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Journal

International Journal of Geomechanics, 16(6)

ISSN

1532-3641

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Publication Date

2016-12-01

DOI

10.1061/(ASCE)GM.1943-5622.0000603

Peer reviewed

**Use of a dual structure constitutive model for predicting the long-term
behavior of an expansive clay buffer in a nuclear waste repository**

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Version Accepted for Publication in

ASCE's International Journal of Geomechanics

[https://doi.org/10.1061/\(ASCE\)GM.1943-5622.0000603](https://doi.org/10.1061/(ASCE)GM.1943-5622.0000603)

Final version published as:

Vilarrasa V., Rutqvist J., Blanco-Martin L., and Birkholzer J. Use of a
dual structure constitutive model for predicting the long-term behavior
of an expansive clay buffer in a nuclear waste repository. ASCE's
International Journal of Geomechanics, 16, article number D4015005
(2016).

21ABSTRACT

22Expansive soils are suitable as backfill and buffer materials in engineered barrier systems to
23isolate high-level nuclear waste in deep geological formations. The canisters containing nuclear
24waste would be placed in tunnels excavated at several hundred meters depth. The expansive soil
25would be used for tunnel backfill and should provide enough swelling capacity to support the
26tunnel walls and thereby reduce the impact of the excavation damaged zone on permeability in
27the near-field that could affect the long-term barrier performance. In addition to their swelling
28capacity, expansive soils are characterized by accumulating irreversible strain upon suction
29cycles and by effects of microstructural swelling on water permeability that for backfill or buffer
30materials can significantly delay the time to reach full saturation. To simulate these
31characteristics of expansive soils, a dual structure constitutive model that includes two porosity
32levels is necessary. We present the formulation of the dual structure model and describe its
33implementation into a coupled fluid flow and geomechanical numerical simulator. We use the
34Barcelona Basic Model (BBM), which is an elasto-plastic constitutive model for unsaturated
35soils, to model the macrostructure, and we assume that the strains of the microstructure, which
36are volumetric and elastic, induce plastic strain to the macrostructure. We test and demonstrate
37the capabilities of the implemented dual structure model by modeling and reproducing observed
38behavior in two laboratory tests of expansive clay. As observed in the experiments, the
39simulations yield non-reversible strain accumulation upon suction cycles and a decreasing
40swelling capacity with increasing confining stress. Finally, we model, for the first time using a
41dual structure model, the long-term (100,000 years) performance of a generic high-level nuclear
42waste repository with waste emplacement in horizontal tunnels backfilled with expansive clay
43and hosted in a clay rock formation. We compare the thermo-hydro-mechanical results of the

44 dual structure model with those of the standard single structure BBM. The main difference
45 between the simulation results using the two models is that the dual structure model predicts a
46 time to fully saturate the expansive clay barrier in the order of thousands of years, while the
47 standard single structure BBM yields a time in the order of tens of years. The saturation
48 evolution of the buffer predicted by the dual structure model follows the short-term (up to 10
49 years) tendency observed in the mock-up test for the FEBEX in situ test, which gives confidence
50 of the performance of the model. These examples show that a dual structure model, like the one
51 presented here, is necessary to properly model the thermo-hydro-mechanical behavior of
52 expansive soils.

53

54 Keywords: expansive soil; engineered barrier systems; unsaturated porous media; swelling;
55 thermo-hydro-mechanical coupling.

56

57 1. INTRODUCTION

58 Expansive soils, among other applications, are suitable as backfill and buffer materials in
59 engineered barrier systems (EBS) to isolate high-level nuclear waste in deep geological
60 formations. The canisters containing nuclear waste would be placed in tunnels excavated at
61 several hundred meters depth. Potential host rocks include granite (Gens et al., 2009, Dupray et
62 al., 2013) and clay/shale formations (Gens et al., 2007; Rutqvist et al., 2014). The excavation of
63 the tunnels will damage the surrounding rock, creating an excavation damaged zone (EDZ). The
64 permeability in the EDZ may increase a few orders of magnitude (Tsang et al., 2005; Blümling et
65 al., 2007; Alonso and Hoffmann, 2007), especially in the direction of the tunnel axis (Vilarrasa et

66al., 2011). This higher transport potential within the EDZ can be minimized by backfilling the
67tunnels with an unsaturated expansive soil, which will swell when hydrated by the host rock. Not
68only can the expansive soil backfill provide enough sustaining pressure to the tunnel wall to
69avoid collapse (Rutqvist et al., 2011), but can also provide enough swelling capacity so that the
70EDZ can be sealed, i.e., a reduction of hydraulic properties, especially in clay host rocks
71(Komine and Ogata, 1994; Tsang et al., 2005; Yu et al., 2014). However, healing, which implies
72not only a decrease in permeability, but also the recovery of the initial mechanical properties, is
73not observed in laboratory and field experiments (Yu et al., 2014).

74Some field experiments, such as the full-scale engineered barriers experiment (FEBEX) (Alonso
75et al., 2005; Martinez-Landa and Carrera, 2005; Gens et al., 2009; Dupray et al., 2013), the
76HE-D in situ heating test (Gens et al., 2007) and the engineered barrier (EB) experiment (Alonso
77and Hoffmann, 2007), have been carried out to gain insight into the thermo-hydro-mechanical
78(THM) processes that occur during the heating and hydration of the EBS. The FEBEX
79experiment was performed at the Grimsel test site (Switzerland), in granite, and the HE-D and
80EB experiments at the Mont Terri site (Switzerland), in Opalinus clay. Though some analytical
81solutions, which can be very useful for probabilistic risk analysis (Tartakovsky, 2007; Jurado et
82al., 2012), have been developed to explain the processes occurring during heating/cooling and
83drying/hydration of the EBS (Chen and Ledesma, 2007), most of the studies use numerical
84models to reproduce the experiments and make long-term predictions (e.g. Gens et al., 2007;
852009; Rutqvist et al., 2008; 2014).

86Some constitutive models exist to model non-isothermal unsaturated soils (Gens, 2010), such as
87the thermo-plasticity model proposed by Laloui and Cekerevac (2003) or the Barcelona Basic
88Model (BBM) (Alonso et al., 1990). The expansive soils forming the EBS, such as bentonite or a

89mixture of sand and expansive clay, have been extensively modeled adopting the BBM (e.g.
90Gens et al., 2007; 2009; Åkesson and Kristensson, 2008; Kristensson and Åkesson, 2008;
91Rutqvist et al., 2011; 2014). Though the BBM is a very appropriate constitutive model for
92unsaturated soils because it can reproduce important features of their behavior, like collapse
93when wetting occurs at a relatively high pre-consolidation stress, it cannot model certain aspects
94of expansive soils. These aspects include accumulation of irreversible strain upon suction cycles
95(Day, 1994; Al-Homoud et al., 1995; Tripathy et al., 2002) or effects of microstructural swelling
96on water permeability. The effect of microstructural swelling on water permeability has been
97observed to have a significant effect on resaturation of expansive soil barriers, for example at the
98mock-up test performed at CIEMAT, Madrid (Spain), which reproduces a large-scale heating test
99of a bentonite buffer (Sánchez et al., 2012).

100To rigorously model these characteristics of expansive soils, it is necessary to use a dual structure
101constitutive model that acknowledges the existence of two porosity levels (Gens and Alonso,
1021992; Alonso et al., 1999; Gens et al., 2006; Sánchez et al., 2005; 2008). Expansive clays present
103a bimodal or trimodal pore size distribution (Figure 1) in which the pores having a diameter
104smaller than $0.1\ \mu\text{m}$ correspond to voids inside clay aggregates and the larger pores correspond
105to pores between clay aggregates (Dixon et al., 1999; Villar, 1999; Delage et al., 2006; Wang et
106al., 2013b). This leads to the differentiation of a microstructure, which is made of the active clay
107minerals, and a macrostructure, which is formed by the global distribution of clay aggregates and
108the macropores between them (Figure 2).

109Fluids can flow solely through the macroporosity (Wang et al., 2013a). As the liquid saturation
110degree of the clay increases (suction decreases), water layers are inserted between the
111microstructure clay layers and thus swelling occurs because the volume of clay particles

112increases (Saiyouri et al., 2000). This causes the microporosity to invade the macroporosity as
113the expansive soil hydrates, which may reduce its permeability by several orders of magnitude
114(Olivella and Gens, 2000; Alonso and Hoffmann, 2007). This permeability reduction as the
115liquid saturation degree increases can explain delays in the saturation time that have been
116observed at both mock-up and in situ experiments involving expansive soil barriers (Sánchez et
117al., 2012). Therefore, the use of a dual structure constitutive model is required to properly
118simulate the THM behavior of expansive soils used as buffer material to backfill the space
119between the canisters containing nuclear waste and the tunnel walls.

120The aims of this paper are to present the dual structure model that has been implemented in the
121TOUGH-FLAC simulator (Rutqvist et al., 2011) and to analyze the differences in the long-term
122performance of a generic nuclear waste repository in a clay host rock when modeling the
123expansive soil backfill either with the standard single structure BBM or the dual structure model.
124To do so, we first present the mathematical formulation of the dual structure model. Then, we
125show the capabilities of the model by reproducing a laboratory test in which irreversible
126expansion accumulates upon suction cycles. Finally, we model the long-term THM response of a
127generic repository for geological disposal of high-level nuclear waste adopting either the
128standard single structure BBM or the dual structure model as a constitutive model for the
129expansive soil. Such long-term simulation, of 100,000 years, is novel and will permit shedding
130light on the long-term performance of the expansive clay that constitutes the buffer using the
131dual structure constitutive model.

132

133 **2. DUAL STRUCTURE MODEL IMPLEMENTATION IN TOUGH-FLAC**

In this section, the development and implementation of a dual structure model for expansive soils into TOUGH-FLAC is presented. First, an overview of the basic equations in the dual structure model following (in part) the developments by Alonso et al. (1999) and Sánchez et al. (2005) is presented. Finally, the implementation of this model into TOUGH-FLAC is summarized.

2.1. *The dual structure approach*

The dual structure model considers the existence of a macrostructure, a microstructure and the interactions between them. The macrostructure can be modeled with a constitutive model for unsaturated soils, such as the BBM. The BBM is able to describe many typical features of the mechanical behavior of unsaturated soils, including wetting-induced swelling or collapse strains (depending on the magnitude of the applied stress), as well as the increase in shear strength and apparent pre-consolidation stress with suction (Gens et al., 2006). The extension of BBM to a dual structure model enables simulating the behavior of expansive soils, such as the dependency of swelling strains and swelling pressures on the initial stress state and on the stress path, strain accumulation upon suction cycles and secondary swelling. It is believed that such behavioral features are mainly related to the existence of coupled chemical-hydrogeological-mechanical phenomena between distinct levels of structure within the material (Alonso et al., 1999).

Conceptually, in a dual structure model, as described by Alonso et al. (1999) and Sánchez et al.

(2005), the total volume, V , of the material consists of the solid phase, V_s , the microstructural

voids V_{vm} , and the macrostructure voids V_{vM}

$$V = V_s + V_{vm} + V_{vM} = V_m + V_{vM}, \quad (1)$$

154 where V_m is the volume of the microstructure.

155 Additionally, the total void ratio, e , and porosity, φ , are the sum of their microstructural and
156 macrostructural components according to

157
$$e = \frac{V_v}{V_s} = \frac{V_{vM}}{V_s} + \frac{V_{vm}}{V_s} = e_M + e_m, \quad (2)$$

158
$$\varphi = \frac{V_v}{V} = \frac{V_{vM}}{V} + \frac{V_{vm}}{V} = \varphi_M + \varphi_m, \quad (3)$$

159 where V_v is the total volume of voids and the subscripts m and M refer to the microstructure
160 and the macrostructure, respectively.

161 The microstructure can swell to invade the macroporosity, depending on the mechanical
162 confinement and load level. This is relevant when considering permeability changes during the
163 expansive soil swelling, because fluid flow takes place through the macroporosity, which is not
164 proportional to the total strain and deformation of the expansive soil.

165 2.2. Macrostructural level

166 The macrostructural behavior is modeled based on the BBM, in which the yield surface is
167 defined in the $p - q - s$ space, where p is net mean stress (i.e., total stress minus gas-phase
168 pressure), q is deviatoric stress (or shear stress), and s is suction (i.e., gas pressure minus liquid
169 pressure). The size of the elastic domain increases as suction increases. This is shown in Figure 3

in the isotropic stress (s - p space) plane. The rate of the increase of the elastic domain, represented by the loading-collapse (LC) curve, is one of the fundamental characteristics of the BBM (Gens et al., 2006).

The suction-dependent loading-collapse (LC) yield surface bounds the elastic region according to

$$f_{LC} = \frac{q^2}{g_y(\theta)^2} - \frac{M^2}{g_y(\theta=0)^2} (p + p_s)(p_0 - p) = 0 \quad (4)$$

where θ is the Lode angle, the function $g_y(\theta)$ describes the shape of the yield surface in the

deviatoric plane, M is the constant slope of the critical state line, $p_s = k_s s$ represents the

increase in cohesion with suction, k_s is an empirical material constant and function

$$p_0 = p^c \left[\frac{p_0^*}{p^c} \right]^{\frac{[\lambda_{PB0} - \kappa_{PB0}]}{[\lambda_{PB} - \kappa_{PB0}]}} \quad (5)$$

is the net mean yield stress (or apparent pre-consolidation stress) at current suction, where p_0^* is

the net mean yield stress (or pre-consolidation stress) at full saturation, p^c is a reference stress,

λ_{ps0} is a compressibility parameter in virgin soil states at zero suction,

183 $\lambda_{ps} = \lambda_{ps0} [(1 - r) \exp(-\xi s) + r]$ is a compressibility parameter in virgin soil states at suction s , r

184 is a constant related to the maximum stiffness of the soil (for an infinite suction), ξ is a

185 parameter that controls the rate of increase of soil stiffness with suction and K_{ps0} is the elastic

186 stiffness parameter for changes in net mean stress at zero suction.

187 The flow rule is given by

188 (6)

$$g_{LC} = \frac{\alpha_a q^2}{g_y(\theta)^2} - \frac{M^2}{g_y(\theta=0)^2} (p + p_s)(p_0 - p)$$

189 where α_a is a parameter that gives rise to a non-associative model, i.e., $g_{LC} \neq f_{LC}$.

190 2.3. *Microstructural level*

191 The following assumptions are adopted related to microstructural behavior and its interaction
192 with the macrostructure:

- 193 • The microstructure is mainly saturated and the effective stress concept holds
- 194 • The microstructural behavior is elastic and volumetric
- 195 • Mechanical, hydraulic, and chemical equilibrium exists between microstructure and
196 macrostructure
- 197 • Coupling between microstructure and macrostructure results in a possible buildup of
198 macrostructural elastoplastic strains when elastic microstructural strains occur

199 With these assumptions, the volumetric microstructural strain, $d\varepsilon_{vm}^e$, depends exclusively on
 200 variations of mean effective stress,

$$201 \quad d\hat{p} = d(\bar{p} - p_l) = d(\bar{p} - p_g + p_g - p_l) = d(p + s), \quad (7)$$

202 where $\bar{p}$ is mean stress, p_l is liquid phase pressure and p_g is gas phase pressure. Therefore, a

203 straight line $p + s = \text{constant}$ can be drawn in the p - s space around the current state of stress and

204 suction along which no microstructural strain takes place (Figure 3). This line, called the Neutral
 205 Line (NL), moves with the current stress state (C) and separates at each instant the zone of

206 microstructural swelling from the zone of microstructural shrinkage in the p - s plane (Figure
 207 3).

208 **2.4. Interaction between structural levels**

209 Microstructural swelling/shrinkage affects the structural arrangement of the macrostructure,
 210 inducing irreversible strains in the macroporosity. These irreversible macrostructural
 211 deformations induced by microstructural effects are considered proportional to the
 212 microstructural strain through interaction functions as

$$213 \quad d\varepsilon_{v\beta}^p = f d\varepsilon_{vm}^e \quad (8)$$

214 where $\varepsilon_{v\beta}^p$ is the macrostructural plastic strain arising from the interaction between both

215 structures. Two interaction functions are defined: $f = f_c$ for microstructural compression or

216 shrinkage paths and $f = f_s$ for microstructural swelling paths. These functions can adopt several

217 forms (Sánchez et al., 2005), but they always depend on the ratio p/p_0

$$218 \quad f_c = f_{c0} + f_{c1} (p/p_0)^{n_c} \quad \text{and} \quad f_s = f_{s0} + f_{s1} (1 - p/p_0)^{n_s}, \quad (9a)$$

219 or

$$220 \quad f_c = f_{c0} + f_{c1} \tanh[f_{c2} (p/p_0 - f_{c3})] \quad \text{and} \quad f_s = f_{s0} - f_{s1} \tanh[f_{s2} (p/p_0 - f_{s3})], \quad (9b)$$

221 where f_{ij} and n_i ($i = c, s$) and $j = 0, 1, 2, 3$) are constants.

222 The ratio p/p_0 is a measure of the distance from the current stress state to the yield locus for the

223 macrostructure LC and has the same meaning as the overconsolidation ratio for an isotropically

224 consolidated soil. A low p/p_0 implies a dense packing of the material. Under such dense

225 packing (dense macrostructure), the microstructural swelling strongly affects the global

226 arrangement of clay aggregates, which becomes more open. This results in a softening of the

227 macrostructure, which implies that the macrostructural yield surface LC shrinks. Under this

condition, expansion accumulates upon suction cycles. On the other hand, a high p/p_0 implies a looser macrostructure. Under such loose packing conditions, the microstructural swelling produces an invasion of the macropores, which tends to close the macrostructure and compression accumulates upon suction cycles. In such a case, the elastic domain increases and LC expands (Alonso et al. 1999; Sánchez et al., 2005).

2.5. Elastic Strain

Equivalently to the BBM model, the macrostructural volumetric elastic strain increment for the dual structure model is associated with changes in net mean stress dp and suction ds (Alonso et al., 1999)

$$d\varepsilon_{vM}^e = \frac{1}{K_M} dp + \frac{1}{K_s} ds, \quad (10)$$

where K_M is the macrostructural bulk modulus and K_s is the macrostructural modulus

associated with suction strain. K_M and K_s are defined as

$$K_M = \frac{(1+e_M)p}{\kappa_{ps}(s)}, \quad (11)$$

$$K_s = \frac{(1+e_M)(s+p_{atm})}{\kappa_{sp}(p,s)} \quad (12)$$

242 where $\kappa_{ps} = \kappa_{ps0} (1 + s \alpha_{ps})$, $\kappa_{sp} = \kappa_{sp0} (1 + \alpha_{sp} \ln(p / p_{ref})) \exp(\alpha_{ss} s)$ and κ_{ps0} and κ_{sp0} are

243 compressibility parameters for changes in net mean stress and suction, respectively. p_{ref} is a

244 reference stress state for relating elastic compressibility to suction and α_{ps} , α_{sp} and α_{ss} are

245 empirical parameters.

246 The microstructural volumetric strain depends on the change in the microstructural effective

247 stress

$$248 \quad d\varepsilon_{vm}^e = \frac{1}{K_m} d\hat{p}, \quad (13)$$

249 where K_m is the microstructural bulk modulus for changes in mean effective stress. Alonso et al.

250 (1999) define two alternative expressions for the microstructural modulus

$$251 \quad K_m = \frac{(1 + e_m) \hat{p}}{\kappa_m}, \quad (14a)$$

$$252 \quad K_m = \frac{e^{\alpha_m \hat{p}}}{\beta_m}, \quad (14b)$$

253 where κ_m , α_m and β_m are compressibility parameters.

254 Thermal strains are purely volumetric

$$d\varepsilon_v^T = (\alpha_0 + 2\alpha_2 \Delta T) dT, \quad (15)$$

where α_0 and α_2 are material parameters corresponding to a temperature-dependent volumetric thermal expansion coefficient and T is temperature.

The deviatoric elastic strain increment of the macrostructure is defined as

$$de_{qM}^e = \frac{1}{3G} dq, \quad (16)$$

where G is the shear modulus and may be obtained using a constant Poisson ratio ν in

$$G = \frac{3(1 - 2\nu)}{2(1 + \nu)} K_M. \quad (17)$$

Thus, the equations for elastic mechanical strain indicate the dependency of bulk modulus on suction (and hence fluid saturation), which in a dry clay can be significantly stiffer than in a water-saturated clay.

In total, the BBM is characterized by 18 parameters and the dual structure model incorporates between 8 and 11 additional parameters, depending on the microstructural bulk modulus and the interaction functions that are used.

2.6. Plastic Strain

Macrostructural plastic strain occurs by two possible mechanisms: either when the stress lies on the LC yield surface, or as a result of microstructural shrinkage/swelling. While the plastic strain

by microstructural shrinkage/swelling is described by Eq. (8), the LC plastic strains are obtained from the plastic flow rule

$$d\varepsilon_{vLC}^p = d\Lambda \frac{\partial g_{LC}}{\partial p}, \quad (18)$$

$$d\varepsilon_{qLC}^p = d\Lambda \frac{\partial g_{LC}}{\partial q}, \quad (19)$$

where $d\Lambda$ is the plastic multiplier obtained from the consistency condition $df_{LC} = 0$ (recall Eq.

(4)). The calculation of the plastic multiplier $d\Lambda$ is detailed in Rutqvist et al. (2011).

The total plastic volumetric strain is the sum of both plastic mechanisms

$$d\varepsilon_v^p = d\varepsilon_{vLC}^p + d\varepsilon_{v\beta}^p. \quad (20)$$

The hardening variable of the macrostructure — the pre-consolidation pressure p_0^* — depends on

the total plastic volumetric strain $d\varepsilon_v^p$ as

$$\frac{dp_0^*}{p_0^*} = \frac{(1 + e_M) d\varepsilon_v^p}{\lambda_{Ps0} - \kappa_{Ps0}}. \quad (21)$$

2.7. Implementation into TOUGH-FLAC

We implemented the dual structure model in TOUGH-FLAC, by extending the previous implementation of the BBM (Rutqvist et al., 2011) to include the microstructural level and its

interactions with the macrostructure. This involves consideration of the sequential coupling of the TOUGH2 and FLAC^{3D} simulators (Rutqvist, 2011), and constitutive stress-strain behavior in FLAC^{3D}. TOUGH2 is a multi-phase non-isothermal finite volume code. FLAC^{3D} is a geomechanics finite difference code. This implementation of the dual structure model in FLAC^{3D} was done using the User Defined constitutive Model (UDM) option in FLAC^{3D}, including C++ coding and dynamic link libraries. Specifically, the following calculation items were added

- 1) Microstructural strain (Eq. 13) and effective stress (Eq. 7)
- 2) Macrostructural strain (Eq. 10)
- 3) Global elastic tensor depending on microscopic and macroscopic structural compliances (Sanchez et al., 2005)
- 4) Micro/macrostructural interaction functions (Eqs. 9a and 9b)
- 5) Plastic macrostructural strain from structural interactions (Eq. 8)
- 6) Plastic corrections in the FLAC^{3D} elastoplastic algorithm (Eqs. 18, 19 and 20)
- 7) Plastic hardening/softening factors (Eq. 21)

Finally, at the end of each FLAC^{3D} step, the hardening parameter, i.e., the pre-consolidation pressure p_0^* , the bulk modulus of both microstructure and macrostructure and the tangential bulk modulus, are updated based on the total plastic volumetric strain and stress state, and these are stored for use in the next step.

3. MODEL CAPABILITIES

305 We test and demonstrate the capabilities of the dual structure model implemented in TOUGH-
 306 FLAC by modeling a laboratory experiment of Pousada (1982), in which an expansive clay
 307 undergoes several suction (wetting-drying) cycles for two net mean stresses (Figures 4 and 5).
 308 Expansive clays show a non-reversible behavior when they undergo successive wetting-drying
 309 cycles. This phenomenon cannot be reproduced with the standard single structure BBM model,
 310 but the incorporation of the interactions between the microstructure and the macrostructure of an
 311 expansive soil allows accumulating plastic strain upon suction cycles. Table 1 shows the
 312 parameters of the dual structure model resulting from the calibration of the laboratory
 313 experiments of Pousada (1982).

314 Figure 4 shows the calibration of a suction cycles test, which comprises 5 suction cycles (suction
 315 ranges from 1.7 to 0.2 MPa in each suction cycle) at a very low net mean stress (0.01 MPa). The
 316 model can reproduce the plastic strain accumulation upon cycles and the tendency to reduce the
 317 amount of plastic strain accumulated between two successive suction cycles as cycles
 318 accumulate. The calibration of the experiment reproduces with a fair accuracy the end points of
 319 the wetting-drying cycles as well as the strain evolution of the first suction cycle, which is
 320 curved. Nevertheless, the strain evolution of the subsequent cycles becomes quite linear in the
 321 laboratory experiment, but the numerical results maintain the curved evolution. To improve this
 322 change in the strain evolution pattern as suction cycles evolve, a more complex bulk modulus of
 323 both the microstructure and macrostructure may need to be proposed.

324 While the microstructure behaves elastically (Figure 4b), the macrostructure undergoes plastic
 325 strain that causes irreversible changes in macroporosity, which is related to the macrostructural

326 void ratio through $\varphi_M = e_M / (1 + e)$ (Figure 4c). Macroporosity is enhanced at low net mean stress

327(low values of the p/p_0 ratio) as a result of the interaction between the two levels of structures.

328Low values of the p/p_0 ratio imply a dense macrostructure, so the swelling of the
329microstructure will open up the macrostructure, inducing expansion upon suction cycles. Thus,
330the plastic strain of the macrostructure induced by the elastic volumetric strain of the
331microstructure is higher during wetting than during drying (Figure 4d).

332Figure 5 displays the results of the same experiment, but performed at a higher net mean stress of
3330.1 MPa. Similarly to the experiment with a lower confining pressure, the numerical calibration
334reproduces fairly well the end points of the wetting-drying cycles and the curved strain evolution
335of the first cycle. But for subsequent suction cycles, the experimental strain evolution becomes
336quasi-linear, while the numerical simulation keeps the curved evolution. Comparison between
337Figures 4 and 5 reveals that the swelling capacity of the material is reduced as the confining
338stress increases. The rest of the characteristics remain the same: the microstructure is elastic,
339plastic strain accumulation is reduced with the number of cycles and expansion accumulates
340upon cycles. The latter occurs because the p/p_0 ratio is still relatively low and therefore, the

341macrostructure is dense.

342For a net mean stress that would yield a high p/p_0 ratio, the macrostructure would be loose and
343micropores would invade macropores upon suction cycles. In this case, given the net mean stress
344and suction values, the microstructure deformation is almost independent of the confining stress
345(recall Figures 4b and 5b) because its stiffness is proportional to the effective stress (Eq. (14)),

346which evolves very similarly in the two experiments. Apart from this, the higher net mean stress
347in the experiment performed under 0.1 MPa implies a higher p/p_0 ratio and therefore, the
348suction cycles are closer to the equilibrium point between the wetting and the drying interaction
349functions. This causes a smaller plastic strain accumulation upon suction cycles due to the
350interaction between the two structural levels (recall Figures 4d and 5d).

351The calibration of the dual structure model with only these two available experiments becomes
352quite complicated due to the large number of degrees of freedom that this model has. Though the
353simulated deformation paths differ somewhat from the experimental results, the global behavior
354of this expansive clay is satisfactorily captured. In general, more experiments would be required
355to adjust most of the parameters of the dual structure model. Actually, this will be needed to
356model bentonite buffers that are intended for use in high-level nuclear waste repositories.

357

358 4. APPLICATION TO A GENERIC REPOSITORY

359We apply the dual structure model and compare the THM results with those of the standard
360single structure BBM in a generic repository similar to that considered in the Swiss nuclear
361waste disposal program. The long-term (100,000 years) behavior of such repository is simulated.
362The host rock is assumed to be Opalinus clay. The tunnels containing the high-level waste are
363placed at 500 m deep and are spaced 50 m. Since the emplacement tunnels may typically be up
364to 1 km long, we model a 2D cross section of the repository and make use of the symmetry to
365model only one tunnel. We further assume that the tunnel is backfilled with FEBEX bentonite
366(Gens et al., 2009; Sanchez et al., 2012). Thus, the dual structure properties of the backfill are

different than those calibrated from the experimental results presented in Section 3. The geometry of the model and the heat load of the waste are displayed in Figure 6 (Rutqvist et al., 2014).

Table 2 compiles the material parameters of the claystone host rock. The properties of the Opalinus clay are taken from Gens et al. (2007) and Corkum and Martin (2007). The relative permeability curves follow the van Genuchten-Mualem model. The properties of the FEBEX bentonite for the standard single structure BBM model were derived by Alonso et al. (2005) and Gens et al. (2009) (Table 3) and were also used in Rutqvist et al. (2014). The properties for the macrostructure of the dual structure model are similar to those used in the single structure BBM model, but some parameters have been adapted to obtain a global behavior of both the microstructure and the macrostructure comparable to that of the BBM model (see Table 4). The properties of the microstructure of the dual structure model for the FEBEX bentonite are based on those proposed by Sanchez et al. (2012), but with some modifications (Table 4).

We assume that the intrinsic permeability varies according to an exponential law that was proposed and calibrated against laboratory measurements by Sanchez et al. (2012) for the dual structure model. This law depends on the porosity of the macrostructure as

$$\mathbf{k} = k_0 \exp[b(\varphi_M - \varphi_{M0})] \mathbf{I}, \quad (22)$$

where $\mathbf{k}$ is the intrinsic permeability tensor, k_0 is the intrinsic permeability at the reference

porosity of the macrostructure φ_{M0} , b is a model parameter and $\mathbf{I}$ is the identity matrix. For the

single structure BBM model, the same law is adopted, but changing macroporosity by total

387porosity and adjusting the value of k_0 , so that the initial permeability is the same in the two cases

388($2.0 \times 10^{-21} \text{ m}^2$). Furthermore, to account for the higher intrinsic permeability of clays to gas than
389to water (Olivella and Gens, 2000), we make use of the relationship given by Klinkenberg (1941)

$$390 \quad k_{gas} = k \left(1 + \frac{b_k}{p_g} \right)^n, \quad (23)$$

391where b_k is the Klinkenberg parameter.

392To calculate consistent initial conditions of the repository once the emplacement tunnel has been
393excavated and the backfill and the waste placed inside the tunnel, a sequence of stages is
394calculated. First, we calculate the pre-excavation equilibrium conditions. Mechanically, the stress
395field is assumed isotropic and the vertical total stress increases linearly with depth and
396proportionally to a bulk density of 24 kN/m^3 . Since the tunnel is located at 500 m depth, the pre-
397excavation mean stress is 11.8 MPa. The mechanical boundary conditions are no displacement
398perpendicular to the lateral and bottom boundaries and a constant pressure equal to atmospheric
399pressure at the upper boundary. Hydraulically, the groundwater table is located at the ground
400surface. Fluid pressure is imposed at the bottom of the model, at 1000 m depth, and is set to 9
401MPa. The ground surface temperature and the temperature at the bottom of the model are fixed to
40210 °C and 40 °C, respectively. Thus, the geothermal gradient is equal to 30 °C/km. Next, the drift
403excavation is simulated by removing the elements in the tunnel and fixing the temperature to 25
404°C and the fluid pressure to 0.1 MPa until steady state is reached. Finally, the nuclear waste
405canister and the bentonite buffer are placed in the tunnel instantaneously and the waste starts to

406 release heat. The bentonite has an initial liquid degree of saturation of 0.65 and the gas pressure
407 is initially fixed at 0.1 MPa.

408 Figure 7 shows the evolution of temperature, liquid saturation degree, fluid pressure and total
409 mean stress at some points within the buffer and in the Opalinus clay obtained with both the
410 BBM and the dual structure model. Temperature evolution is similar for both mechanical
411 constitutive models, though the temperature peak is slightly higher close to the canister for the
412 dual structure model because the buffer becomes drier than for the standard single structure
413 BBM (Figure 7a). However, the hydration of the buffer is significantly affected by the
414 mechanical constitutive model (Figure 7b). While the buffer close to the canister becomes fully
415 saturated after 60 years for the BBM, it takes up to 2780 years when using the dual structure
416 model. This is the first time that the time for full saturation of the buffer has been predicted,
417 because previous simulations did not go beyond some tens of years (recall that we simulated
418 100,000 years). Though the exact time at which the buffer will become fully saturated is very
419 uncertain because we do not know with precision all the parameters of the dual structure model,
420 the difference of two orders of magnitude between the saturation time predicted by the BBM and
421 the dual structure model shows the importance of using a constitutive model that accounts for
422 two structural levels to reproduce the thermo-hydro-mechanical behavior of expansive clays.

423 This difference in the saturation time of the buffer occurs because in the dual structure model the
424 porosity through which fluids flow is only the porosity of the macrostructure and not the total
425 porosity, like in the BBM. The deviation in the saturation evolution in the inner part of the buffer
426 between the two models starts at early times (2-3 years), which is in agreement with the
427 observations of the 10 year-long mock-up test for the FEBEX in situ test performed at the
428 laboratory at CIEMAT, Madrid (Spain) (see Sanchez et al., 2012 for details). Furthermore, the

429delay in the saturation of the bentonite buffer causes a delay in its pressurization close to the
430canister (Figure 7c). Figure 7c displays that, close to the canister, the increase in fluid pressure,
431which equals the maximum pressure of the fluids filling the pores, i.e., gas pressure if the soil is
432unsaturated and liquid pressure if the soil is saturated, is significantly delayed. But once the
433buffer is fully saturated, the thermal pressurization is similar to that of the buffer close to the
434tunnel wall. Despite this significant delay in saturation at the inner parts of the buffer, the overall
435buffer swelling stress evolution is not severely retarded (Figure 7d). Indeed, the buffer is still
436functioning to provide sufficient swelling and support load to the tunnel wall and the EDZ
437(Figure 8). The swelling stress of a few MPa has the potential to close the fractures of the EDZ,
438significantly reducing permeability of the EDZ and assuring sealing in the long-term.

439Figure 9 displays the variables that control the dual structure constitutive model, i.e., suction,
440mean net stress and effective stress. While suction and mean net stress are used to calculate the
441behavior of the macrostructure according to the BBM, the mean effective stress determines the
442elastic volumetric strain of the microstructure in the dual structure model. Suction close to the
443tunnel wall decreases from the beginning of the simulation because the host rock, which is fully
444saturated, supplies groundwater that gradually saturates the bentonite buffer (Figure 9a).
445However, suction increases initially close to the canister because the heat of the high-level
446nuclear waste dries the bentonite. Subsequently, the saturation of the whole bentonite buffer
447starts to take place and suction decreases. The net mean stress (Figure 9b) is similar for both
448models close to the tunnel wall because of the relatively quick saturation of this part of the
449buffer, which leads to a comparable high stiffness of the expansive clay (Figure 9d). However,
450close to the canister, the net mean stress becomes much higher for the dual structure model than
451for the BBM because the higher suction (recall Figure 9a) leads to a stiffer bentonite (Figure 9d).

452The effective mean stress evolution (Figure 9c) is similar to the suction evolution because the net
453mean stress is relatively low.

454Figure 10 illustrates porosity evolution for simulation results of both constitutive models. The
455total porosity changes, though larger in the dual structure model, are relatively similar for both
456models, especially in the region of the buffer close to the tunnel wall. However, a higher porosity
457reduction occurs close to the waste overpack, where a stronger drying takes place when
458accounting for the dual structure model. Interestingly, the reduction in macroporosity is larger
459than the reduction in total porosity close to the waste overpack. This larger macroporosity
460reduction in the dual structure model leads to a greater permeability reduction close to the waste
461overpack that impedes hydration of the buffer (Figure 11).

462Figure 12 schematically illustrates the evolution of the microporosity and the macroporosity in a
463point close to the canister and in another point close to the tunnel wall. The expansive clay close
464to the tunnel wall becomes saturated at a low mean stress. Thus, both the microstructure and the
465macrostructure swell (strain is negative according to the sign criterion of geomechanics) and
466since the interaction function of swelling at low stress is positive (Figure 12b), the plastic strain
467of the macrostructure due to interaction between the two structural levels is negative, i.e., the
468macrostructure expands (Figure 12a). Therefore, the permeability of the clay increases and full
469saturation occurs relatively quickly.

470On the other hand, close to the canister, the buffer dries during the first year of simulation,
471leading to shrinkage at low stress (strain is positive). In this case, since the interaction function of
472shrinkage at low stress is positive, the plastic strain of the macrostructure due to interaction
473between the two structural levels is positive, which implies shrinkage of the macrostructure and

474therefore, a permeability reduction. Later, the permeability is reduced even further because the
475mean stress of the buffer increases, which causes a compression of the pores. Finally, the region
476around the canister is saturated at high stress. Under these conditions, the microstructure swells
477(strain is negative), but the interaction function of swelling at high stress is negative (Figure
47812b). As a result, the plastic strain of the macrostructure due to interaction between the two
479structural levels is positive, i.e., the macrostructure shrinks. This shrinkage of the macrostructure
480is caused by an invasion of the microstructure, which closes the macropores when the expansive
481clay swells at high stress, contributing to reduce the permeability. This greater permeability
482reduction around the waste overpack when using the dual structure model causes a significant
483delay in the time at which the buffer becomes fully saturated.

484These results are in agreement with the short-term results of Sanchez et al. (2012), who modeled
485a large-scale heating test—a mock-up test for the FEBEX in situ test—performed at the
486laboratory that lasted for 10 years. Their modeling results reproduce the experimentally observed
487delay of the saturation of the buffer in the short-term when using the dual structure model instead
488of the BBM. Here, we show how such a delay might affect the long-term THM evolution of a
489repository. Future code comparison of the dual structure model will be valuable. The independent
490implementation of the dual-structure model into a different code, as conducted in this study,
491provides the possibilities of performing such code comparison and additional validations. This
492will lead to increased confidence in the long-term predictions of these complex and important
493processes.

494 5. CONCLUSIONS

495The dual structure model accounts for two structural levels to model the THM behavior of an
496expansive soil, i.e., the microstructure and the macrostructure, and the interactions that occur
497between them. We have presented the formulation of the dual structure model and described its
498implementation into the coupled fluid flow and geomechanical simulator TOUGH-FLAC.
499Furthermore, we have shown the capabilities of the dual structure model by modeling and
500reproducing observed behavior for two laboratory tests performed by Pousada (1982) on
501expansive clay under increasing confining stress. In agreement with observations in the
502laboratory, the simulations yielded non-reversible strain accumulation upon suction cycles and a
503decreasing swelling capacity as the confining stress increases. Finally, we have modeled the
504long-term performance of a generic high-level nuclear waste repository with a bentonite back-
505filled waste emplacement tunnel and compared the results of both the dual structure model to
506that of a standard single structure model equivalent to the Barcelona Basic Model (BBM).

507The main difference between the two models is that the dual structure model predicts that the
508time for full saturation of the expansive clay is of thousands of years, while the BBM yields a
509time of tens of years. The numerical simulation shows that this delay is caused by the fact that
510the fluid flow conducting macrostructure is invaded by the microstructure with associated
511reduction in permeability for water flow. Such a delay has previously been observed in large-
512scale laboratory and in situ experiments and here we show this might affect the long-term
513performance of a repository. This result shows evidence that to properly simulate the THM
514behavior of expansive soils, a dual structure model, like the one presented here, should be used.
515However, the modeling results also showed that despite a significant delay in saturation at the
516inner parts of the buffer, the overall buffer swelling stress evolution was not severely retarded.

517 That is, the buffer is still functioning to provide sufficient swelling and support load to the tunnel
518 wall and the EDZ.

519

520 ACKNOWLEDGEMENTS

521 Funding for this work was provided by the Used Fuel Disposition Campaign, Office of Nuclear
522 Energy, of the US Department of Energy under Contract Number DE-AC02-05CH11231 with
523 Berkeley Lab.

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525 REFERENCES

526 Al-Homoud, A.S., Basma, A.A., Malkawi, A.I.H., Al-Bashabsheh, M.A. Cyclic swelling
527 behavior of clays. *J. Geotech. Engrg.*, **121**, 562–565 (1995).

528 Alonso, E.E., Gens, A., Josa, A. A constitutive model for partially saturated soils. *Geotechnique*,
529 **40**, 405–430 (1990).

530 Alonso, E.E., Vaunat, J., Gens, A. Modelling the mechanical behaviour of expansive clays.
531 *Engineering Geology*, **54**, 173–183 (1999).

532 Alonso, E.E., Alcoverro, J., Coste, F., Malinsky, L., Merrien-Soukatchoff, V., Kadiri, I., Nowak,
533 T., Shao, H., Nguyen, T.S., Selvadurai, A.P.S., Armand, G., Sobolik, S.R., Itamura, M.,
534 Stone, C.M., Webb, S.W., Rejeb, A., Tijani, M., Maouche, Z., Kobayashi, A., Kurikami,
535 H., Ito, A., Sugita, Y., Chijimatsu, M., Borgesson, L., Hernelind, J., Rutqvist, J., Tsang,
536 C., Jussila, P. The FEBEX benchmark test: case definition and comparison of modeling
537 approaches. *Int. J. Rock Mech. Min. Sci.*, **42**, 611–638 (2005).

538Alonso, E.E., Hoffmann, C. Modelling the field behaviour of a granular expansive barrier.
539 *Physics and Chemistry of the Earth*, **32**, 850–865 (2007).

540Åkesson, M., Kristensson, O. Mechanical modeling of MX-80 – Development of constitutive
541 laws. *Physics and Chemistry of the Earth*, **33**, S504–S507 (2008).

542Blümling, P., Bernier, F., Lebon, P., Martin, C.D. The excavation damaged zone in clay
543 formations time-dependent behaviour and influence on performance assessment. *Phys*
544 *Chem Earth*, **32**, 588–599 (2007).

545Chen, G.J., Ledesma, A. Coupled solution of heat and moisture flow in unsaturated clay barriers
546 in a repository geometry. *Int. J. Numer. Anal. Meth. Geomech.*, **31**, 1045–1065 (2007).

547Corkum, A.G., Martin, C.D. The mechanical behaviour of weak mudstone (Opalinus Clay) at
548 low stresses. *Int. J. Rock Mech. Min. Sci.*, **44**, 196–209.

549Day, R.W. Swell-shrink behavior of compacted clay. *J. Geotech. Engrg.*, **120**, 618–623 (1994).

550Delage, P., Marcial, D., Cui, Y.J., Ruiz, X. Ageing effects in a compacted bentonite: a
551 microstructure approach. *Geotechnique*, **56**(5), 291–304 (2006).

552Dixon, D.A., Graham, J., Gray, M.N. Hydraulic conductivity of clays in confined tests under low
553 hydraulic gradients. *Can. Geotech. J.* **36**, 815–825 (1999).

554Dupray, F., François, B., Laloui, L. Analysis of the FEBEX multi-barrier system including
555 thermoplasticity of unsaturated bentonite. *Int. J. Numer. Anal. Meth. Geomech.*, **37**, 399–
556 422 (2013).

557Gens, A., Alonso, E. A framework for the behaviour of unsaturated expansive clays. *Can.*
558 *Geotech. J.* **29**, 1013–1032 (1992).

559 Gens, A., Sánchez, M., Sheng, D. On constitutive modelling of unsaturated soils. *Acta*
560 *Geotechnica*, **1**, 137–147 (2006).

561 Gens, A., Vaunat, J., Garitte, B., Wileveau, Y. In situ behaviour of a stiff layered clay subject to
562 thermal loading, observations and interpretation. *Geotechnique*, **57**(2), 207–228 (2007).

563 Gens, A., Sanchez, M., Guimaraes, L. do N., Alonso, E.E., Lloret, A., Olivella, S., Villar, M.V.,
564 Huertas, F. A full-scale in situ heating test for high-level nuclear waste disposal:
565 observations, analysis and interpretation. *Geotechnique*, **59**(4), 377–399 (2009).

566 Gens, A. Soil - environmental interactions in geotechnical
567 engineering. *Geotechnique*, **60**, 3–74 (2010).

568 Jurado, A., de Gaspari, F., Vilarrasa, V., Bolster, D., Sánchez-Vila, X., Fernández-García, D.,
569 Tartakovsky, D.M. Probabilistic analysis of groundwater-related risks at subsurface
570 excavation sites. *Engineering Geology*, **125**, 35–44 (2012).

571 Klinkenberg, L.J. The Permeability of Porous Media to Liquids and Gases, in *API Drilling and*
572 *Production Practice*, 200–213 (1941).

573 Komine, H., Ogata, N. Experimental study on swelling characteristics of compacted bentonite.
574 *Can. Geotech. J.* **31**, 478–490 (1994).

575 Kristensson, O., Åkesson, M. Mechanical modeling of MX-80 – Quick tools for BBM parameter
576 analysis. *Physics and Chemistry of the Earth*, **33**, S508–S515 (2008).

577 Laloui, L., Cekerevac, C. Thermo-plasticity of clays: An isotropic yield mechanism. *Computers*
578 *and Geotechnics*, **30**, 649–660 (2003).

579Lloret, A., Villar, M.V., Sanchez, M., Gens, A., Pintado, X., Alonso, E.E. Mechanical behaviour
580 of heavily compacted bentonite under high suction changes. *Géotechnique*, **53**(1), 27-40
581 (2003).

582Martinez-Landa, L., Carrera, J. An analysis of hydraulic conductivity scale effects in granite
583 (Full-scale Engineered Barrier Experiment (FEBEX), Grimsel, Switzerland). *Water*
584 *Resources Research*, **41**, W03006, doi:10.1029/2004WR003458 (2005).

585Olivella, S., Gens, A. Vapour transport in low permeability unsaturated soils with capillary
586 effects. *Transport In Porous Media*, **40**, 219–241 (2000).

587Pousada, P.E. Deformabilidad de arcillas expansivas bajo succión controlada. *Ph. D. Thesis*,
588 Technical University of Madrid, Spain (1982).

589Rutqvist J., Barr D., Birkholzer J.T., Chijimatsu M., Kolditz O., Liu Q.-S., Oda Y, Wang W.-Q.
590 and Zhang C.-Y. Results from an international simulation study on coupled thermal,
591 hydrological, and mechanical (THM) processes near geological nuclear waste
592 repositories. *Nuclear Technology*, **163**, 101–109 (2008).

593Rutqvist, J., Ijiri, Y. Yamamoto, H. Implementation of the Barcelona Basic Model into TOUGH-
594 FLAC for simulations of the geomechanical behavior of unsaturated soils. *Computers &*
595 *Geosciences*, **37**, 751–762 (2011).

596Rutqvist, J., Zheng, L., Chen, F., Liu, H.-H., Birkholzer, J. Modeling of coupled thermo-hydro-
597 mechanical processes with links to geochemistry associated with bentonite-backfilled
598 repository tunnels in clay formations. *Rock Mech. Rock Eng.*, **47**, 167–186 (2014).

599 Saiyouri, N., Hicher, P., Tessier, D. Microstructural approach and transfer water modeling in
600 highly compacted unsaturated swelling clays. *Mechanics of Cohesive-Frictional*
601 *Materials*, **5**, 41–60 (2000).

602 Sánchez, M., Gens, A., Guimarães, L. do N., Olivella, S. A double structure generalized plasticity
603 model for expansive materials. *Int. J. Numer. Anal. Meth. Geomech.*, **29**, 751–787 (2005).

604 Sánchez, M., Gens, A., Guimarães, L. do N., Olivella, S. Implementation algorithm of a
605 generalised plasticity model for swelling clays. *Computers & Geotechnics*, **35**, 860–871
606 (2008).

607 Sánchez, M., Gens, A., Olivella, S. THM analysis of a large-scale heating test incorporating
608 material fabric changes. *Int. J. Numer. Anal. Meth. Geomech.*, **36**, 391–421 (2012).

609 Tartakovsky, D.M. Probabilistic risk analysis in subsurface hydrology. *Geophysical Research*
610 *Letters*, **34**, L05404 (2007).

611 Tripathy, S., Subba Rao, K.S., Fredlund, D.G. Water content – void ratio swell-shrink paths of
612 compacted expansive soil. *Can. Geotech. J.* **39**, 938–959 (2002).

613 Tsang, C.F., Bernier, F., Davies, C. Geohydromechanical processes in the Excavation Damaged
614 Zone in crystalline rock, rock salt, and indurated and plastic clays—in the context of
615 radioactive waste disposal. *International Journal of Rock Mechanics and Mining*
616 *Sciences*, **42**(1), 109-125 (2005).

617 Vilarrasa, V., Koyama, T., Neretnieks, I., Jing, L. Shear-induced flow channels in a single rock
618 fracture and their effect on solute transport, *Transport In Porous Media*, **87**, 503–523
619 (2011).

620Villar, M.V. Investigation of the behaviour of bentonite by means of suction-controlled
621 oedometer tests. *Engineering Geology*, **54**, 67–73 (1999).

622Wang, Q., Cui, Y.-J., Tang, A.M., Barnichon, J.-D., Saba, S., Ye, W.-M. Hydraulic conductivity
623 and microstructure changes of compacted bentonite/sand mixture during hydration.
624 *Engineering Geology*, **164**, 67–76 (2013a).

625Wang, Q., Tang, A.M., Cui, Y.-J., Barnichon, J.-D., Ye, W.-M. Investigation of the hydro-
626 mechanical behaviour of compacted bentonite/sand mixtures based on the BExM model.
627 *Computers and Geotechnics*, **54**, 49–52 (2013b).

628Yu, L., Weetjens, E., Sillen, X., Vietor, T., Li, X., Delage, P., Labiouse, V., Charlier, R.
629 Consequences of the thermal transient on the evolution of the damaged zone around a
630 repository for heat-emitting high-level radioactive waste in a clay formation: a
631 performance assessment perspective. *Rock Mechanics and Rock Engineering*, **47**, 3-19
632 (2014).

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638FIGURE CAPTIONS LIST

639Figure 1. Schematic representation of the two structural levels considered in the dual structure
640 model. Clay particles are represented by the gray lines.

641 Figure 2. Schematic representation of the dual structure model in the isotropic plane, including
 642 the neutral line (NL) and the loading-collapse (LC) yield surface. The NL moves with the
 643 current stress state, so that the current stress state is always contained within the NL. The
 644 stress state can change along one of the following three stress paths: (i) microstructural
 645 shrinkage, if it moves to the right of the NL, (ii) microstructural swelling, if it moves to
 646 the left of the NL and (iii) neutral loading, if it moves along the NL, in which case the
 647 microstructure does not deform.

648 Figure 3. Evolution of (a) volumetric strain, (b) microstructural void ratio, (c) macrostructural
 649 void ratio and (d) plastic strain of the macrostructure due to micro/macrostructure
 650 interaction upon suction (wetting-drying) cycles for a net mean stress, p , of 0.01 MPa.
 651 The experimental volumetric deformation of Pousada (1982) is also displayed in (a).

652 Figure 4. Evolution of (a) volumetric strain, (b) microstructural void ratio, (c) macrostructural
 653 void ratio and (d) plastic strain of the macrostructure due to micro/macrostructure
 654 interaction upon suction (wetting-drying) cycles for a net mean stress, p , of 0.1 MPa.
 655 The experimental volumetric deformation of Pousada (1982) is also displayed in (a).

656 Figure 5. Schematic representation of the generic repository model, detail of the grid around the
 657 waste showing the monitoring points and heat power evolution for the generic repository.

658 Figure 6. Evolution of (a) temperature (see Figure 5 for the location of the observation points),
 659 (b) liquid saturation degree, (c) liquid pressure and (d) total mean stress for the dual
 660 structure model (DSM) and the standard single structure Barcelona Basic Model (BBM).

Figure 7. Evolution of the total and effective radial stress at point V3 located at the tunnel wall for the dual structure model (DSM) and the standard single structure Barcelona Basic Model (BBM).

Figure 8. Evolution of (a) suction, (b) net mean stress, (c) effective mean stress and (d) global bulk modulus for the dual structure model (DSM) and the standard single structure Barcelona Basic Model (BBM).

Figure 9. (a) Total porosity evolution for the dual structure model (DSM) and the standard single structure Barcelona Basic Model (BBM). (b) Macroporosity and microporosity evolution of the dual structure model.

Figure 10. Permeability evolution for the dual structure model (DSM) and the standard single structure Barcelona Basic Model (BBM). Permeability is a function of the macroporosity in the dual structure model.

Figure 11. (a) Schematic evolution of the microporosity, macroporosity, plastic strain of the macrostructure due to micro/macrostructure interaction and permeability and (b) evolution of the interaction functions for a point close to the canister (V1) and a point close to the tunnel wall (V2).

TABLES

Table 1. Parameters used to reproduce the suction cycles test of Pousada (1982).

Parameters defining the Barcelona Basic Model for macrostructural behavior

κ_{ps0}	κ_{sp0}	λ_{ps0}	p^c	r	ξ	p_0^*
=0.005	=0.01	=0.024	(MPa)=0.01	=0.85	(MPa ⁻¹)=0.2	(MPa)=0.75

Parameters defining the law for microstructural behavior

$$\alpha_m \text{ (MPa}^{-1}\text{)}=1.2 \quad \beta_m \text{ (MPa}^{-1}\text{)}=0.02$$

Interaction functions between the microstructure and the macrostructure

$$f_c = 1.975 + 0.185 \tanh[5(p/p_0 - 0.275)] \quad f_s = 1.825 - 0.4 \tanh[-0.4(p/p_0 - 0.3)]$$

$$e_{micro}=0.45 \quad e_{macro}=0.55$$

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703Table 2. Properties of the clay host rock (Gens et al., 2007; Corkum and Martin, 2007).

Property	Value
Porosity, φ (-)	0.15

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Young's modulus, E (GPa)	5
Poisson ratio, ν (-)	0.3
Grain density, ρ_s (kg/m ³)	2400
Grain Specific heat, C_s (J/kg/°C)	900
Thermal conductivity, λ_T (W/m/K)	2.2
Thermal expansion coefficient, α_0 (°C ⁻¹)	1.0x10 ⁻⁵
Intrinsic permeability, k (m ²)	5.0x10 ⁻²⁰
van Genuchten water retention parameter m (-)	0.41
van Genuchten entry pressure, P_0 (MPa)	48
Residual liquid saturation, S_{lr} (-)	0.1
Residual gas saturation, S_{gr} (-)	0.01

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719 Table 3. Material parameter values for the bentonite buffer used in the BBM model (Gens et al.,
720 2009).

Property	Value
Initial dry density, ρ_d (kg/m ³)	1600
Compressibility parameter for stress-induced elastic strain, κ_{ps0} (-)	0.05
Compressibility parameter for suction-induced elastic strain, κ_{sp0} (-)	0.25
Poisson ratio, ν (-)	0.4
Parameter for stress-induced elastic strain, α_{ps} (MPa ⁻¹)	-0.003
Parameter for suction-induced elastic strain, α_{sp} (-)	-0.161
Parameter for suction-induced elastic strain, α_{ss} (-)	0
Reference stress state for relating elastic compressibility to suction, p_{ref} (MPa)	0.01
Thermal expansion coefficient, α_0 (°C ⁻¹)	1.5x10 ⁻⁵
Compressibility parameter in virgin state soils at zero suction, λ_{ps0} (-)	0.15
Parameter defining soil stiffness associated with loading collapse yield, r (-)	0.925
Parameter for the increase of soil stiffness with suction, ξ (MPa ⁻¹)	0.1
Parameter that describes the increase of cohesion with suction, k_s (-)	0.1
A reference stress state for compressibility relation in virgin states, p^c (MPa)	0.5
Slope of the critical state line, M (-)	1.0

Non-associativity parameter in the plasticity flow rule, α_a (-)	0.53
Specific volume at reference stress state p^c in virgin state, v^c (-)	1.937
Net mean yield stress for saturated conditions at reference temperature, p_0^* (MPa)	12.0
Initial porosity, φ_0 (-)	0.398
Saturated reference permeability at reference porosity φ_0 , k_0 (m ²)	4.5×10^{-27}
Reference porosity for the permeability model, φ_0 (-)	0.14
Model parameter for permeability, b (-)	50
Relative permeability to liquid, k_{rl} (-)	$k_{rl} = S_l^3$
Relative permeability to gas, k_{rg} (-)	$k_{rg} = 1$
Klinkenberg parameter, b_k (MPa)	2.5×10^5
van Genuchten water retention parameter m (-)	0.32
van Genuchten entry pressure, P_0 (MPa)	30
Residual liquid saturation, S_{lr} (-)	0.1
Residual gas saturation, S_{gr} (-)	0
Grain Specific heat, C_s (J/kg/°C)	800
Thermal conductivity, λ_T (W/m/K)	$0.5 + S_l(1.3 - 0.5)$

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732 Table 4. Material parameter values of the bentonite buffer used in the dual structure model (only
 733 the parameters of the macrostructure that differ from those used for the BBM model
 734 (Table 3) are included here) (Sanchez et al., 2012).

Property	Value
Compressibility parameter for stress-induced elastic strain, κ_{ps0} (-)	0.079
Compressibility parameter for suction-induced elastic strain, κ_{sp0} (-)	0.08
Reference stress state for relating elastic compressibility to suction, p_{ref} (MPa)	0.03
Specific volume at reference stress state p^c in virgin state, v^c (-)	1.4935
Initial void ratio of the macrostructure, e_M (-)	0.35
Initial void ratio of the microstructure, e_m (-)	0.3
Parameter controlling the microstructural soil stiffness, α_m (MPa ⁻¹)	0.006

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Parameter controlling the microstructural soil stiffness,	β_m (MPa ⁻¹)	0.0027
Interaction function for microstructural swelling paths	$f_s = 0.8 - 1.1 \tanh[20(p/p_0 - 0.25)]$	
Interaction function for microstructural compression paths	$f_c = 1.0 + 0.9 \tanh[20(p/p_0 - 0.25)]$	
Saturated reference permeability at reference porosity	φ_0, k_0 (m ²)	3.0×10^{-23}
Reference porosity of the macrostructure for the permeability model,	φ_{M0} (-)	0.14

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742**FIGURES**

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744 Figure 1. Bimodal pore size distribution of an expansive soil measured from mercury intrusion
 745 porosimetry (adapted from Lloret et al., 2003).

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748Figure 2. Schematic representation of the two structural levels considered in the dual structure
 749 model. Clay particles are represented by the gray lines.

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752Figure 3. Schematic representation of the dual structure model in the isotropic plane, including
 753 the neutral line (NL) and the loading-collapse (LC) yield surface. The NL moves with the
 754 current stress state, so that the current stress state is always contained within the NL. The
 755 stress state can change along one of the following three stress paths: (i) microstructural
 756 shrinkage, if it moves to the right of the NL, (ii) microstructural swelling, if it moves to
 757 the left of the NL and (iii) neutral loading, if it moves along the NL, in which case the
 758 microstructure does not deform.

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Figure 4. Evolution of (a) volumetric strain, (b) microstructural void ratio, (c) macrostructural void ratio and (d) plastic strain of the macrostructure due to micro/macrostructure interaction upon suction (wetting-drying) cycles for a net mean stress, p , of 0.01 MPa. The experimental volumetric deformation of Pousada (1982) is also displayed in (a).

771

774 Figure 5. Evolution of (a) volumetric strain, (b) microstructural void ratio, (c) macrostructural
 775 void ratio and (d) plastic strain of the macrostructure due to micro/macrostructure
 776 interaction upon suction (wetting-drying) cycles for a net mean stress, p , of 0.1 MPa.
 777 The experimental volumetric deformation of Pousada (1982) is also displayed in (a).

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780Figure 6. Schematic representation of the generic repository model, detail of the grid around the
 781 waste showing the monitoring points and heat power evolution for the generic repository.

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Figure 7. Evolution of (a) temperature (see Figure 5 for the location of the observation points), (b) liquid saturation degree, (c) liquid pressure and (d) total mean stress for the dual structure model (DSM) and the standard single structure Barcelona Basic Model (BBM).

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795 Figure 8. Evolution of the total and effective radial stress at point V3 located at the tunnel wall
 796 for the dual structure model (DSM) and the standard single structure Barcelona Basic
 797 Model (BBM).

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Figure 9. Evolution of (a) suction, (b) net mean stress, (c) effective mean stress and (d) global bulk modulus for the dual structure model (DSM) and the standard single structure Barcelona Basic Model (BBM).

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Figure 10. (a) Total porosity evolution for the dual structure model (DSM) and the standard single structure Barcelona Basic Model (BBM). (b) Macroporosity and microporosity evolution of the dual structure model.

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811 Figure 11. Permeability evolution for the dual structure model (DSM) and the standard single
 812 structure Barcelona Basic Model (BBM). Permeability is a function of the macroporosity
 813 in the dual structure model.

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Figure 12. (a) Schematic evolution of the microporosity, macroporosity, plastic strain of the macrostructure due to micro/macrostructure interaction and permeability and (b) evolution of the interaction functions for a point close to the canister (V1) and a point close to the tunnel wall (V2). Note that the sign criterion of geomechanics is adopted, i.e., strain is positive in compression and negative in extension.