameters: In one side, heating changes stress distribution which is the generator of damage; in the other hand, there is extraction of solid skeleton at the zones near the thermal source, and there is contraction of it at the further zones, which leads closure of openings and reducing of generated stresses. Further, the suction increase is equivalent to a compressive loading, since it diminishes damage stresses. Therefore, we can say that at first, factors generating damage forces induce cracks; afterward, in the following times damage force reduction factors beget to drop damage force which has been produced at former times.

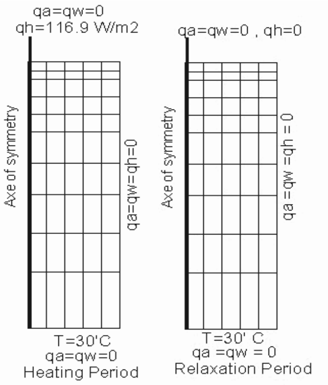

Figure 1. Bentonite heating test. Boundary conditions.

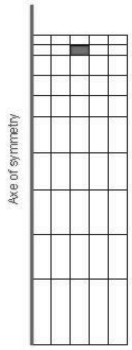

Figure 2. Element number 22

Table 1. Parameters of the five Van Genuchten water retention curves

Graph	α(VG)	n (VG)
A	1.87E+08	1.2
B	1.87E+08	1.429
C	2.87E+08	1.429
D	3.87E+08	1.429
E	3.87E+08	1.5

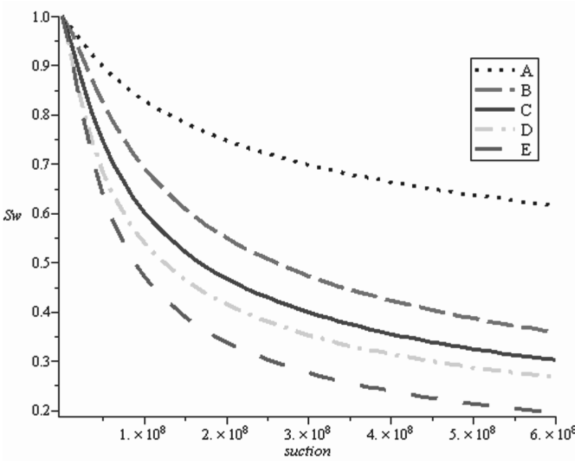

Figure 3. Five used Van Genuchten water retention curves

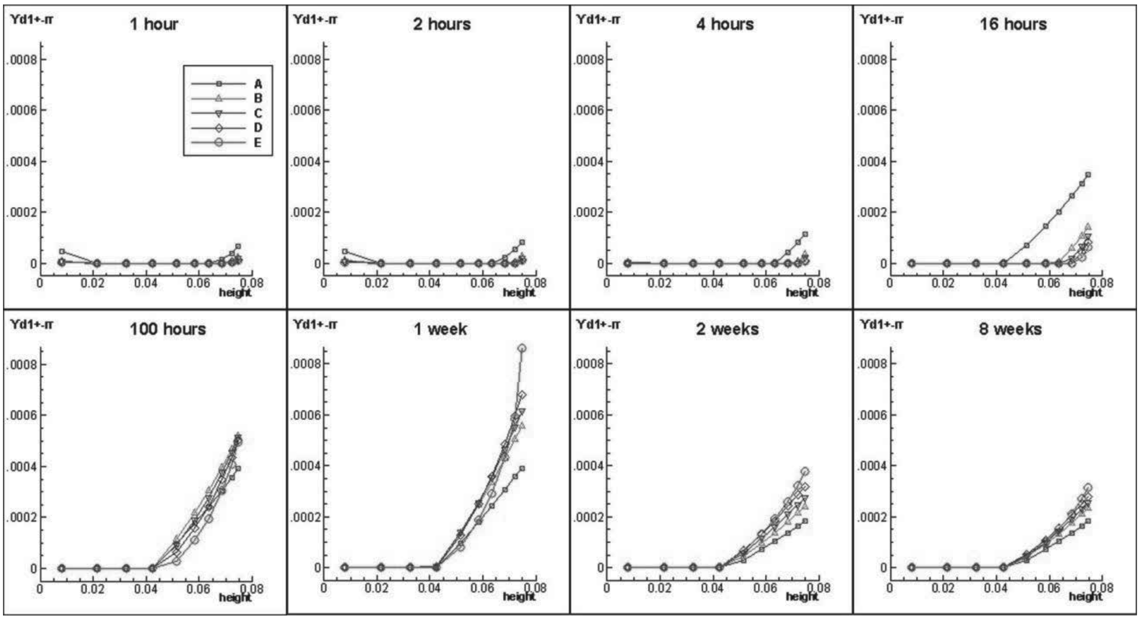

Figure 4. Evaluation of damage in all specimens at the whole testing time

Though the heat source is shut down at the time of one week, the magnitude of damage at the height of about 0.0585 to 0.0665 meters above the bottom of samples is increased at second week in comparison with one week. The increase of damage in mentioned part of the sample even after shutting down the heat source can be discuss as below: It explained before that in the loading phase, there is extraction of solid skeleton at the zones near the thermal source, and there is contraction of it at the further zones. After removing thermal loading, the distribution of temperature in all elements of upper part of sample has got relatively uniform; therefore, the zones with extraction of skeleton get smaller, also the zones with contraction of skeleton extract. The extraction of this part causes the pores get bigger and so that the crack opening rises in this part.

Figure 5, illustrates the damage parameter versus temperature for an element which is located near the heat source (element number 22 which is shown in Figure 2). The samples can be divided into two upside part and downside parts, and the trends of drying or wetting are investigated. With this strategy, during the heating period the upside part of the sample loses its water while the downside part of the sample gets wetter. At the top part of the samples, using the water retention curves shown in Figure 3, it can be concluded that specimen E has the highest amount of moisture and samples D, C, B, A, respectively get drier. Since the chosen element is in up part of the sample, according the above arguments, the specimen A is the drier sample. It can be clearly seen in Figure 5, that this sample behaves more brittle in comparison with other samples.

In order to investigate the trend of water permeability, the variation of this parameter due to saturation degree, and damage is drawn respectively in Figures 6 and 7, for an element (No.22) near the heater.

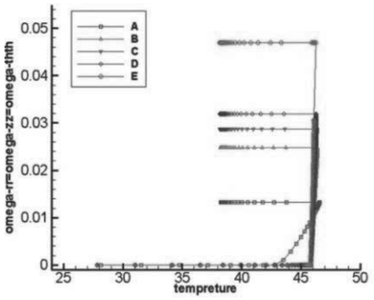

Figure 5. Variation of damage parameter respect to the temperature for all specimens for element22.

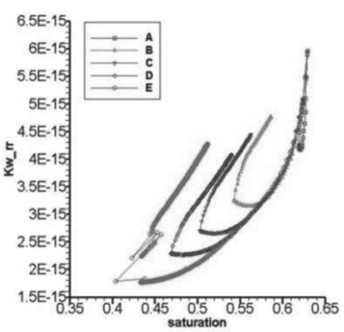

Figure 6. Variation of water permeability respect to the saturation degree for all specimens for element 22.

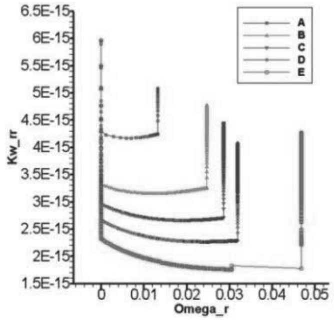

Figure 7. Variation of water permeability respect to the damage parameter for all specimens for element22.

As it shown in Figures 6 and 7 water permeability reduces from A toward E. This is why the specimens get dry from A to E. First that there is no crack in samples, and pores are in their initial size, increasing of saturation degree leads to water permeability reduction. After occurrence of cracks, pores get larger. This factor prompts to grow the permeability, but graphs trend shows that the saturation degree reduction conquers this factor. Therefore, the coupling of these two parameters causes falling trend in water permeability. After removing thermal loading, the magnitude of damage almost remains constant, while by reversing water direction in samples, saturation degree rises and therefore permeability increases.

4 CONCLUSIONS

Theoretical framework of a damage model of Arson and Gatmiri dedicated to non-isothermal unsaturated porous media and formulated in independent state variables (net stress, suction and thermal stress) is presented. The damage model has been implemented in θ-stock Finite Element code. A parametric study on initial damage is then performed to assess the influence of the Excavation Damage Zone (EDZ) on the response of the nuclear waste repository during the heating phase. Different parameters such as suction and thermal stress effect on generation of damage. It is observed that water permeability is mostly affected by the variation of saturation degree of the specimen. Overall, the trends meet the theoretical expectations.

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