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- 1 Assessment of a high-level spent nuclear fuel disposal model
- 2
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- 11

Abstract: This paper assesses a model for the full-scale engineered barrier experiment 12 (Febex) in situ test, simulating the disposal of heat-emitting, high-level spent nuclear fuel. 13 The model has been developed using Code_Bright and is based on previous modelling 14 efforts. The model focuses on the thermo-hydro-mechanical behaviour of a bentonite 15 barrier surrounding a heater that simulates the heat production of radioactive spent fuel. 16 The new model incorporates the new dismantling operations and has been compared with 17 new in situ measurements. Once calibrated, the long-term response of the model has been 18 analysed. Furthermore, the implementation of additional processes and their impact on 19 hydration and stress development have been assessed. In this assessment, it has been 20 found that the bentonite barrier does not fully saturate near the canister in any case, which 21 is an important goal for the isolation of the spent nuclear fuel. The intrinsic permeability 22 has been found to give results closer to measurements when its value is doubled. The 23 24 double-structured model has given interesting results, but the authors found that it does not have a great influence in the general behaviour of the model. 25

- **Keywords**: FEBEX, CODE_BRIGHT, numerical modeling, nuclear waste disposal.
- 27

28 **1. Introduction**

Deep geological storage or disposal remains the preferred option for waste management
 of heat-emitting, high-level radioactive nuclear waste (HLW) in several countries.

- Excavation of deep underground repositories is limited to rock units that are reasonably
- 32 stable and without major groundwater flow, and to depths of a few hundred metres
- below the surface.
- 34 The required degree of waste isolation needed for HLW is provided by a combination of
- engineered and natural barriers placed between the potentially harmful radionuclides
- and the biosphere. The natural barrier is fundamentally the host rock, and the artificial
- barriers are the solid matrix of the waste itself, the metallic canister enclosing the waste,
- and the backfill –the sealing material placed around the canisters. This backfill, also
- 39 called an 'engineered barrier', is often constructed using compacted expansive clay.
- 40 Bentonite has generally been chosen because of its high swelling capacity, low
- 41 permeability and favorable retardation properties (Gens et al., 2009).

42 The bentonite barrier fulfills several important functions. In the first instance, a very

- 43 low hydraulic conductivity restricts water penetration and retards significantly solute
- transport due to its low diffusion coefficient and to additional sorption effects. It should
- 45 also provide a favorable chemical environment and be able to self-heal if subjected to

46 physical perturbation such as cracking and fissuring events (Gens, 2003). The

47 engineered clay barrier and adjacent host rock (usually called the 'near field') will be

48 subjected to the heating effect of the nuclear waste, and also to various associated

49 hydraulic and mechanical phenomena that interact in a complex way.

- 50 In addition, compacted bentonite is initially unsaturated, and will therefore be subjected
- to hydration from the surrounding rock, triggering further coupled thermo-hydro-

52 mechanical (THM) phenomena. In order to achieve a safe and robust repository design,

it is necessary to have a good understanding of the processes that occur in the near field,

and of their evolution over time (Gens et al., 2009).

55 Given the importance of the problem, it has proved useful to perform large-scale and medium-scale heating tests simulating repository conditions in underground laboratories 56 around the world (Dixon et al., 2002; Pusch et al., 1985; Selvadurai, 1997; Volckaert et 57 al., 1996). Because of the low permeability of the materials involved, such experiments 58 usually require long testing times, measured in years, in order to obtain meaningful 59 results. The complexity of the phenomena involved, and of their interactions, implies 60 that process understanding and interpretation of results are limited unless supported by 61 suitable numerical models able to reproduce the main features of the test. Owing to the 62 coupled nature of the THM interactions, coupled THM formulations are inevitably 63

64 required.

The present paper contains the description of an updated model for the large scale in 65 66 situ heating test FEBEX. In this test, after five years of heating, one of the heaters was switched off and the experiment was partially dismantled, allowing the final state of the 67 barrier to be observed directly. In this way, very valuable information on the state of the 68 69 bentonite at the end of the test was obtained. The test has received attention during the initial (Gens et al., 1998) and intermediate stages (Alonso & Alcoverro, 2005). Finally, 70 Gens et al. (2009) discussed the thermal, hydraulic and mechanical observations in the 71 bentonite barrier and in the host rock, paying special attention to the progress of 72 hydration in the barrier, the effects of heating and vapor transport, and the development 73 of swelling pressures in the barrier. 74

- 75 In the FEBEX experiment, heaters are emplaced in the axis of a tunnel excavated in
- 76 granite to simulate the heat production of radioactive waste. The test is fully
- instrumented, and attention is focused on the thermo-hydro-mechanical (THM)

behavior of the near-field region constituted by the compacted bentonite barrier

surrounding the heater and the immediately adjacent rock. Interpretation of the test is

80 assisted by the performance of a coupled numerical analysis based on a formulation that

81 incorporates the relevant THM phenomena. Further description of the FEBEX in situ

- test can be found in Gens et al. (2009).
- 83 The model of this test has been developed using CODE_BRIGHT (Olivella et al.,
- 84 1996), a Finite Element Method program that enables coupled thermo-hydro-
- 85 mechanical analysis in geological media. This is a code version that incorporates
- 86 customized pre- and post- process interfaces so that simulation models that use
- 87 CODE_BRIGHT -available from: <u>https://deca.upc.edu/en/projects/code_bright</u>- can be
- developed more easily. It allows easy modification of parameters, boundary conditions,
- 89 excavation protocols, meshing and organization of calculation intervals. The reason is

- 90 that it has been developed using the GiD interface (<u>http://www.gidhome.com</u>) that
- 91 permits pre- and post- process of data in a user-friendly way.
- 92 The updated model for FEBEX is based on the geometry and material properties of the
- previous modeling efforts (Gens et al., 2009). The main objective of this work is to
- develop a new model of the well-known FEBEX experiment that can be further
- exploited in terms of two main goals: (1) comparison with new measurements and (2)
- 96 implementation of additional processes such as coupled flows and double structure
- 97 models to investigate their impact of hydration and stress development.
- 98 This updated model is intended to be complementary with the work done by Sanchez et
- al. (2012) who also made long term predictions about the FEBEX model but didn't
- 100 contemplate the introduction and assessment of the additional processes that are101 included in this article.
- 102

103 2. The FEBEX updated model

Figure 1 shows the model geometry and materials considered in this model. The host 104 105 rock, the bentonite buffer, and the concrete plug are the geomaterials considered. In 106 addition, a steel liner confines the bentonite and plug. The model assumes axisymmetry along the tunnel axis. The geometry and material distribution are prepared to simulate 107 108 the partial dismantling of the test which was carried out during the performance of the test in such a way that one of the heaters has continued operating. Boundary conditions 109 are modified accordingly for the excavation of the plug and part of the bentonite is 110 removed from the model thus simulating excavation. 111

112 This model takes advantage of the unstructured mesh development for the discretization 113 of the host rock. However, the buffer is discretized with structured mesh as this is more

- adequate in the zone of interest to reduce numerical errors and to facilitate the
- 115 monitoring of calculated variables that should be compared with measurements.
- 116 Table 1 shows the intervals considered in the analysis up to 2500 days, i.e. before
- dismantling operations. In order to match the measured evolution of temperature during
- the experiment (see more details about this in Gens et al., 2009), the heat power was
- 119 progressively modified (see table 1) until the 100°C target temperature was reached.
- 120 From that point on, the temperature was prescribed at the value of 100°C in both
- heaters. Later, one of the heaters was removed but the other continued heating.
- A mechanical boundary condition restraining the normal displacements has been
 applied all along the external boundary. Also, a constant pressure of 0.9 MPa is imposed
- 124 on the external boundary. As indicated above, during intervals 3 to 5 the power of the
- heaters is prescribed and therefore the temperature increases. Once the temperature
- reaches the target value on the surface canister $(100^{\circ}C)$ the boundary condition on the
- heater is changed from constant power to constant temperature (more information about
- boundary condition implementation in the Code_Bright User's Guide, downloadable
- 129 from the Code_Bright web page -<u>https://deca.upc.edu/en/projects/code_bright</u>).
- 130 Tables 2 and 3 show the constitutive laws used in the model and the properties
- 131 corresponding to the FEBEX bentonite as considered with single porosity and
- 132 considering that it can be represented with the Barcelona Basic Model or BBM (Alonso
- et al., 1990), van Genuchten model, Darcy's law, power relative permeability and
- 134 geometric mean for thermal conductivity. The parameters are divided in hydraulic and
- 135 mechanical parameters and correspond to the Code_Bright materials input window

- 136 (more information about this parameters in Code_Bright User's Guide). More precise
- 137 information may be obtained from the model, which is available by request to the
- authors.



- 140 Figure 1. Model geometry, materials and mesh considered for FEBEX updated
- 141 modeling (some materials are differentiated to simulate excavation only).
- 142

143 Table 1. Time intervals considered for the simulation up to 2500 days

Time interval	Initial Time	Final Time	Prescribed heat	Prescribed
	(days)	(days)	flow (W/heater)	Temperature (°C)
1 (stress equilibrium)	0	20	-	12
2 (construction)	20	155	-	12
3	155	176	1200	-
4	176	197	2000	-
5	197	207	2400	-
6	207	2500	-	100

144

Figure 2a shows the distribution of temperature around the 2 heaters at 21 days, 1.5
years and 5.5 years, i.e. during normal operation of the test and thus before dismantling.
It can be observed that the temperature in the vicinity of the heaters rises till it reaches a
value close to 100°C and the temperature of the surrounding host rock continues

increasing after that.

150 Figure 2b shows the distribution of degree of saturation. In general, the rock remains

saturated except at early times. As the bentonite is installed in the tunnel with a high

initial suction, some desaturation of the rock takes place. This zone is re-saturated very

- soon as the water from the host rock is mobilized. At 5.5 years, the bentonite buffer is
- not fully saturated, but the drying near the canister is less intense than at 1.5 years,
- 155 indicating that the saturation process continues.
- 156 Figure 2c shows the distribution of porosity in the bentonite. Clearly, swelling of the
- 157 bentonite takes place near the hydration boundary (i.e. the contact with the rock) while
- 158 contraction takes place in the zone of drying (i.e. the contact with the heaters). As it can
- be seen in the figure, the range of porosity variation after 5.5 years is 0.378 to 0.413,
- 160 with an average very close to the initial value of 0.4.
- 161

Table 2. Hydraulic parameters for bentonite. See Code_Bright User's Guide for furtherdetails.

Retention curve					
20	Van Genuchten model:				
0.072	$(1 - \lambda) = \left[(1 - \lambda) + \frac{1}{2} \right]^{-\lambda}$				
0.18	$S_e = \frac{S_l - S_{rl}}{S_r} = \left[1 + \left(\frac{P_g - P_l}{P_r}\right)^{1-\lambda}\right] \qquad P = P_o \frac{\sigma}{r}$				
0.01	$S_{ls}-S_{rl}$ [(P)] δ_0				
Intrinsic permeability					
1.9E-21	Darcy's law: $\mathbf{q}_{l} = -\frac{\mathbf{k}k_{rl}}{(\nabla P_{l} - \rho_{l}\mathbf{g})}$				
1.9E-21	Durcy shaw. $\mathbf{q}_l = \frac{1}{\mu_l} (\mathbf{v}_l + \mathbf{p}_l \mathbf{g})$				
1.9E-21	$13 (4 +)^2$				
0.4	Kozeny's model: $\mathbf{k} = \mathbf{k}_0 \frac{\phi^2}{(1-\phi_0)^2} \frac{(1-\phi_0)^2}{\phi^3}$				
0.001	$(1-\varphi)^2 \varphi_0$				
Liquid phase relative permeability					
6					
1	$k_{rl} = AS_e^{\lambda}$				
3					
Diffusive flux of vapor					
1	Fick's law for molecular diffusion:				
5.9E-6	$\mathbf{W} = -(\tau \phi_0 S D^W \mathbf{I}) \nabla_{(v)} v^{a p o r} - D \left[\frac{(273.15+T)^n}{(273.15+T)^n} \right]$				
2.3	$\mathbf{r}_{g} = -(\mathbf{r} \boldsymbol{\psi} \boldsymbol{\mu}_{g} \boldsymbol{\sigma}_{g} \boldsymbol{\nu}_{m} \mathbf{I}) \mathbf{v} \boldsymbol{\omega}_{g} \boldsymbol{\nu}_{m} = \boldsymbol{\nu} \begin{bmatrix} \mathbf{p}_{g} \end{bmatrix}$				
0.8	$\tau = \text{constant} = \tau_o$				
Conductive flux of heat 1					
1	Fourier's law: $\mathbf{i}_{c} = -\lambda \nabla T$				
0.47	$\lambda = \lambda_{act}^{S_l} \lambda_{dru}^{(1-S_l)}$				
1.15	sut ury				
	20 0.072 0.18 0.01 y 1.9E-21 1.9E-21 1.9E-21 0.4 0.001 e permeabil 6 1 3 por 1 5.9E-6 2.3 0.8 meat 1 1 0.47 1.15				

Figure 3 shows the variation of temperature at some points within the bentonite and the comparison between the Operational Base Case (OBC) model calculations –

- 167 corresponding to the analysis reported in Gens et al. (2009)– and the current model. It
- 168 can be seen that the temperature is reproduced in the same way by the model as it was
- 169 obtained with the OBC model, so this new model is equivalent to that one. It is
- important to recall that one of the objectives of this contribution was to prepare a newgeometry and mesh (GiD environment) to be able to consider additional cases.

A similar response is obtained in terms of relative humidity (Figure 4) and the

- 172 A similar response is obtained in terms of relative numberly (Figure 4) and the 173 correspondence of the present model with the OBC model shows that no significant
- variation has occurred. Actually, small variations on the parameters or shapes of the
- 175 constitutive equations do not produce a significant variation of relative humidity. This

- shows that it is possible that some additional mechanisms of water flow (in addition to
- 177 Darcy and Fick equations) may play a role and may help to explain the different
- 178 hydration rates.
- 179 The evolution of stresses in the bentonite is represented in Figure 5. The response shows
- 180 the same limitations as observed in the OBC especially concerning the overestimation
- 181 of stress development at early stages of hydration. The low measured stresses can be
- interpreted qualitatively in different ways, one of them being the possible hydration of
- 183 the bentonite aggregates controlled by double structure effects.
- 184

185	Table 3. Mechanical parameters for bentonite. Thermo-elasto-plastic (TEP) model. See
186	Code_Bright User's Guide for further details.

Elastic parameters		
ITYCL	1	
P1: <i>k</i> _{io}	-0.05	
P2: <i>kso</i>	0.25	$d\varepsilon^e = \frac{\kappa_i(s)}{\alpha} \frac{dp}{dr} + \frac{\kappa_s(p,s)}{\alpha} \frac{ds}{ds} + (\alpha) dT$
P3: K _{min} (MPa)	0.1	$1+e \ p' \ 1+e \ s+0.1$
P5: <i>v</i>	0.4	
P8: α_i	-0.003	where:
P9 : <i>αsp</i>	-0.161	$k(s) = k \left(1 \pm \alpha \cdot s \right)$
P10: pref (MPa)	0.01	$\kappa_i(s) - \kappa_{io}(1 + \alpha_i s)$
Thermal parameters		$k_{s}(p',s) = k_{so} \left(1 + \alpha_{sp} \ln p' / p_{ref} \right)$
ITYCL	1	
P1: α_o	1.5E-4	
P5: $T_{ref}(^{o}C)$	20	
Plastic parameters 1		
ITYCL	1	$\lambda(o)-kio$
P1: λ(0)	0.15	$p = p^{c} \left(\frac{p_{o}^{*}(T)}{p_{o}} \right)^{\lambda(s)-kio}$
P2: <i>r</i>	0.925	$P_o P \left(p^c \right)$
P3: β (MPa ⁻¹)	0.05	$n^{*}(T) - n^{*}$
P4: ρ (°C ⁻¹)	0.2	$p_o(\mathbf{r}) - p_o$
P5: <i>k</i>	0.1	F () 1
P6: p_{so} (MPa)	0.1	$\lambda(s) = \lambda(o) (1-r) \exp(-\beta s) + r $
Plastic parameters 2		
ITYCL	1	$p = p + k \operatorname{sexp}(-\rho \Lambda T)$
P1: <i>p^c</i> (<i>MPa</i>)	0.5	$P_s = P_{so} + K B CAP(P \square I)$
P2: <i>M</i>	1	
Ρ3: α	0.53	$\Delta I = I - I_{ref}$
P4: <i>e</i> _o	0.6	
P5: $p_o * (MPa)$	12	

188 Finally, the evolution of water pressure in the rock is represented in Figure 6. This

189 model uses 0.9 MPa as a boundary condition in the outer boundary. From the

190 observation of the results (overestimated pressure in the rock roughly by 0.05 MPa), it

is probable that 0.85 MPa would be more appropriate. This will be modified in future

models but the effect on the other variables is expected to be very small taking into

account the large suction gradients in the bentonite.

195 **3. Long term results**

196 Once the presented model was calibrated with real measurements, a long term

197 prediction has been performed. This section contains some results corresponding to the

model considering a maximum calculation time of 20 years and the incorporation of the

199 operations of shut down and dismantling of one canister, concrete abutment and

200 bentonite. The distribution of temperatures is shown in Figure 7a. It can be observed

that the operations of dismantling affect the canister close to the access drift together

- with part of the barrier, while the second canister heating continues. Figure 7b shows
- the distribution of degree of saturation and Figure 7c the distribution of mean stresses.
 Degree of saturation indicates that at 20 years, full saturation has not been achieved yet.
- Degree of saturation indicates that at 20 years, full saturation has not been achieved y
- 205 The evolution of temperatures is presented in Figure 8. Temperatures near the

dismantled heater show that the cooling takes place quite fast and that it has only a

small influence on section D1. In section F2 and G, the effect is very important and the model captures well the rapid fall of the temperature rapid down to the measured lower

208 model captures well the rapid fall of the temperature rapid down to the r 209 values due to the new configuration of the test after partial dismantling.

210 Pore pressures are represented in Figure 9. The negative pore pressures correspond

actually to suction. The strong evaporation induced by heating near the canister

produces a large increase of suction. The maintained heating in section F2 delays the

pore pressure increase near the canister. This is because the evaporation is strong and

vapor migration compensates the water flow from the rock. In section G, which

undergoes cooling caused by the canister removal, the water pressure recovers more

216 rapidly at the same time that cooling takes place. The rate of water pressure recovery 217 increases rapidly.

Relative humidity (HR) depends on pressure and temperature and can be calculated from these variables at any point. This is necessary in order to compare the calculated variables with the measurements of relative humidity at the sensors. The comparison is shown in Figure 10. Note that there is not real data for r = 0.52 m at section F2. While in section F2, near the heater, relative humidity does not reach 100%, which would correspond to full saturation, the 100% relative humidity is reached after 20 years at section H, indicating that when the heating stops, full saturation is reached more

225 rapidly.

226 Figure 10 also shows the evolution of stresses at sections F2 and G. Note that sections H and G can be considered equivalent sections, since they are very close to each other (see 227 Figure 3) and since neither there is data for stress at section H nor there is data for 228 229 relative humidity at section G. The stress development shows also the effect of the dismantling but it is less pronounced in the central zone of the prevailing heater. 230 231 Stresses reach a value in the range of 4 to 5 MPa according to the model calculations. The correspondence with the measurements is quite good at F2. In contrast, at section G 232 in which the measurements show a delay in the response, the sensor seems to have been 233 reactivated when dismantling took place. This model will be considered the base case 234

for the additional processes assessment that will be described next.

236

237 4. Additional processes assessment

The model presented above will be considered from now on as a base case for the
comparison with the results from alternative models including additional processes such
as the incorporation of a coupled flow induced by a thermal gradient, the variation of

- the intrinsic permeability or the introduction of a double porosity model, for which the
- impact on hydration and stress development has been assessed.
- 243



Figure 2. Distributions at 21 days, 1.5 years and 5.5 years of: a) temperature; b) degree

246 of saturation; c) porosity.

247



249 Figure 3. Temperature evolution at different points.

250

251 4.1. Thermal gradient induced water flow

The water flow induced by a thermal gradient can be expressed as an additional flux to the usual Darcy's flux. The generalized advective flux including thermal osmosis is expressed as in Eq. (1):

255
$$\mathbf{q}_{l} = -\frac{\mathbf{k}k_{rl}}{\mu_{l}}(\nabla p + \rho_{l}g\nabla z) - k_{rl}k_{T}\nabla T$$
(1)

256 Where **k** [m²] denotes the intrinsic permeability tensor, k_{rl} [-] denotes the relative 257 permeability of the liquid, *g* is the gravity vector, μ_l is the dynamic viscosity, *p* [MPa] 258 is the hydraulic pressure, *T* [K] is temperature, ρ_l is liquid density, and k_T [m²/K/s] is 259 the thermo-osmotic permeability.

This is the flux of liquid phase induced by both pressure and temperature gradients. It is
an advective flux in the sense that it drags the water. The total flux of water is then
written as in Eq. (2):

263
$$\mathbf{j}_l^w = -D\rho_l \nabla \mathbf{w}_l^w + \rho_l \mathbf{q}_l$$

Where D $[m^2/s]$ is the diffusion coefficient, which actually corresponds to the dissolved species, in this case the air, which is dissolved in the water.

(2)

266



267





a) Results from OBC case as compared with measurements



271 Figure 5. Evolution of stresses

272

270







275

b) Results from the current new model 0.9 Borehole SF23







Figure 7. Distributions for 2500 days and for 20 years of: a) temperature; b) distribution

- 278 of degree of saturation; c) distribution of mean stress.
- 279



Figure 8. Evolution of temperature at sections D1, F2 and G.





Figure 9. Evolution of pressure at sections F2 and G.





Figure 10. Evolution of relative humidity (up) and stress (down) at different sections for the base case.



- at an average temperature of 25 °C and various temperature gradients and porosities, 293
- range between 10^{-14} and $3 \cdot 10^{-13}$ m²/K/s. In another study [11] thermal osmosis across a 294 kaolinite membrane was investigated. An estimate of k from the data of this study 295
- (Srivastava, 1975), corresponding to conditions similar to the ones giving the high k
- 296 297
- values (Dirksen, 1969), yields a value of $2.6 \cdot 10^{-10} \text{ m}^2/\text{K/s}$, which is three orders of magnitude greater. As a first approximation, the values of k mentioned above can be 298
- used to define a range of values $k_T = 10^{-14} 10^{-10} \text{ m}^2/\text{K/s}^{\circ}$. 299
- 300 In order to compare this value with the value corresponding to the pressure gradient (i.e. the dominant effect), it is necessary to calculate the ratio between intrinsic permeability 301 and viscosity. For the intrinsic permeability value of the Febex bentonite a value of 302 $1.9 \cdot 10^{-21}$ m² which divided by the viscosity of water 0.001 Pa·s, leads to: $1.9 \cdot 10^{-12}$ 303 $m^2/MPa/s$. These two values are comparable. 304
- 305 In order to discriminate the relative dominance of fluxes in this case, it is also necessary 306 to introduce the gradients of pressure and temperature. While the temperature gradient can be estimated easily and does not change very much with time (although temperature 307 308 and water content change), the pressure gradient varies more, in space and time. 309 Therefore, depending on the zone in the bentonite and the time, the advective flux may be influenced by thermal osmosis and this should be investigated. 310
- 311 In order to implement in an easy way the thermal gradient term, Equation (1) can be written as: 312

313
$$\mathbf{q}_{l} = -\frac{\mathbf{k}k_{rl}}{\mu_{l}} (\nabla p + \alpha \nabla T + \rho_{l} g \nabla z)$$
(3)

314 In FEBEX, the pressure and the temperature gradients are opposite in sign. Actually the thermo-osmotic flux delays hydration and therefore it may explain some delayed 315 316 effects. The parameter α in this equation is the ratio between the thermo osmotic 317 conductivity and the hydraulic conductivity following Equation (3). As we have seen 318 that the order of magnitude can be similar, it follows that $\alpha=1$ gives a condition in which the thermal osmosis induced flux is comparable to the hydraulic flux. This 319 320 situation occurs because the bentonite has very low hydraulic conductivity and therefore it is possible to find a value of the conductivity for thermal osmosis which leads to $\alpha=1$ 321 (i.e. $1.9 \cdot 10^{-12}$ m²/K/s, the value calculated above but in the units of k_T). 322

The evolution of relative humidity in the case in which the thermal gradient induced 323 324 flux is incorporated is shown in Figure 11 (upper left) and Figure 12 (upper left), for 325 section F2. The water flow induced by the temperature gradient delays hydration. Actually, for the values of the parameters considered, it manages to compensate the 326 water inflow up to a point that for steady state temperature conditions, the relative 327 328 humidity stabilizes and does not tend to 100%. This means that the bentonite barrier is 329 not fully saturated and hence the isolation would be achieved.

- 330 The evolution of the stress development is also shown in Figure 11 (lower left) and 331 Figure 12 (lower left). Since the hydration reaches a point that does not progress, and
- relative humidity stabilizes, the stress also stabilizes below the swelling pressure. 332
- 333 Compared to the base case (see Figure 10), we can observe that the results of the base case are closer to the real data than those obtained considering this thermal gradient 334
- 335 induced flux. In fact, considering this induced flux, the relative humidity seems to stay
- constant with time, at least at points not far from the heater, which is not the result that 336
- the real measurements are given. 337
- 338

339 4.2. Sensitivity to permeability

An analysis about the sensitivity of the model to permeability changes has also been 340 performed, since permeability is the variable subjected to bigger variations due to 341 changes in density, structure and construction of the barrier, measurement difficulties, 342 343 etc. For the base case presented in this paper, permeability of the bentonite has been increased by a factor of 2, which is a reasonable variation. This accelerates somewhat 344 the hydration as the permeability of the buffer controls the hydration rate in FEBEX. 345 Moreover, as liquid pressure increases faster due to permeability increase, the stress 346 developed also increases faster leading to values which are still comparable to the 347 measurements (Figures 11 and 12). 348

349



Figure 11. Evolution of relative humidity (up) and stress (down) at section F2 for two additional excess thermal and iont induced flux (left) and double normachility (right)

additional cases: thermal gradient induced flux (left) and double permeability (right).

Actually, the stress development in the case of double permeability is quite consistent with measurements, giving closer values to the real data than the base case. It can also be observed that even doubling the permeability, full saturation of the bentonite barrier is not achieved, even after 20 years.

357





361

362 **4.3. Double porosity model**

The effect on the hydration and swelling including a double structure model is considered in this section. The double porosity model is an extension of the BBM approach presented above. The double structure effects are considered in the following way: two structural

- levels are considered with different suctions. The two suctions are related by aninteraction term.
- 368 Equation 4 shows the simplified mass balance equations incorporating the microstructure.
- 369 It is assumed that porosity can be decomposed into two adding contributions.

$$\frac{\partial}{\partial t} \left(\phi_{M} \rho_{lM}^{w} S_{lM} + \phi_{M} \rho_{gM}^{w} S_{gM} \right) + \nabla \left(\mathbf{j}_{lM}^{w} + \mathbf{j}_{gM}^{w} \right) = -\Gamma^{w} \qquad (M) \qquad (4)$$
$$\frac{\partial}{\partial t} \left(\phi_{m} \rho_{lm}^{w} S_{lm} \right) = \Gamma^{w} \qquad (m)$$

Where an interchange term has been introduced. This term is calculated as a function of the suctions in the micro pores and the macro pores (Eq. 5).

$$\Gamma^{w} = \alpha_{micro-macro} \left(s_{m} - s_{M} \right) \tag{5}$$

Where S_m is the suction micro and S_M corresponds to the suction macro. The macro and micro porosities are defined following Eq. 6.

$$\phi = \phi_M + (1 - \phi_M) \phi_{m'} = \phi_M + \phi_m \tag{6}$$

Where the porosity of the microstructure may be defined in two different ways, i.e. with respect to the volume of the microstructure or with respect to the total volume. The backfill material in the FEBEX is composed by blocks. The macro porosity is assumed to be 0.40 while the micro porosity is set to 0.15 in these model calculations.

The combination of the double structure and the BBM model consists –in the model used
here– in using the suction in the microstructure for the mechanical calculations. For
instance, for the swelling terms, the volumetric elastic deformation is calculated as in Eq.
7.

$$d\varepsilon_{v} = \frac{\kappa_{p}}{1+e} \frac{dp'}{p'} + \frac{\kappa_{s}}{1+e} \frac{ds_{m}}{\left(s_{m}+p_{atm}\right)}$$
(7)

In addition, the micropores contribute to water storage and a specific retention curve isconsidered, which essentially imposes that the micropores remain saturated (Eq. 8).

$$S_{lm} = \exp\left(-\frac{\left(s_{m}\right)^{\beta_{micro}}}{P_{o\ micro}}\right)$$
(8)

384 Where $\alpha_{\text{micro-macro}} = 5 \times 10^{-12} \text{ kg/MPa/m}^3/\text{s}$, $\beta_{\text{mic}} = 1.150 \text{ and } P_o_{\text{micro}} = 700 \text{ MPa}$.

The results of suction development are shown in figure 13. The micro suction shows a smoothed response when sharp variations of macro suction take place. This is an expected response as the water flow from macro to micro and vice-versa is delayed by the interaction parameter α . 389 Moreover, the results of the stress development when the double porosity is considered are quite similar to the results obtained in the base case, and thus are not shown in this 390 391 paper for the sake of briefness. The swelling stress in the FEBEX experiment is an integrated response of expansion of the backfill in a heterogeneous way as the process of 392 hydration is modified by the heating. The suction in the micro and macro pores is not 393 394 equal but it may happen that the averaged values are not so different. Actually, this is controlled by the capacity to hydrate and this, in turn, is controlled by the permeability of 395 the backfill. 396

397



398

Figure 13. Evolution of macro and micro suction. Dashed line is considered for micro suction while the continuous line corresponds to the macro suction.

401

402 **5. Conclusions**

403 This paper presents a model that has been prepared based on previous modeling efforts 404 performed for FEBEX. The model produces similar results as the previous models taking into account that some slight modifications have been introduced on the 405 constitutive equations (for instance, the retention curve). Once calibrated, the long term 406 407 response of the model predictions up to 20 years has also been performed, taking in 408 consideration the operations of shut down and dismantling of the first canister, concrete abutment and bentonite. The evolution of temperature, degree of saturation, stress, 409 water pressure, relative humidity have been analyzed. 410

The model has been used to analyze the effect of various processes, such as the

- 412 incorporation of thermal osmosis, the variation of intrinsic permeability and the
- 413 introduction of a double porosity model. The incorporation of thermal-osmosis leads to
- the possibility of developing a steady state situation in which the water flow induced by
- the thermal gradient is compensated by the water flow induced by the hydraulicgradient. This implies that the clay will not reach a full saturation even for long term
- 416 gradient. This implies that the clay will not reach a full saturation417 conditions.
- The vapor flux, although it can also be related to a thermal gradient is no able to reach this condition as it vanishes when the gas degree of saturation reduces. As the material
- 420 progressively saturates, the vapor flux reduces and finally is zero at full saturation. In
- 421 contrast, the liquid water flow induced by a thermal gradient increases with water
- 422 saturation and reaches its maximum for a given thermal gradient, at full saturation.

- The intrinsic permeability has been shown to be a parameter that permits a significant
- 424 improvement simply by varying it by a factor of two. In fact, the results obtain for the
- double permeability case are closer to real data than the base case, meanwhile the
- thermal gradient induced flux case gives worse results than the base case, if we comparethem with the real data.
- 427
- Finally, the double structure model has given different results for micro and macro
- suction but we found that does not have great influence in the general behavior of the model as the stress development obtained is guite similar to the base case
- model, as the stress development obtained is quite similar to the base case.
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