

International
Progress Report

IPR-04-34

Äspö Hard Rock Laboratory

Prototype Repository

Buffer – backfill interface displacement simplified THM modelling approach

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ANDRA

May 2004

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Report no.
IPR-04-34

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May 2004

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Keywords: Prototype, THM modelling, Displacement, Temperature, Saturation, Total stress

This report concerns a study which was conducted for SKB. The conclusions and viewpoints presented in the report are those of the author(s) and do not necessarily coincide with those of the client.

Abstract

Within the framework of the Prototype Repository Project performed by SKB at the Äspö HRL, deposition holes are filled with casks surrounded by a buffer and the deposition tunnel is backfilled. Question addressed by this report concerns the buffer-backfill interface displacement during natural hydration of the system. Simplified THM predictive modelling is applied in two extreme cases:

- Case Hole N.1: Hydration by water inflow inside the hole, which gives displacement of around 0.1 to around 0.2 m after 100 years depending on the elasto-plastic behaviour of the backfill.
- Case Hole N.3: Hydration by water inflow in the backfill with displacement of 0.1 m after 100 years.

Sammanfattning

I försöket Prototype Repository som genomförs vid Äspö Hardrock Laboratory har kapslar omgivna av högkompakterad bentonit placerats i deponeringshål. Tunneln och de övre delarna av deponeringshålen har även återfyllts med en blandning av krossat berg (70 %) och bentonit (30 %). Denna rapport behandlar deformationen av skiktet mellan buffert och återfyllnaden under naturlig bevätning. Förenklad THM modellering har gjorts för två extremfall:

- Fall 1 Deponeringshål 1: Hydratisering av buffert genom inrinning från deponeringshålet. Detta fall ger en förskjutning på mellan 0.1 – 0.2 m efter 100 år beroende på återfyllningens antagna elsto-plastiska beteende.
- Fall 2 Deponeringshål 3: Hydratisering genom inflöde till återfyllningen ger en förskjutning på 0.1 m efter 100 år.

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1 Context and objective of the study

1.1 Questions asked and modelling method

1.1.1 Questions asked

Within the framework of the Prototype Repository Project performed by SKB at the Äspö Hard Rock Laboratory, six heated copper casks have been emplaced in deposition holes drilled into the floor of a deposition tunnel. Within deposition holes, casks are embedded with bentonite buffer and the deposition tunnel has been backfilled with a mixture of 30 % bentonite and 70 % crushed rock. Buffer and backfill are in direct contact under initial gravity equilibrium (see Fig. 2-1).

One characteristic of the KBS-3 repository concept is the hydration of buffer and backfill through natural water inflows from the fractured surrounding rock. During the hydration process, both buffer and backfill mechanical properties evolve, as both materials contain bentonite swelling clays developing a hydro-mechanical coupling.

This major experiment is managed by SKB and involves many National Operators (Agencies) and their associated research teams. Among them, ANDRA is especially interested in the following operational question:

How is the position of the backfill-buffer interface dependent

- Of the hydration scenario (through the deposition tunnel, through a fracture inside a deposition hole, etc.)
- Of the mechanical behaviour (elastic / plastic) of the materials (buffer and backfill)?

On a pure scientific point of view, the *in situ* experiment is also a unique opportunity to test, in complex and realistic conditions, the capability of theoretical models and modelling tools to represent, at least qualitatively, the evolution of a structure at the scale of a deposition structure.

At the request of ANDRA, EDF realised a first modelling attempt with basic THM models representing transfers and mechanical elastic interactions in an unsaturated clay barrier. Among – at least – the three following mechanisms which influence the prediction:

- Geometric and boundary conditions;
- Practical importance of the plastic displacement of the backfill;
- Practical importance of the shear strength at the rock-barrier interface.

The first and second one were partially considered, with help of simplified assumptions, whereas the last one has been totally left to future studies.

1.1.2 Presentation of the results: contents of the modelling work

The analysis of the problem can be divided in two successive phases:

1. Dehydration scenario (and associated kinetics) of the buffer and backfill, which depend strongly on the thermo-hydraulic conditions imposed to the structure. For seek of simplicity and as a first modelling attempt, two “extreme” thermo-hydraulic configurations were considered: one with water coming from the tunnel; the other with water coming inside a hole (*via* a circular fracture).
2. Buffer-backfill mechanical interaction, involving the elasto-plastic behaviour of the materials. For seek of simplicity and as a first step of the modelling work, and also because of relative stiffness and “consolidation” state of the two geomaterials, only the plastic behaviour of the backfill was taken into account.

As expressed above, these two modelling stages are separated, meaning a weak coupling between the hydraulic kinetics (resaturation) and its mechanical consequences. The first phase is a pure elastic THM modelling whereas the second phase is a pure mechanical elasto-plastic modelling of the backfill. The link between phases 1 and 2 is realised by injecting the swelling of the clay calculated in phase 1 (under elastic assumptions for both the buffer and the backfill) as a mechanical boundary condition, expressed in terms of (total) stress, for the prediction made in phase 2 of the pure mechanical behaviour of the backfill alone.

Despite its approximate aspect, this method seems a simplified approach able to give tendencies and orders of magnitude of a buffer-backfill interaction involving plasticity and therefore, according to the hydration scenario followed, giving different final positions of the buffer-backfill interface at the end of the THM evolution (full resaturation).

1.2 Description of the test

1.2.1 Geometry

The test area can approximately be described as the association of 2 sections in the deposition tunnel, separated and sealed by concrete plugs and backfilled by a mixture of bentonite and crushed rock (see Fig. 2-1):

- A group of four deposition holes in section 1 of the tunnel: N.1 is 13 m away from the dead end, the distance between the boreholes is 6 m; the distance between N.4 and the concrete plug is 9 m.
- A group of two deposition holes in section 2: borehole N.5 is 9 m away from the concrete plug separating the two sections and borehole N.6 is 8 m away from the second sealing; the distance between the two boreholes is 6 m.

1.2.2 Instrumentation

Boreholes N.1 and 3 are equipped with sensors measuring total pressure, pore pressure and temperature and displacement of the buffer-backfill interface. The overall instrumentation is detailed in [BOR2].

1.2.3 Material data

The information followed for the behaviour of the materials and the corresponding data are:

- Clay buffer: same data as for the modelling of CRT and TBT (see EDF Reports [GAT2] and [SEM]), extracted from [BOR1] and [HÖK3], with special attention to the initial and associated parameters of the clay blocks;
- Backfill: THM data on the bentonite-crushed rock backfill are available in [JOH] and in [GUN];
- Pellets: THM data on pellets have been determined by [SUG] (however not considered in our study).

Modelling parameters, as well as modelling geometry and boundary conditions, will also be chosen with help of data adopted by other modelling teams, particularly by [LED2] and [CHI].

2 Geometry and modelling strategy

2.1 Geometry simplifications

From the information gathered in different reports, several conclusions and decisions were adopted:

- In spite of the 3D configuration of the test and of the interaction between boreholes, axi-symmetric modelling of an isolated borehole seems a good qualitative compromise (see [LED2, p. 4], in spite of the more controversial advice of [CHI, p. 7-8]).
- The numerical calculations will focus on the two instrumented boreholes N.1 and N.3.

2.2 Phase 1: elastic THM modelling of the resaturation kinetics

With help of some simplified assumptions, holes N.1 and N.3 can stand for two “extreme” typical situations (see Fig. 2-2):

- Because closer to the end of the tunnel and less submitted to the interaction with the other holes, N.1 is representative of a unique borehole in an infinite host rock. Experimental measurements revealed that resaturation is probably coming, through a fracture, directly inside the borehole, whereas the gallery remains nearly dry. This situation is represented, in our simulations of Borehole N.1, by a punctual water injection at hydrostatic pressure $p=4$ MPa inside the hole, equidistant from the bottom and the top (altitude $z=3$ m from the bottom, scan line LZ3 at $r=0.875$ m).
- On the contrary, according to in situ measurements and under the assumption that the host rock is undamaged around hole N.3 (which is transcribed by a zero hydraulic flux condition on the lateral surface of the buffer), the rehydration of hole N.3 comes preferentially from the tunnel (at hydrostatic pressure $p=4$ MPa). For seek of simplicity, hole N.3 is also modelled in axi-symmetric conditions as a unique hole in an infinite host rock [1].

Thanks to all simplifying assumptions made on geometry and on thermal-hydraulically-mechanical loading, the THM simulation can be separated into two successive sub-phases (See Fig. 2-2):

- Pure thermal simulation of the simplified geometry including the host rock;
- Fully coupled THM simulation on the tunnel (backfill) and the buffer alone, with imposed temperatures deduced from the previous stage and constant hydraulic boundary conditions ($p=4$ MPa and/or $q_w=0$) due to the simplifications listed above.

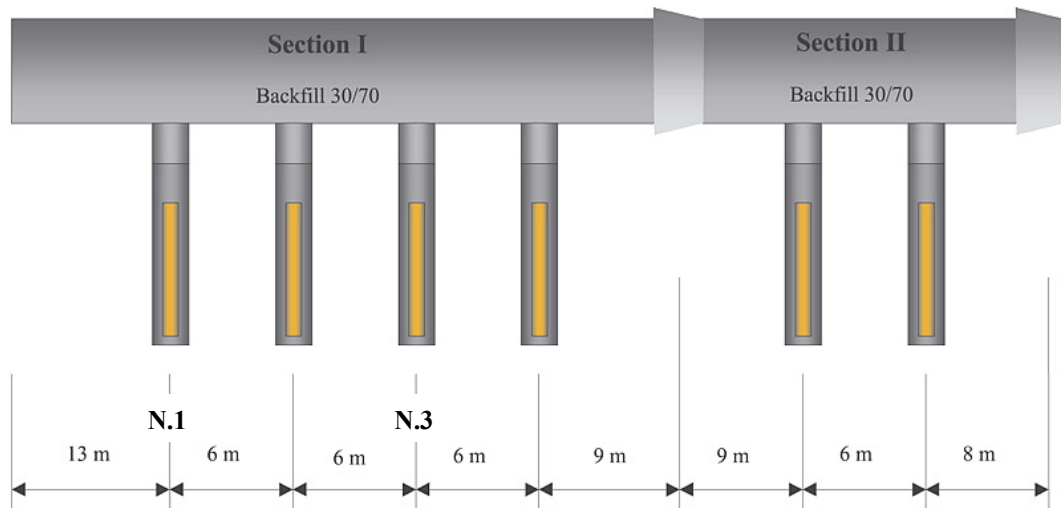


Figure 2-1. Schematic view of the layout of the Prototype Repository

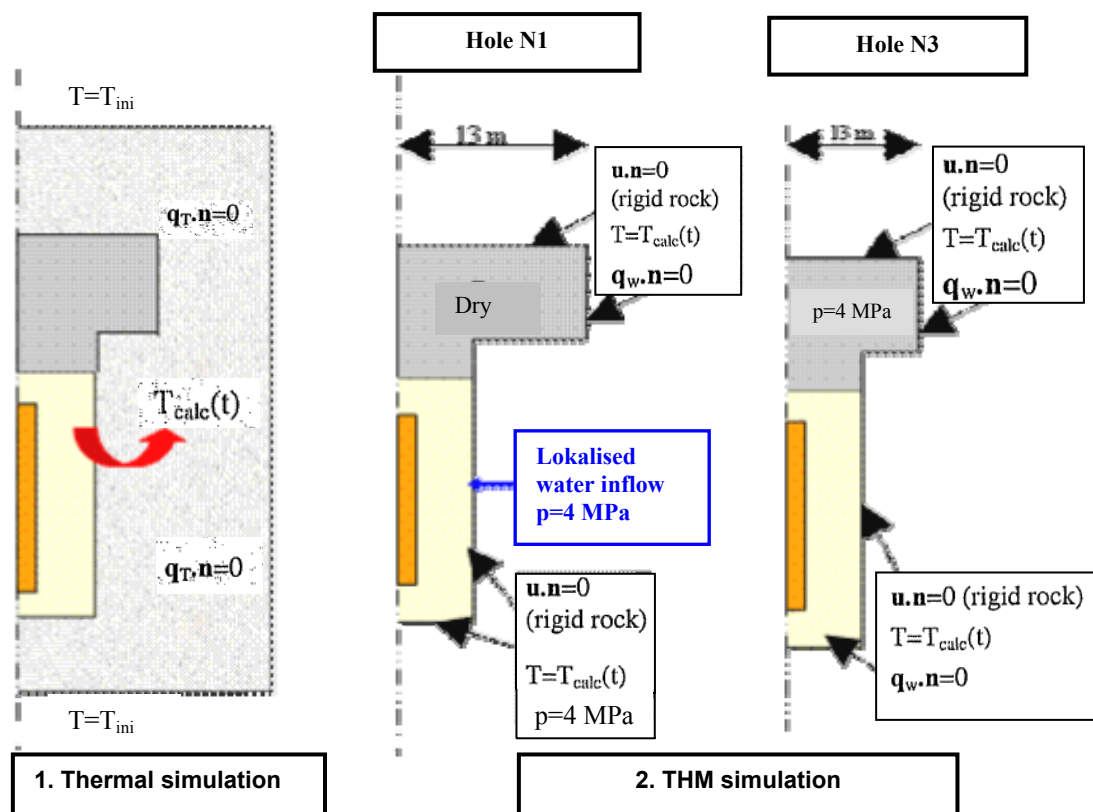


Figure 2-2. Schematic representation of modelling phase 1: THM (boundary conditions)

2.3 Phase 2: plastic behaviour of the backfill

Once THM evolution with time calculated (phase 1), total stress at the buffer-backfill interface is extracted from it and imposed, as a boundary condition, in a new simulation purely mechanical and concerning the backfill alone.

This new simulation is devoted to the influence of the plastic behaviour of the backfill, modelled with a Ducker-Prager criterion, corresponding to a cohesion $C=1$ MPa and a internal friction angle $\phi=33^\circ$.

3 Precise set of THM material data

With help of the bibliographic references listed below and also of previous studies performed by EDF on Projects CRT and TBT, the following complete and precise set of THM data was adopted for all materials:

Host rock: same data as in the modelling of TBT.

Clay buffer:

- when looking at values adopted by UPC [LED2, p. 10-11], and more specially to porosity and saturation value (resp. 0.366 and 0.83, p. 11), one deduce that the MX80 based clay buffer considered at the beginning of the test is close to the area called “upper ring” in the EDF report on TBT [SEM, p. 21]. Therefore, characteristics of the clay buffer are considered to be those defined in Table 3 (p. 21), column “Clay barrier - Upper ring”, of EDF Report [SEM]. However, some slight differences will be considered:
- intrinsic permeability $k_{int}=1.2 \cdot 10^{-21} \text{ m}^2$, which is consistent with $k(e)$ relations given in Clay’s report (Hökmark & Fälth, p. 12), as remarked in EDF’s report [SEM, p. 16] and will allow, in a second phase of the simulation, to approach reality by taking into account the measured evolution of the permeability with the void ratio; however, this value is much lower than the intrinsic permeability chosen by UPC in hole N.3 [LED2, p. 10: why such a difference with Hole N.1?] and will cause big discrepancies between the results of UPC and EDF;
- thermal data for the pure thermal calculation (phase 1, sub-phase 1) are: $C_{moy}=1355 \text{ J/(kg.K)}$ and $\rho_{moy}=2019 \text{ kg.m}^{-3}$;
- thermal data for the THM calculation (phase 1, sub-phase 2) are: $C_{grains}=800 \text{ J/(kg.K)}$ and $\rho_{hom_ini}=1983 \text{ kg.m}^{-3}$;

Backfill:

As given by [GUN, p. 11] and also adopted by [LED2, p. 10], the following data are considered for the backfill (assumed an homogeneous and continuous equivalent porous medium):

- dry density: $\rho_d=1700 \text{ kg.m}^{-3}$;
- intrinsic permeability: $k_{int}=4. \cdot 10^{-17} \text{ m}^2$, corresponding to hydraulic conductivity $K_{ws}=4. \cdot 10^{-10} \text{ m.s}^{-1}$;
- initial porosity: $\phi_0=0.4$ [LED2];
- Poisson’s ratio: $\nu=0.3$ [LED2];

- Young's modulus in drained conditions: $E=30$ MPa (this value is adopted by UPC, but the name "Compressibility: M" given by [GUN] introduces a possible confusion with the drained bulk modulus $K = \frac{E}{3(1-2\nu)}$; but, due to the value taken for Poisson's ratio $\nu=0.3$, this does not make any significant numerical difference);
- heat capacity: $C_{\text{clay grain}}=C_{\text{rock grains}}=800$ J/(kg.K), then $C_{\text{mixt grains}}=800$ J/(kg.K);
- density in saturated state (assumed in the calculation): $\rho_{\text{sat}}= \rho_d + \phi \rho_w = 2100$ kg.m⁻³;
- equivalent homogeneous volumetric heat (for pure thermal simulation): $C_{\text{hom}}=3.032 \cdot 10^6$ J/(m³.K).

Data material synthesis

Table 3.1 Thermal parameters

Parameter	Buffer (BO)	Rock (BG)	Backfill	Remarques
λ (W/m/K)	1.268	2.7	1.5	
ρ (kg.m ³)	2019			ρ_{moy}
C_p (J/kg/K)	1355			C_{moy}
$\rho \cdot C_p$ (J/m ³ /K)	$2.7357 \cdot 10^6$	$2.08 \cdot 10^6$	$3.032 \cdot 10^6$	

Table 3.2 Plastic parameters

Parameter	Buffer (BO)	Rock (BG)	Backfill
Friction angle (°)			33
Cohesion (MPa)			1

Table 3.3 THM parameters

Parameter	Buffer (BO)	Rock (BG)	Backfill	
			Hole3	Hole1
Young's modulus (MPa)	66	-----	30	
Poisson's ratio	0.4	-----	0.3	
Solid density (kg.m ⁻³)	2670	-----	2833	
Solid thermal expansion	10 ⁻⁵	-----	10 ⁻⁵	
Porosity (initial)	0.368	-----	0.40	
Reference vapour pressure (Pa)	1519	-----	1	906
Reference initial saturation	0.803	-----	1	0.4
Initial global density (kg.m ⁻³)	1983	-----	2100	
Initial capillary pressure (MPa)	15.745	-----	0	85.75
Initial enthalpy of water	-15745.	-----	0	-85750.
Liquid thermal expansion (K ⁻¹)	3. 10 ⁻⁴	-----	3. 10 ⁻⁴	
Viscosity of liquid water				
Viscosity of gas (Pa.s)	1.8 10 ⁻⁵	-----	1.8 10 ⁻⁵	
Liquid thermal conductivity (W/m/K)	3.363	-----	0	
Solid thermal conductivity	λ _{sol} =0.24	-----	2.5	
Capillary curve	$S_w = \frac{a}{a + \left \frac{p_c}{p_w g} \right ^b}$ <p style="text-align: center;">with $a=1.08 \cdot 10^4$ and $b=1.07$</p>			
Relative permeability to liquid phase	$k_{rl}(S_w) = S_w^3$			
Relative permeability to gas phase	$k_{rg}(S_w) = (1-S_w)^3$			
Intrinsic permeability (m ²)	3. 10 ⁻²¹	-----	4. 10 ⁻¹⁷	
Fick's Coefficient (global)(m ² s ⁻¹)	10 ⁻⁵	-----	10 ⁻⁵	

4 Results of phase 1: Thermal and THM modelling

4.1 Hole N.1

4.1.1 Saturation process (Fig. 4-3 and 4-4)

Punctual resaturation of the buffer: a diffusive process

Hole N.1 is submitted to a punctual rehydration coupled with temperature and mechanics (swelling). Fig. 4-3 and 4-4 show very clearly the diffusion of water inside the EBS, from its injection point (axi-symmetric representation of an horizontal fracture parallel to the tunnel) to the inner part of the clay buffer. Fig.4-3 shows strikingly that the saturation process is still running and far from its end after 100 years, and that the diffusive peak of saturation around the injection cote remains visible.

Water redistribution with temperature

Fig. 4-3 also shows that this saturation process is neither regular nor monotonous. When looking at what happens at the bottom of the buffer (near altitude $z=0$ in Fig. 4-3), one can notice that during the first year, this area is rehydrating more slowly than the rest of the clay buffer, consistently with its remote position from the water injection. But after 1 or 2 years, this tendency is inverted: surprisingly, the bottom ($z=0$) of the buffer becomes more saturated than areas that are yet closer to the injection point. This apparent paradox is explained by a strong coupling with temperature gradients, which are very strong between the interface of the hot zone near the canister and the cold zone around the bottom of the buffer, and which contribute to vaporisation-condensation circulations able to redistribute significant amounts of water [SEL, LAS2].

This phenomenon is even more visible in Fig. 4-4, located on the section of the injection: whereas saturation $S_w=1$ is imposed on the outer radius $r=0.875$ in contact with the fracture, a slight transient desaturation (-14%) due to heating occurs during the first 3-5 years of the experiment; then, the hydraulic diffusion of water becomes dominant and resaturates the whole section LZ3.

4.1.2 Thermal process (Fig. 4-1 and 4-2)

This T→H coupling has nearly no effect on the thermal evolution, which is very similar to those found by ENRESA [LED2, p. 6, 7 & 9]: a maximal temperature of 63°C at the heater-clay interface is obtained after 1 year only (on section LZ3: see Fig. 4). After 1 year, a very little redistribution of temperature can be noticed (with a cooling of 2°C in the hottest part), probably due to the resaturation of the inner part of the clay (for section LZ3: see Fig. 4-4), which contributes to a slight increase of the thermal conductivity.

4.1.3 Swelling profiles (Fig. 4-5 and 4-6)

Despite the localised aspect of the dehydration the swelling of the clay barrier (and the corresponding swelling pressure) is homogeneously distributed in space, vertically (Fig. 4-5) as well as radially (Fig. 4-6). The total stress value reached after 100 years is around -11 MPa.

However, this state of total stress “collapses” in the backfill (see Fig. 4-5 at altitude $z > 7$ m), revealing the great contrast of stiffness between the two materials.

Mechanical aspects will be more deeply commented in section 5 dealing with plasticity.

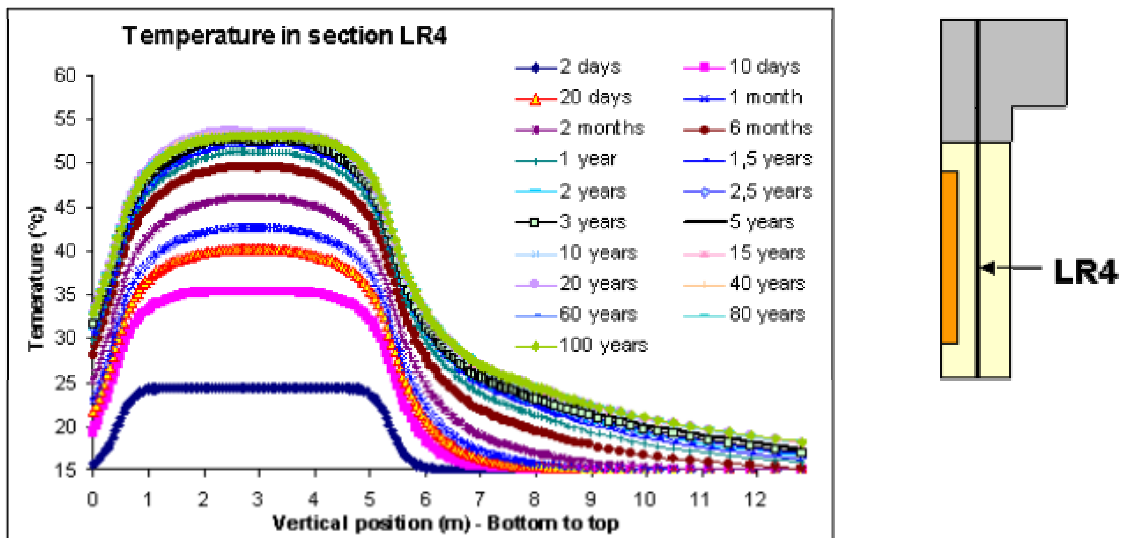


Figure 4-1. Temperature profiles at different instants in vertical section LR4 of Borehole N.1

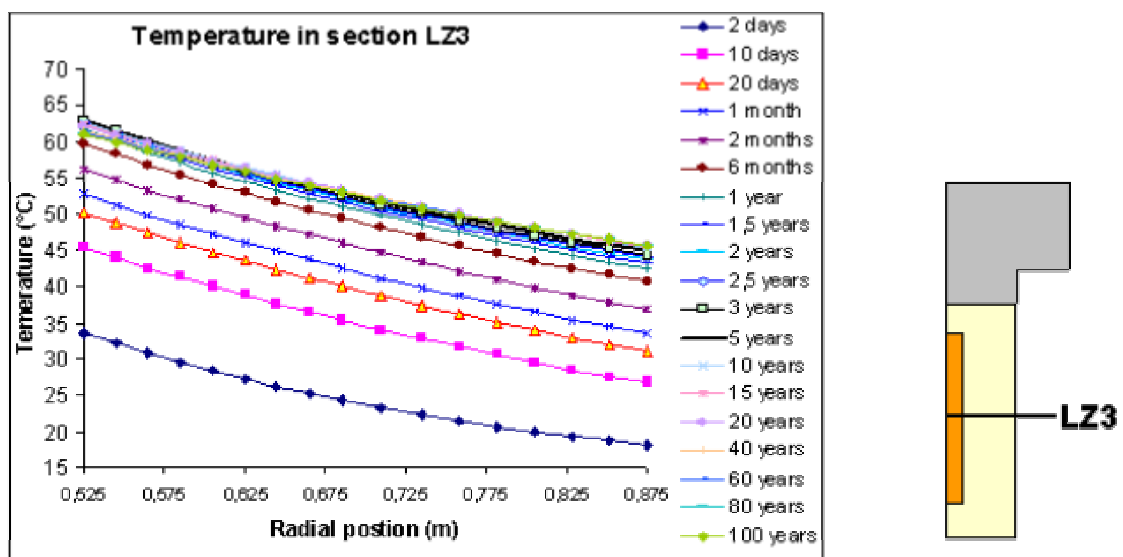


Figure 4-2. Temperature profiles at different instants in horizontal section LZ3 of Borehole N.1

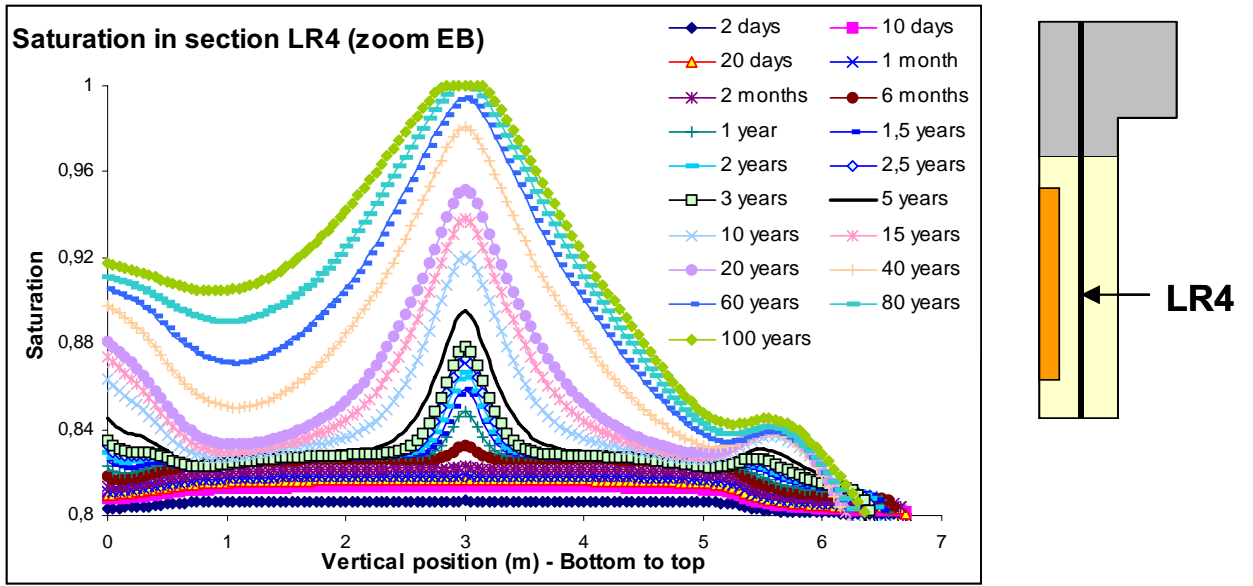


Figure 4-3. Saturation profiles at different instants in vertical section LR4 of Borehole N.1

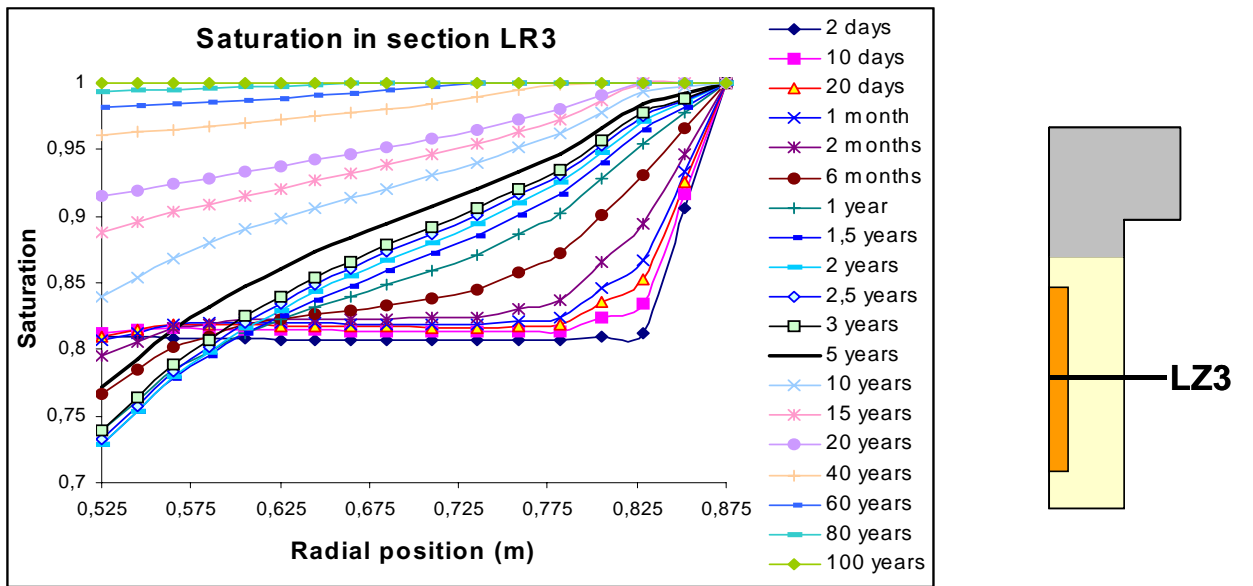


Figure 4-4. Saturation profiles at different instants in horizontal section LZ3 of Borehole N.1

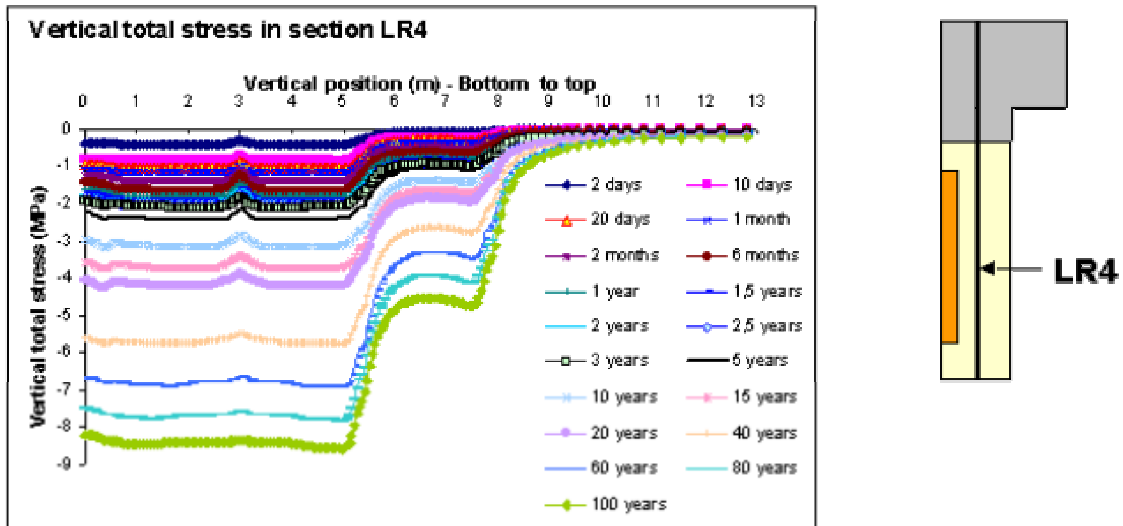


Figure 4-5. Vertical total stress profiles at different instants in vertical section LR4 of Borehole N.1

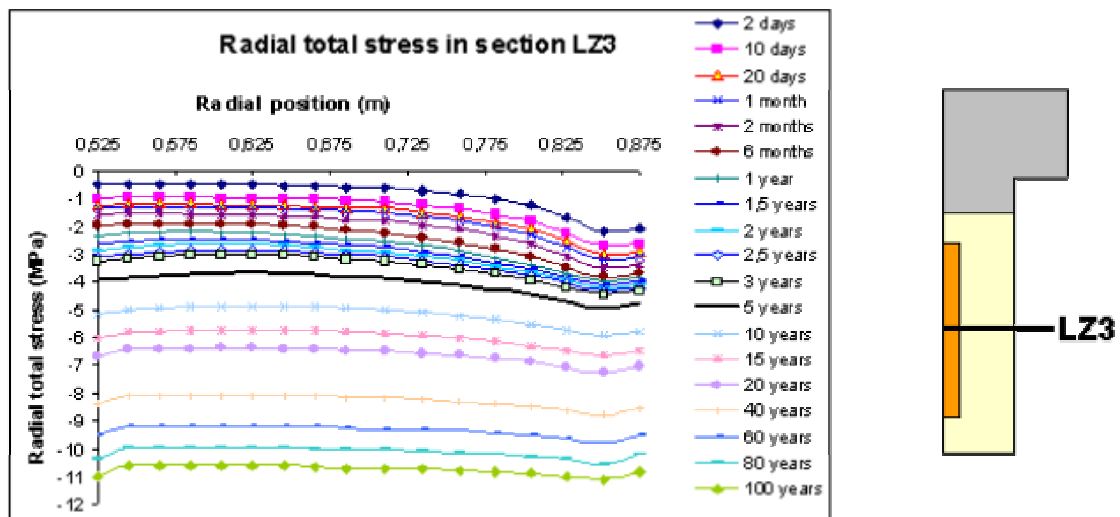


Figure 4-6. Radial total stress profiles at different instants in horizontal section LZ3 of Borehole N.1

4.2 Hole N.3

4.2.1 Saturation process (Fig 4-7 and 4-8)

Rehydration by the tunnel (backfill) vertical diffusive evolution in section LR4

Borehole N.3 is submitted to a rehydration by the drift alone. Fig.4-7 shows clearly this diffusive water inflow, which is now vertical from the top ($z=7$ m) to the bottom of the clay buffer. However, this resaturation seems very slow, and slower than the previous one by punctual injection. After 100 years, the process is far from being achieved and the central part of the clay barrier remains even less saturated than initially.

Water redistribution with temperature

Again, this apparent paradox is explained by the same water redistribution phenomenon as explained in § 4.1.1. Thermal gradients provoke a desaturation of the hottest zone (central zone) to the benefit of the coldest zones located near (namely: the bottom of the buffer, at $z=0$), despite their remote position from the hydration front.

This local water redistribution under thermal gradient is here clearer than in hole N.1, specially in section LZ3 (Fig. 4-8). In section LZ3, which is very far from the hydration front, no water is provided by the outside (tunnel), and the water redistribution that occurs from the inner part (desaturating from 82% to 63%) to the outer part of the section (rehydrating from $S_w=0.82$ to $S_w=0.88$), is only due to radial displacement of water under thermal gradient inside the section.

4.2.2 Thermal process

Thermal evolution in sections LR4 and LZ3 of hole N.3 is very similar to those concerning hole N.1. Slight differences can be noticed: hotter temperatures in section LZ3 (67°C instead of 63°C at the contact with the heater) and a very negligible redistribution of the thermal profiles after 1 year can easily be explained by the fact that, in hole N.3 (especially in LZ3), the resaturation is delayed, and consequently its influence on thermal parameters.

4.2.3 Swelling profiles (Fig. 4-9 and 4-10)

The total stress profiles on vertical section LR4 (Fig. 4-9) show, unsurprisingly, the link between the saturation evolution and the swelling pressure evolution. As expected, the area which is hydrating faster is also swelling (or developing swelling pressure) faster: this occurs clearly at the buffer-backfill interface – first in the buffer only, but the swelling pressure is finally transmitted to the whole bentonite-crushed rock filling the top of the hole and it seems that the “collapse” in stress which can be noticed in the backfill at altitude $z=7.8$ m is more a question of structure (intersection borehole-tunnel) than a question of material and its behaviour.

In section LZ3 (Fig. 4-10), a slight and non monotonous increase of swelling pressure (maximum value of 1.4 MPa after 6 months, decreasing to less than 1 MPa after 100 years) is only due to inner water redistribution under thermal gradient.

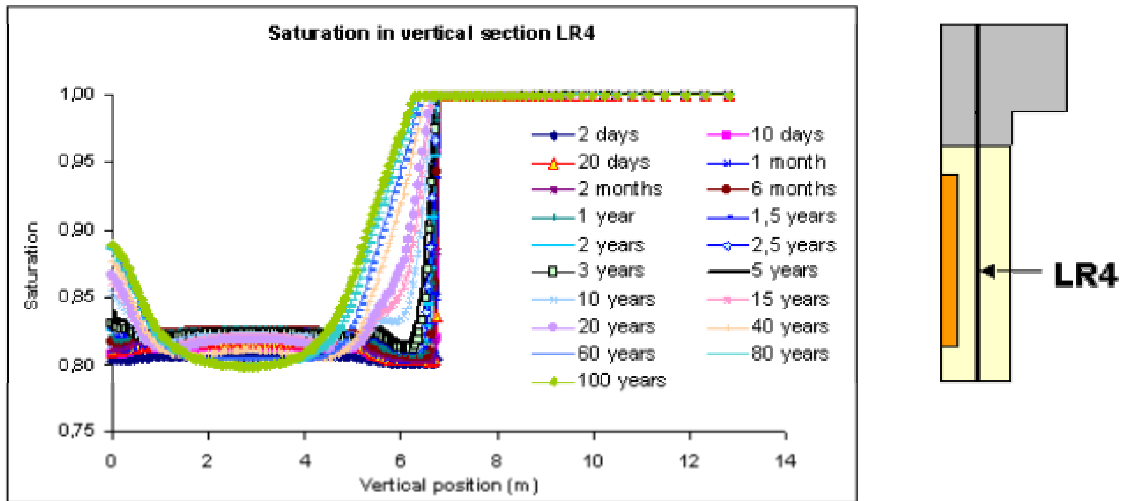


Figure 4-7. Saturation profiles at different instants in vertical section LR4 of Borehole N.3

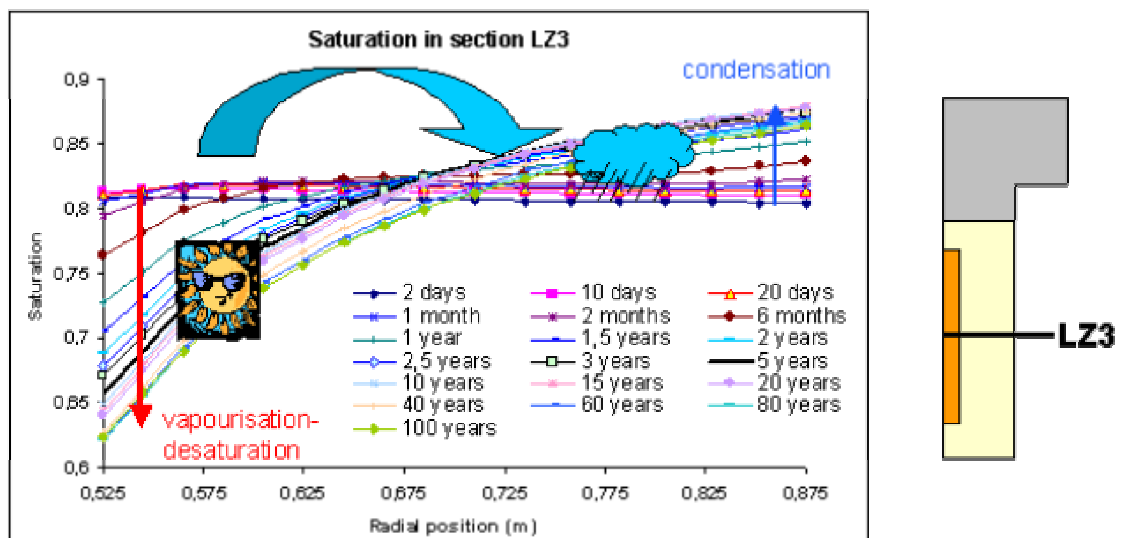


Figure 4-8. Saturation profiles at different instants in horizontal section LZ3 of Borehole N.3

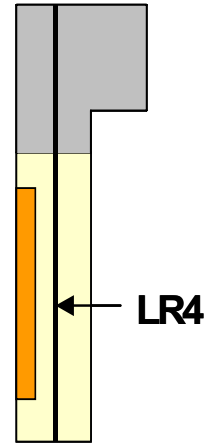
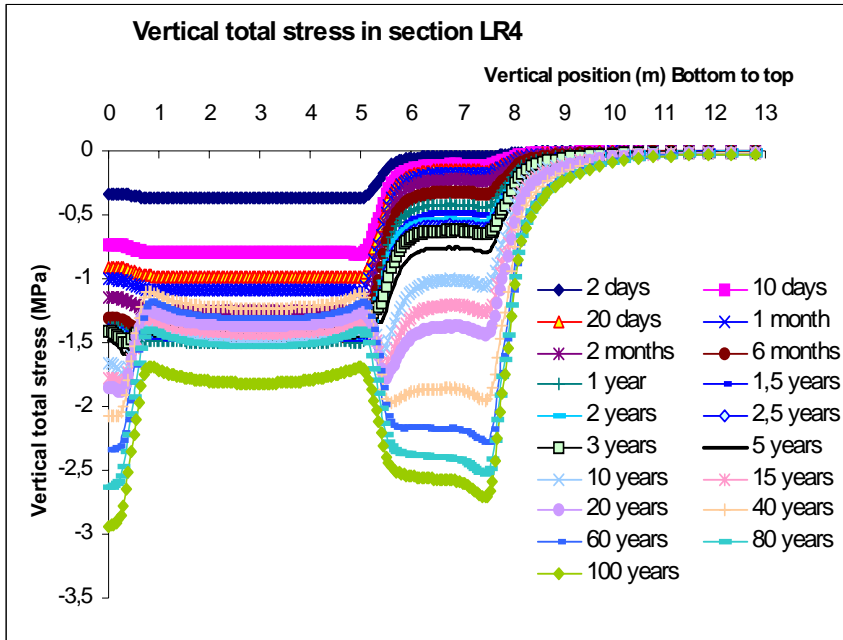


Figure 4-9. Vertical total stress profiles at different instants in vertical section LR4 of Borehole N.3

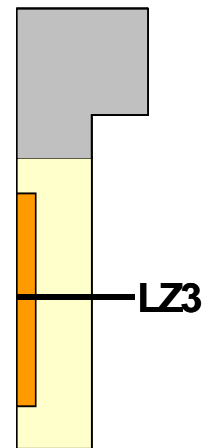
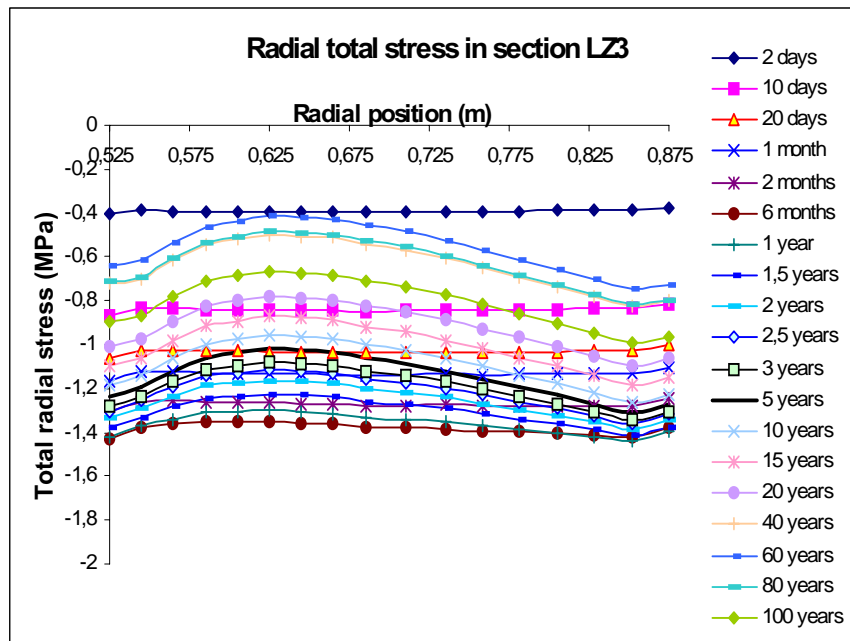


Figure 4-10. Radial total stress profiles at different instants in horizontal section LZ3 of Borehole N.3

5 Results of phase 2: Plasticity of the backfill

In order to answer the question of the position of the buffer-backfill interface according to the hydration scenario (borehole vs. tunnel), it was necessary.

1. To predict the kinetics associated to the two scenarios;
2. To account for irreversible effects dependent on the loading path associated to each scenario.

In this section, the loading path is “measured” at the buffer-backfill interface and applied, as a pure mechanical loading, to the backfill considered alone. More precisely, the total stress calculated in phase 1 at the buffer-backfill-interface is recorded and applied again in a new simulation, which is an elasto-plastic modelling of the backfill^[2].

Then, the corresponding displacement is calculated, with contribution of both its plastic and its elastic component. These two contributions can be distinguished when comparing these new results to the displacements formerly calculated in the pure elastic simulation of Phase 1^[3]. This comparison is made in Fig. 5-1 (hole N.1) and 5-2 (hole N.3) below, which show:

- A big influence of the plastic component of the vertical displacement at the buffer-backfill interface in hole N.1: the vertical displacement is about 17 cm instead of 6 cm (at $z=7\text{m}$) after 100 years (full saturation not yet reached);
- A much smaller influence of the same plastic component in hole N.3, responsible for an increase of 0.8 cm only (total displacement of 10.6 cm) for the same value of the elastic displacement: 9.8 cm.

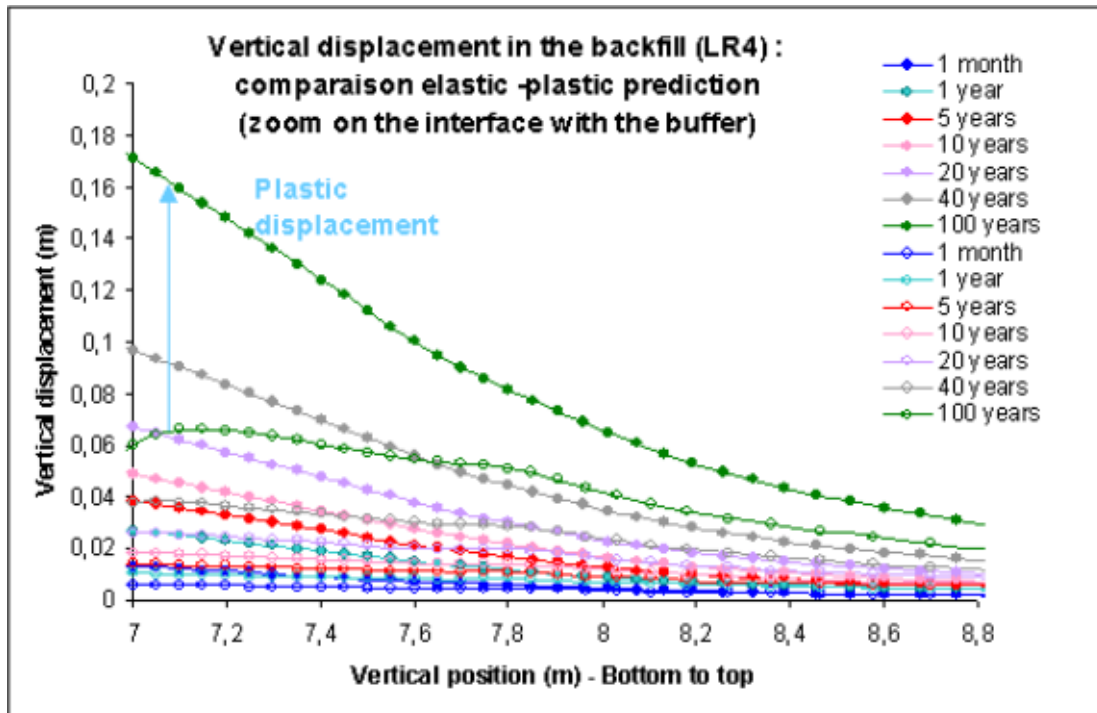
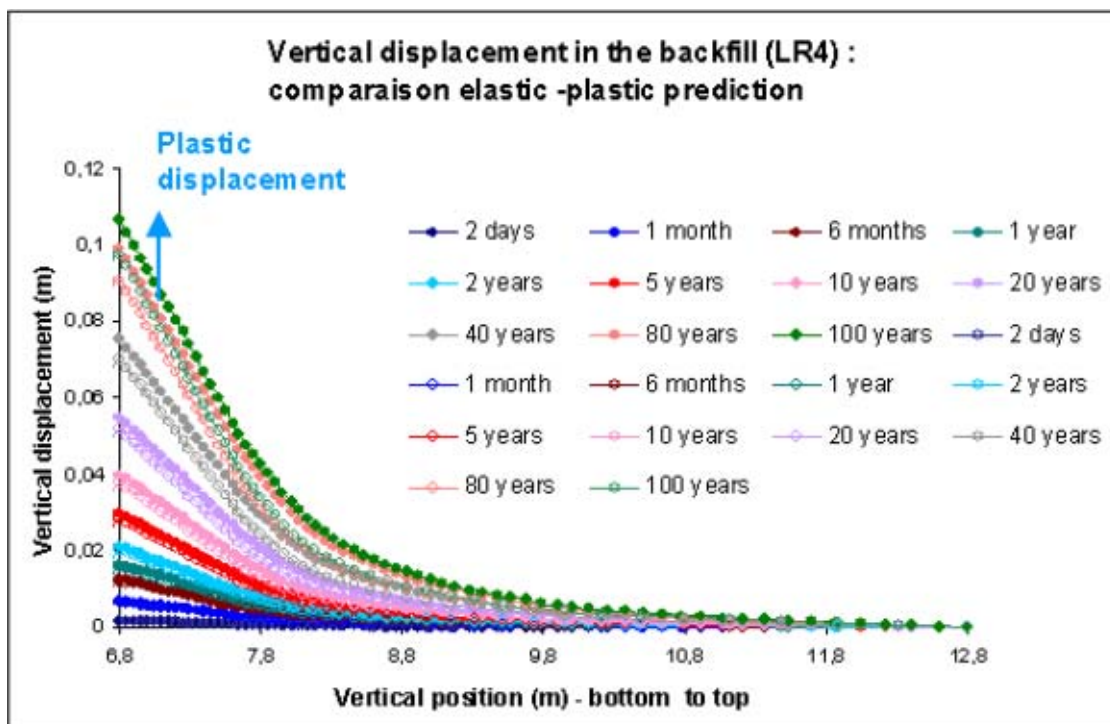


Figure 5-1. Vertical displacement in the backfill of Borehole N.1 (section LR4).



*Figure 5-2. Vertical displacement in the backfill of Borehole N.3 (section LR4).
Elasto-plastic modelling (plain symbols) and comparison to elastic modelling (white symbols)*

References

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^[1] Even if such a simplification seems less defensible in the case of N.3 which, due to its position in the middle of section 1 of the tunnel, develops a maximal interaction with all the other holes. In fact, a first modelling attempt was made by considering hole N.3 as representative of a generic borehole in a periodic repository, with symmetry conditions implying no hydraulic and thermal flux as well as no displacement in the median plan with the neighbouring boreholes. In the perspective of a 2D axisymmetric representation, the “characteristic distance” of the gallery in interaction with the borehole was then 3 m – which is also representative of a no-displacement mechanical condition in all directions: in the median plan because of symmetry (distance: 3 m) and at the rock-backfill interface, because of the quasi undeformability of the host rock (distance: 2.5 m, radius of the gallery). This simplification in geometry, which stands for the other extreme representation of hole N.3, leads to too high temperatures.

^[2] Let us notice that, as the backfill remains either nearly totally dry (hole N.1) or totally saturated at constant pressure (hole N.3), the hydro-mechanical part of its behaviour is not – or nearly not – activated. Additionally, one can admit that this hydro-mechanical part (*ie* the attached HM properties) is much lower for the backfill than for the bentonite buffer. For this reason, it seems reasonable to consider only the purely mechanical loading on the backfill, that is to say the total stress applied on it by the swelling clay.

^[3] The equivalence of the elastic component in Phase 2 and the displacement of Phase 1 is justified by the purely mechanical behaviour of the backfill, for reasons explained in the previous footnote.