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Thermal Impact on the Damaged Zone Around a Radioactive Waste Disposal in Clay Host Rocks

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Deliverable D13 – Annex 2 Hollow cylinder tests on COX argillite

Editor(s): Robert Charlier Authors : Robert Charlier, Frédéric Collin, Pierre Gerard, Chunliang Zhang

Laboratories: ULg, GRS

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1 Introduction

Hollow cylinder tests have been performed by GRS on COX argillite samples within Timodaz WP 3.3 (Deliverable 7). The experimental results have evidenced the axial permeability increase by fracturing due to the mechanical and thermal loading.

Within Timodaz WP5.3 ULg and GRS perform thermo-hydro-mechanical modelling of this experiment. New hydro-mechanical couplings are proposed in order to reproduce the increase of the permeability with the mechanical load. ULg uses a hydro-mechanical model where an additional coupling between the permeability and the tensile strains is associated. This embedded fracture model allows the reproduction of the development of preferential pathways along fractures generated by tensile strains. This model is introduced in the finite element code Lagamine developed by ULg. GRS uses a damage-elastoplastic model, which takes into account the permeability evolution with porosity according to the Kozeny relationship. The modelling from GRS is performed with the Code Bright finite element code. In this report the experimental procedures and the main tests results are firstly reminded. Then the proposed thermo-hydro-mechanical models by each team are developed. Comparisons between numerical and experimental results are then presented.

2 Executive summary

Hollow cylinder tests have been performed by GRS on COX argillite samples within Timodaz WP 3.3 (Deliverable 7). The experimental results have evidenced the axial permeability increases by fracturing due to the mechanical and thermal loadings. Within Timodaz WP5.3 ULg and GRS perform thermo-hydro-mechanical modelling of this experiment. New hydro-mechanical couplings are proposed in order to reproduce the increase of the permeability with the mechanical load:

- ULg uses a hydro-mechanical model where an additional coupling between the permeability and the tensile strains is associated. This embedded fracture model allows the reproduction of the development of preferential pathways along fractures generated by tensile strains. This model is introduced in the finite element code Lagamine developed by ULg.
- GRS uses a damage-elastoplastic model, which takes into account the permeability evolution with porosity according to the Kozeny relationship. The modelling from GRS is performed with the Code_Bright finite element code.

2.1 Large hollow cylinder tests on COX argillite

Within TIMODAZ-WP3.3 (Deliverable 7), GRS carried out EDZ-simulation tests on four large hollow cylinders of the COX argillite to investigate fracturing and sealing processes of the host rock around HLW disposal boreholes. The large COX cores were extracted from the MHM-URL at Bure and prepared to hollow cylinders of ~0.5 m length and 280 mm outer diameter with axially-drilled central boreholes of 100 mm diameter. High saturation degrees were achieved between 82 % and 100 %.

Regarding damage development and recovery in the host clay rock around HLW disposal boreholes, the tests were designed and carried out in the GRS big triaxial apparatus by simulation of the relevant processes such as borehole excavation, backfilling / lining, heating, and cooling. Figure 1 illustrates a typical test layout and the pictures of a large hollow cylinder before and after testing.



Figure 1 : Test layout of EDZ-simulation with large hollow cylinders of COX argillite

The main observations from the four large hollow cylinder tests are:

- 1. The <u>borehole excavation</u> simulated by reducing the inner borehole pressure from 15 MPa down to 1 MPa resulted in convergence of the borehole but not any increase in permeability along the cylinder axis, indicating no build up of pathway through the samples. Further increase of the external confining stress beyond 20 to 24 MPa (corresponding to depths of 800 1000 m) led to fracturing and flow pathway, indicated by the drastic increase in gas permeability from 10^{-21} m² to 10^{-14} m².
- 2. The <u>backfill impact</u> simulated by increasing the inner borehole pressure from 1 to 15 MPa led to a strong reduction of the gas permeability by several orders of magnitude from 10⁻¹⁷ down 10⁻²¹ m², depending on the initial characteristics of the excavation-induced fractures in the argillite.
- 3. The <u>water transport</u> through the fractures in the claystone led clay minerals swelling into the interstices and thus sealing the fractures, whereby the permeability decreased drastically to $2 \cdot 10^{-18}$ m², four orders of magnitude lower than that by gas flowing.
- 4. <u>Heating</u> from 29 °C to 74 °C accelerated the borehole convergence and the water inflow. The thermal impact on the water conductivity of fractured claystone is governed by the change of the water viscosity, while the intrinsic permeability is less affected by heating.
- 5. <u>Cooling</u> down slowed the deformation and the water transport through the fractured claystone. The permeability after cooling was between $1.0 \cdot 10^{-18}$ and $3.5 \cdot 10^{-18}$ m², nearly the same as that before heating.
- 6. The <u>post-investigation</u> on a tested sample showed a significant increase of the water content up to 9.3 % at the inlet side to 6.2 % at the outlet. The most part of the sample was "over saturated", i.e. the water content was higher than that in the natural and saturated state (w \approx 7.0 %). The water uptake was accompanied by volume expansion of the clay matrix into the fracture space under confined conditions.

Details of the test results are given in Deliverable 7.

2.2 Numerical results of ULg

ULg numerical modelling of hollow cylinder tests is performed by using Lagamine finite element code. One EDZ-simulation test is modelled: the BMT4 hollow cylinder test. Initial state of argillite is desaturated ($S_{rw} \square 0.86$), which implies the need of a thermo-hydromechanical model for unsaturated media. The initial stress state is isotropic.

2.2.1 Constitutive models

The main relationships of the thermo-hydro-mechanical model for unsaturated media are based on Bishop effective stress. The mechanical model used for the COX argillite is a nonassociated elastoplastic constitutive law. The yield surface is defined by a Van Eekelen criterion. Isotropic hardening of the friction angle is considered in the model.

The mass flow into the porous medium is defined by the sum of the advection of the liquid water (Darcy's law for unsaturated cases) and the diffusion of water vapour (Fick's diffusion law). The advective flux of the gaseous phase is neglected. The water retention curve is given by the van Genuchten relationship and the water relative permeability function proposed by van Genuchten is also adopted.

The heat transport is related to three effects: conduction, convection by the fluids and evaporation. The enthalpy of the system is given by the sum of each component's enthalpy. Further details about the balance equations and the coupled thermo-hydraulic formulation can be found in Collin et al. (2002) and in Deliverable 10.

2.2.2 Permeability-strain coupling model

A specific permeability model (Olivella and Alonso, 2008; Levasseur et al., 2010) is considered in order to reproduce the development of preferential pathways into argillite. It adds new hydro-mechanical coupling between permeability and the strain state. The basic idea consists in the appropriate representation of single discontinuity representing the rock bedding, which is embedded in a continuous finite element. As presented in Deliverable 10, the increase of permeability in the damage zone is linked with the development of tensile strains:

$$K_{ij} = K_0 \left(1 + \lambda \left(\varepsilon^T - \varepsilon_0 \right) \right)^3 \quad \text{if } \varepsilon^T > \varepsilon_0 \tag{1}$$

with K_0 the initial permeability, ε^T the tensile strain, ε_0 a threshold strain for the permeability increases and λ a fitting parameter corresponding to the fracture density. The threshold strain could be considered as the strain corresponding to the tensile strength of the rock. Aperture opening can not therefore be initiated before a failure by tension occurs.

2.2.3 Experiment numerical idealization

A 2D axisymetric modelling of the BMT4 hollow cylinder test is performed. Injection filter is taken into account in the modelling (Porous disk), because it influences the water volume injected during the four injection steps. Indeed when the injection system is shut-off the water in the porous disk continues flowing into the sample. The porous volume of the injection system influences thus the water volume injected in the sample. The geometry and the initial conditions of the modelling are presented in Figure 2.



Figure 2 : BMT4 hollow cylinder test (a) Geometry and initial conditions – (b) Mesh for finite element modelling

There are 6 steps in the thermo-hydro-mechanical modelling of the BMT4 hollow cylinder test: the consolidation, the borehole excavation, the EDZ intensification, the water injection tests, the cooling and the heating stages. Gas permeability tests are performed at the end of the consolidation stage and during the borehole excavation and EDZ intensification stages. However they are not modelled, which should not influence a lot the numerical results owing to the low gas volume injected in argillite. Gas pressure remains thus constant at the atmospheric pressure during the modelling.

Concerning the filter, high permeability is defined and the water relative permeability curve is based on a cubic law. A small air entry value and a sharp decrease are used for the retention curve of the filters. A linear elastic model is used for the mechanical behaviour with the same Young modulus and Poisson ration as for argillite. It allows avoiding the development of stresses concentration and traction strains at the contact between the filter and argillite. The porosity of the filters is provided by GRS and is needed in order to reproduce the correct porous volume of the injection system. The thermal characteristics are the same as for argillite.

2.2.4 Conclusion on ULg modelling

An elastoplastic model with a hardening of the friction angle provides a good reproduction of the experimental strains measured at the sample inner and outer during the different mechanical loading steps.

The embedded fracture model has been used for the modelling of the different steps. It allows the increase of the permeability assuming the development of preferential pathways in the zones where tensile strains are developed (Figure 3). Aperture of discrete paths is the main variable that controls the permeability evolution. This model allows the reproduction of the permeability increase observed at the inner of the COX hollow cylinders submitted to mechanical load. Nevertheless the experimental results seem to be strongly influenced by the initial desaturation of the porous disk, which makes difficult an accurate reproduction of the injected water volume through the sample during the water hydraulic tests.



During the heating and the cooling stages, the modelling could reproduce the general tendency of the water inflows or outflows (Figure 4 and Figure 5), but underestimate the experimental water volume. The thermo-mechanical model of the COX hollow cylinder does not take into account the influence of temperature on the mechanical characteristics, but argillite seems to behave as a normally consolidated rock with the development of compressive strains when the temperature increases. For long term predictions, the modelling underestimates the experimental radial strains, but the development of potential thermo-plasticity is not taken into account in the model.



Figure 3 : Water volume injected during the injection tests – Comparison between experimental and numerical results



Figure 4 : Inner radial strain during heating and cooling stages (V and VI) – Comparison between experimental and numerical results

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Figure 5 : Outer radial strain during heating and cooling stages (V and VI) – Comparison between experimental and numerical results

2.3 Numerical results of GRS

GRS benchmark modelling was performed by using CODE_BRIGHT (version cdv3, 2004). Two EDZ simulation tests BMT1 and BMT4 were modelled.

2.3.1 Constitutive models

Considering the complex testing procedure and boundary conditions of the large hollow cylinder tests, coupled THM calculations were carried out by solving a set of balance equations of energy, solid mass, water mass, air mass and stress equilibrium with selected constitutive models. The main assumptions were made:

- 1. The COX clay rock is relatively isotropic and homogeneous because of the insignificant bedding planes;
- 2. Heat transport includes conduction (Fourier's law) through the porous medium, advection of liquid water and vapour flow;
- 3. Water transport is controlled by liquid water advection (Darcy's law), vapour diffusion in air (Fick's law), and liquid / gas phase changes (psychrometric law);
- 4. Gas migration is governed by advection (Darcy's law), dissolution in liquid (Henry's law) and the ideal gas law;
- 5. The damage-elastoplastic model developed by UPC for argillaceous rocks (Vaunat et al., 2003; 2004; 2009) is applied for description of the mechanical behaviour of the COX claystone. COX is considered as a composite material made of a clay matrix connected by bonds (Figure 6). The clay matrix behaves like a typical elastoplastic soil Hoek and Brown's criterion as yield surface, while the bonds behave like a typical quasi-brittle material that can be represented by a damage elastic law. Bond damage or degradation occurs as the result of apparition of micro-fissures within the bonds, which reduces the surface on which stresses and strains are active. Any load applied to an element of cemented material is distributed itself between the soil matrix and the bonds according to a ratio that depends on the geometric arrangement of both components.







Figure 6 : Conceptual model of claystone as composite material with clay matrix and bonds

Details of the formulations and applications of the applied balance equations and constitutive models are given in a number of UPC's publications (Gens et al., 2006; 2007; Vaunat et al., 2003; 2004; 2009).

2.3.2 Permeability porosity coupling model

The Kozeny's model is employed for the relationship of permeability k with porosity φ :

$$k = k_o \frac{\varphi^3}{(1-\varphi_0)^2} \frac{(1-\varphi_0)^2}{\varphi_0^3}$$
(2)

with the initial permeability value of $k_0 = 2 \cdot 10^{-20} \text{ m}^2$ at the initial porosity of $\phi_0 = 15\%$ for the COX argillite.

2.3.3 Experiment numerical idealizations

BMT1

The EDZ-simulation test BMT1 was performed on a COX hollow cylinder (DIR2003-K4) of D/d/L= 280/100/525 mm at ambient temperature of 26 °C in four steps:

- i. <u>Initial state</u> at the same outer and inner borehole pressure of $\sigma_R = \sigma_r = 15$ MPa and axial stress of $\sigma_a = 17$ MPa;
- ii. <u>Borehole excavation</u> by decreasing the inner pressure down to $\sigma_r = 2.6$ MPa;
- iii. <u>Unloading</u> in radial direction down to $\sigma_R = 3$ MPa for 4 days;

iv. <u>Loading</u> in axial direction to failure.

During the test, gas flow was recorded at injection pressure of 1.5 MPa at the bottom. This test was simulated in a hydro-mechanical coupling way using an axisymmetric model. Because the sample was initially not saturated at a degree of 82 %, the corresponding suction of s = 22 MPa is adapted as the initial condition in the sample. The modelling steps with application of the corresponding boundary conditions are illustrated in Figure 7.





Figure 7 : Geometry and boundary conditions for modelling of the hollow cylinder test BMT1

BMT4

The EDZ-simulation test BMT4 was performed on a COX hollow cylinder (DIR1004-EST27312) of D/d/L= 280/100/460 mm. The test procedure involved six phases with respective boundary conditions:

- I. <u>Initial state</u> at the same outer and inner borehole pressure of $\sigma_R = \sigma_r = 15$ MPa and at fixed axial strain ($\Delta \epsilon_a = 0$);
- II. <u>Borehole excavation</u> by reducing the borehole pressure down to $\sigma_r = 1.0$ MPa;
- III. <u>EDZ-intensification</u> by increasing the external radial load till gas breaking through;
- IV. <u>Water injection</u> to the top of the fractured sample at pressures of 0.5 to 0.3 MPa for 17 days;
- V. <u>Heating</u> by increasing the temperature from 29 °C to 74 °C at the outer surface during 3 days and kept constant for 19 days;
- VI. <u>Cooling</u> down by reducing the temperature to the initial level of 29 °C over 3 days and kept for 18 days.

Considering the complex testing procedure and conditions, coupled THM calculations were carried out. The initial porosity of 15.8 % and saturation degree of 90 % (suction s = 10 MPa) are taken into account. An axisymmetric model is adopted for the hollow cylinder (Figure 8). The realized test procedure with the above mentioned steps is simulated by applying the corresponding conditions to the model.

The following boundary conditions are applied: (1) instead of the fixed axial strain, the recorded axial stress of 1.7 MPa is applied in the model within the first three steps (I-III) because the poor control of the axial strain and possible weak contacts between the load pistons and the end faces of the sample; (2) the gas migration test during the first three steps





(I-III) is not simulated by keeping the gas pressure atmosphere; (3) the temperature measured at the inner borehole wall is applied as a boundary condition because some amounts of heat lost from the sample ends; and (4) various values of the intrinsic permeability between $4 \cdot 10^{-20}$ and $5 \cdot 10^{-18}$ m² are examined by comparing the water flow and pressure with the measured data.



Figure 8 : Geometry and boundary conditions for modelling of the hollow cylinder test BMT4

2.3.4 Conclusion on GRS modelling

In the GRS benchmark modelling, the capabilities of the THM constitutive models in CODE_BRIGHT (cdv3), particularly the damage-elastoplastic model for argillaceous rocks, have been examined by comparison with the results of the large hollow cylinder tests on the COX claystone in regard to the development and recovery of the EDZ around HLW disposal boreholes. The results indicate that:

- The short-term deformation behaviour of the hollow cylinders is reasonably represented by the model with indication of micro-damage evolution, but the post-failure behaviour could not be modelled due to earlier stop of the computation.
- The drastic increase in permeability by fracturing and the permeability decrease by recompaction of the fractures can not be captured by the Kozeny's permeability – porosity relationship for porous media without fractures (Figure 9).
- The observed water inflow into the fractured claystone is significantly underestimated by the modelling even though the real permeability value of the fractured claystone is used.
- The significant responses of deformation in the damaged claystone to heating and cooling are weakly revealed by the modelling (Figure 10).



Generally speaking, the THM behaviour of damaged claystones can not reasonably be approached by the constitutive models for continuum porous media without involving effects of discontinuities. From our knowledge, the behaviour of damaged claystones is not yet well characterized and understood. Further research work is obviously necessary to improve the constitutive models for the prediction of the development and recovery of the EDZ and to enhance the certainty of the long-term performance and safety assessments of HLW repositories in argillaceous formations.



Figure 9 : Calculated permeability variations in comparison with the measured data



Figure 10 : Calculated and observed deformations before, during and after heating

2.4 Conclusion

Numerical results obtained by ULg and GRS show that the embedded fracture model (permeability-strain coupling model) allows the reproduction of the permeability increase of the damaged sample, whilst the Kozeny relationship is not sufficient to reproduce the drastic increase of the permeability. Nevertheless the experimental results seems to be strongly influenced by the initial desaturation of the porous disk, which modifies the injected water volume during the water injection tests and complicates an accurate reproduction of the numerical results.



3 Brief description of the large hollow cylinder tests on COX argillite

Within TIMODAZ-WP3.3 (Deliverable 7), GRS carried out EDZ-simulation tests on four large hollow cylinders of the COX argillite to investigate fracturing and sealing processes of the host rock around HLW disposal boreholes. The results serve as database for validation of the THM constitutive models used by the project partners within WP5.2. The large COX cores were extracted from the MHM-URL at Bure and prepared to hollow cylinders of ~0.5 m length and 280 mm outer diameter with axially-drilled central boreholes of 100 mm diameter. Due to the long storage periods of months to years, even though the cores were carefully confined and sealed, they were more or less de-saturated. In order to attain the natural state of the claystone, a re-saturation phase was performed before testing with water vapour over several months. High saturation degrees were achieved between 82 % and 100 %. The basic characteristics of the prepared samples are summarized in Table 1.

		Size	Grain	Bulk	Dry		Water	Saturation	Initial
Test	Sample	D/d/L	density	density	density	Porosity	content	degree	suction
No.		(mm)	(g/cm^3)	(g/cm^3)	(g/cm^3)	(%)	(%)	(%)	(MPa)
BMT1	DIR2003-	D280							
	EST19387	d100	2.70	2.41	2.28	15.4	5.5	82.0	23.0
	(-460m)	L525							
BMT2	DIR1004-	D280							
	EST27319	d100	2.70	2.43	2.28	15.7	6.8	98.0	5.0
	(-501m)	L520							
BMT3	DIR2004-	D280							
	EST27315	d100	2.70	2.45	2.29	15.0	6.8	100.0	0.0
	(-461m)	L520							
BMT4	DIR2004-	D280							
	EST27312	d100	2.70	2.41	2.26	15.8	6.2	89.0	10.0
	(-463m)	L460							

Table 1 : Basic characteristics of the large COX hollow cylinders

Regarding damage development and recovery in the host clay rock around HLW disposal boreholes, the tests were designed and carried out in the GRS big triaxial apparatus by simulation of the relevant processes such as borehole excavation, backfilling / lining, heating, and cooling. Figure 11 illustrates a typical test layout and the pictures of a large hollow cylinder before and after testing. During the tests, responses of the COX hollow cylinders were monitored by various instruments for measurements of external confining stress, axial / radial strain, borehole pressure / convergence, gas / water injection pressure and inflow / outflow, and temperature. The stress conditions in the COX formation at the depth of ~500 m in the URL Bure were taken into account in the tests, i.e. $\sigma_1 = 16$ MPa, $\sigma_2 = \sigma_3 = 12$ MPa.





de too mm axia load before testing instrumentation after testing **Figure 11 : Test layout of EDZ-simulation with large hollow cylinders of COX argillite**

The main observations from the four large hollow cylinder tests are:

- 1. The <u>borehole excavation</u> simulated by reducing the inner borehole pressure from 15 MPa down to 1 MPa resulted in convergence of the borehole but not any increase in permeability along the cylinder axis, indicating no build up of pathway through the samples. Further increase of the external confining stress beyond 20 to 24 MPa (corresponding to depths of 800 1000 m) led to fracturing and flow pathway, indicated by the drastic increase in gas permeability from 10^{-21} m² to 10^{-14} m².
- 2. The <u>backfill impact</u> simulated by increasing the inner borehole pressure from 1 to 15 MPa led to a strong reduction of the gas permeability by several orders of magnitude from 10⁻¹⁷ down 10⁻²¹ m², depending on the initial characteristics of the excavation-induced fractures in the argillite.
- 3. The <u>water transport</u> through the fractures in the claystone led clay minerals swelling into the interstices and thus sealing the fractures, whereby the permeability decreased drastically to $2 \cdot 10^{-18}$ m⁻², four orders of magnitude lower than that by gas flowing.
- 4. <u>Heating</u> from 29 °C to 74 °C accelerated the borehole convergence and the water inflow. The thermal impact on the water conductivity of fractured claystone is governed by the change of the water viscosity, while the intrinsic permeability is less affected by heating.
- 5. <u>Cooling</u> down slowed the deformation and the water transport through the fractured claystone. The permeability after cooling was between $1.0 \cdot 10^{-18}$ and $3.5 \cdot 10^{-18}$ m², nearly the same as that before heating.
- 6. The <u>post-investigation</u> on a tested sample showed a significant increase of the water content up to 9.3 % at the inlet side to 6.2 % at the outlet. The most part of the sample was "over saturated", i.e. the water content was higher than that in the natural and saturated state (w \approx 7.0 %). The water uptake was accompanied by volume expansion of the clay matrix into the fracture space under confined conditions.



Details of the test results are given in Deliverable 7. Some data are also presented below in comparison with modelling results.

4 Numerical results of ULg

ULg numerical modelling of hollow cylinder tests is performed by using Lagamine finite element code. One EDZ-simulation test is modelled: the BMT4 hollow cylinder test.

4.1 Constitutive models and parameters

The main relationships of the thermo-hydro-mechanical model for unsaturated media are presented hereafter. Further details about the balance equations and the coupled thermo-hydraulic formulation can be found in Collin et al. (2002) and in Deliverable 10.

A Bishop effective stress is considered in the momentum balance equation and in our thermohydro-mechanical model:

$$\sigma' = \sigma - b \left(S_{rw} p_w + \left(1 - S_{rw} \right) p_g \right) \tag{1}$$

with b the Biot coefficient, S_{rw} the degree of saturation, p_w the water pressure and p_g the gas pressure.

4.1.1 Mechanical model

The mechanical model used for the COX argillite is a non-associated elastoplastic constitutive law. The yield surface is defined by a Van Eekelen criterion. The yield function f uses a linear relationship between the first stress tensor invariant and the second deviatoric stress tensor invariant.

The Van Eekelen yield limit is given by the following equation:

$$f \equiv II_{\hat{\sigma}} + m \left(I_{\sigma} - \frac{3c}{\tan \varphi} \right) = 0$$
⁽²⁾

with φ the friction angle and c the cohesion; $I_{\sigma} = \sigma_{ii}$ the first stress invariant; $II_{\hat{\sigma}} = \sqrt{\frac{1}{2}\hat{\sigma}_{ij}\hat{\sigma}_{ij}}$ the second deviatoric stress invariant with $\hat{\sigma}_{ij} = \sigma_{ij} - \frac{I_{\sigma}}{3}\delta_{ij}$; $(3\sqrt{3}III_{\sigma})$ 1

$$m = a \left(1 + b \sin 3\beta\right)^n \text{ and } \sin 3\beta = -\left(\frac{3\sqrt{3}}{2}\frac{III_{\hat{\sigma}}}{II_{\hat{\sigma}}^3}\right) \text{ with } III_{\hat{\sigma}} = \frac{1}{3}\hat{\sigma}_{ij}\hat{\sigma}_{jk}\hat{\sigma}_{ki} \text{ the third stress}$$

invariant.

Isotropic hardening of the friction angle is considered in the model. The plastic flow is assumed to induce hardening of the yield surface, which is introduced via a hyperbolic variation of the internal variables (φ) as a function of the Von Mises equivalent plastic strain \mathcal{E}_{eq}^{p} :

$$\varphi = \varphi_0 + \frac{(\varphi_f - \varphi_0)\varepsilon_{eq}^p}{\beta_{\varphi} + \varepsilon_{eq}^p}$$
(3)

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where the Von Mises equivalent plastic strain is obtained by integration of the Von Mises equivalent plastic strain rate $\dot{\varepsilon}_{eq}^{p}$:

$$\varepsilon_{eq}^{p} = \int_{0}^{t} \dot{\varepsilon}_{eq}^{p} dt \quad \text{with} \quad \dot{\varepsilon}_{eq}^{p} = \sqrt{\frac{2}{3}} \dot{\hat{\varepsilon}}_{ij}^{p} \dot{\hat{\varepsilon}}_{ij}^{p} \tag{4}$$

Coefficient β_{φ} represents the value of the equivalent plastic strain for which the half of the hardening of the frictional angle is achieved.

4.1.2 Hydraulic model

The mass flow into the porous medium is defined by the sum of the advection of the liquid water (Darcy's law for unsaturated cases) and the diffusion of water vapour (Fick's diffusion law) :

$$m_{i} = f_{i,w} + i_{i,v}$$

$$= -\rho_{w} \frac{\kappa k_{r,w}}{\mu_{w}} \left(\frac{\partial p_{w}}{\partial x_{i}} + \rho_{w} g_{i} \right) - D\tau \phi \left(1 - S_{r,w} \right) \frac{\partial \rho_{v}}{\partial x_{i}}$$
(5)

where κ is the intrinsic permeability, $k_{r,w}$ is water relative permeability, μ_w is the water dynamic viscosity, D is the molecular diffusion coefficient of the mixture of gaseous air and water vapour, τ the tortuosity, ρ_w the water density and ρ_v the vapour density.

The advective flux of the gaseous phase is neglected, because the gas pressure remains constant.

The water retention curve is given by the van Genuchten relationship:

$$S_{r,w} = \left[1 + \left(\frac{p_c}{P_r}\right)^{\frac{1}{1-m}} \right]^{-m} \text{ and } S_{r,w} = 1 \text{ if } p_c < 0$$
(6)

The water relative permeability function proposed by van Genuchten is also adopted:

$$k_{r,w} = \sqrt{S_{r,w}} \left[1 - \left(1 - S_{r,w}^{1/m} \right)^m \right]^2$$
(7)

4.1.3 Thermal model

The heat transport is related to three effects: conduction, convection by the fluids and evaporation:

$$t_{i} = -\lambda \frac{\partial T}{\partial x_{i}} + \left(c_{p,w} \rho_{w} f_{i,w} + c_{p,v} i_{i,v}\right) \left(T - T_{0}\right) + L i_{i,v}$$

$$\tag{8}$$

with λ the medium conductivity, $c_{p,w}$ the water specific heat, $c_{p,v}$ the vapour specific heat and L the latent heat for vaporization.

The enthalpy of the system is given by the sum of each component's enthalpy:

$$h = \rho C_{p} \left(T - T_{0} \right) + \phi \left(1 - S_{r,w} \right) \rho_{v} L$$
(9)

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with ρC_p the volumetric heat capacity of the whole porous medium and ρ_v the vapour density.

The standard expressions of the evolution of the dynamic viscosity, the water and solid grains densities with the temperature can be found in Deliverable 10.

4.1.4 Permeability-strain coupling model

A specific permeability model (Olivella and Alonso, 2008; Levasseur et al., 2010) is considered in order to reproduce the development of preferential pathways into argillite. It adds new hydro-mechanical coupling between permeability and the strain state. The basic idea consists in the appropriate representation of single discontinuity representing the rock bedding, which is embedded in a continuous finite element. As presented in Deliverable 10, the increase of permeability in the damage zone is linked with the development of tensile strains.

The relationship between permeability and the strain state can then be written (see Deliverable 10 for further details):

$$K_{ij} = K_0 \left(1 + \lambda \left(\varepsilon^T - \varepsilon_0 \right) \right)^3$$
 if $\varepsilon^T > \varepsilon_0$

with K_0 the initial permeability, ε^T the tensile strain, ε_0 a threshold strain for the permeability increases and λ a fitting parameter corresponding to the fracture density. The threshold strain could be considered as the strain corresponding to the tensile strength of the rock. Aperture opening can not therefore be initiated before a failure by tension occurs.

4.2 Boundary value problem

A 2D axisymetric modelling of the BMT4 hollow cylinder test is performed. During this experiment several small half holes of 5 mm diameter had been drilled respectively from the top and the bottom to a depth of 60 mm along the borehole wall. It allows fluid supplying directly into the middle region near the borehole wall and avoids the local densification that may take place at the ends of the samples (Deliverable 7). These small boreholes are not taken into account in our modelling, because the contact between the samples and the load pistons is assumed perfect and no densification zone can be developed at the ends of the hollow cylinder in our modelling. Nevertheless the injection filter is taken into account in the modelling, because it influences the water volume injected during the four injection steps. Indeed when the injection system is shut-off the water in the porous disk continues flowing into the sample. The geometry and the initial conditions of the modelling are presented in Figure 12.

Initial state of argillite is desaturated ($S_{rw} \square 0.86$), which implies the need of a thermo-hydromechanical model for unsaturated media. The initial stress state is isotropic.





Figure 12 : BMT4 hollow cylinder test (a) Geometry and initial conditions – (b) Mesh for finite element modelling

There are 6 steps in the thermo-hydro-mechanical modelling of the BMT4 hollow cylinder test: the consolidation, the borehole excavation, the EDZ intensification, the water injection tests, the cooling and the heating stages. Gas permeability tests are performed at the end of the consolidation stage and during the borehole excavation and EDZ intensification stages. However they are not modelled, which should not influence a lot the numerical results owing to the low gas volume injected in argillite. Gas pressure remains thus constant at the atmospheric pressure during the modelling.

During the consolidation stage the radial stresses are increased to 15 MPa and remains constant during one day (Figure 13). No axial displacement is allowed at the ends of the hollow cylinder during all the experiment. No water flux is allowed at the top and the bottom of the experiment. The temperature remains constant at 29° C.

Then inner radial stress is decreased from 15 MPa to 1 MPa and maintains constant during the 4,8 days of the borehole excavation stage ($t_{tot} = 5,8$ days), whilst the outer radial stress remains constant at 15 MPa during this stage (Figure 13). The hydraulic boundary conditions are the same as previously. The temperature remains constant at 29°C.

During the EDZ intensification step outer radial stress is increased from 15 MPa to 24 MPa and then immediately reduced down to 15 MPa for another 2 days ($t_{tot} = 7,8$ days). The inner radial stress remains constant at 1 MPa (Figure 13). The hydraulic boundary conditions are the same as in the previous stage. The temperature remains constant at 29°C.





Figure 13 : Inner and outer radial stresses during the consolidation, borehole excavation and EDZ intensification stages

During the water injection stage the mechanical boundary conditions remain constant. The temperature remains constant at 29°C. Four injection tests are modelled increasing the water pressure to 0.5 MPa at the top of the injection porous disk, interrupted by no flux boundary condition at the top in order to reproduce the shut-off of the injections. The water injection tests are performed between the following total times (Figure 14):

- $t_{tot} = 7,8$ days and $t_{tot} = 8,185$ days
- $t_{tot} = 11,8$ days and $t_{tot} = 12,23$ days
- $t_{tot} = 12,76$ days and $t_{tot} = 13,23$ days

Then a water pressure of 0.3 MPa is imposed at the top of the sample from $t_{tot} = 13,76$ days to $t_{tot} = 25,77$ days. At the bottom of the sample a seepage condition at the atmospheric pressure is imposed, which makes possible water outflow but no water inflow.



Figure 14 : Injection water pressure evolution during water injection tests

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During the heating and cooling stages the mechanical and hydraulic boundary conditions remain the same as at the end of the injection test stage. Temperatures of 74° and 69°C are respectively imposed in 3 days at the outer and the inner surfaces of the hollow cylinders and then maintained constant during 20 days ($t_{tot} = 48,77$ days). Then the outer and inner temperatures are decreased in 3 days down the initial temperature (29°C), and maintained constant during 18 days ($t_{tot} = 69,77$ days) (Figure 15).



Figure 15 : Inner and outer temperatures boundary conditions during heating and cooling stages

4.3 Thermo-hydro-mechanical parameters

4.3.1 COX argillite

The thermo-hydro-mechanical parameters for COX argillite used for the modelling are presented in Table 2, Table 3 and Table 4. Hardening of the friction angle is considered in the Van Eekelen elastoplastic model. An anisotropic permeability is considered for COX argillite. The retention and water relative permeability curves are fitted on experimental (see Gerard et al., 2010) for more details. Figure 16 presents the retention curve based on the van Genuchten relationship. Initial porosity is based on pre-test characterization performed by GRS (Deliverable 7). The thermal conductivity (assumed constant) and volumetric heat capacity of COX argillite are based on previous thermo-hydro-mechanical modelling performed by ULg for Andra (Gerard et al., 2006).





Geomechanical characteristics		COX argillite
Young elastic modulus [MPa]	E_0	4000
Poisson ratio [-]	υ	0.3
Cohesion [MPa]	С	3
Initial friction angle [°]	φ_0	12.5
Final friction angle [°]	φ_{f}	20
Hardening parameter [-]	$eta_{_{arphi}}$	0.01
Biot's coefficient [-]	b	1

Table 2 : COX argillite mechanical characteristics

Table 3 : COX argillite hydraulic characteristics

Hydraulic characteristics	COX argillite	
Initial porosity [-]	\$ 0	0.15
Initial radial permeability [m ²]	K _r	10 ⁻¹⁹
Initial axial permeability [m ²]	κ_{ax}	8 10 ⁻²⁰
Tortuosity [-]	τ	0.25
Air entry pressure [MPa]	P_r	15
van Genuchten retention parameter [-]	п	1.49
van Genuchten water relative permeability parameter [-]	т	0.55
Vapour diffusion coefficient [m ² /s]	D	2.78 10 ⁻⁵
Water specific mass [kg/m ³]	ρ_w	1000
Fluid dynamic viscosity [Pa.s]	μ_w	10 ⁻³
Water bulk modulus [MPa]	Χw	2000

Table 4 : COX argillite thermal characteristics	
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Thermal characteristics	COX argillite	
Thermal conductivity [W/(mK)]	λ	1.9
Volumetric heat capacity [J m ⁻³ .K ⁻¹]	$ ho C_p$	1007
Linear solid thermal expansion coefficient [K ⁻¹]	β_s	-1 10 ⁻⁵
Volumetric liquid thermal expansion coefficient [K ⁻¹]	β_w	4.37 10 ⁻⁴
Liquid dynamic viscosity thermal coefficient [K ⁻¹]	α_w	0.01

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4.3.2 Filter

The thermo-hydro-mechanical models used for the filter are presented in Table 5, Table 6 and Table 7. High permeability is defined and the water relative permeability curve is based on a cubic law. A small air entry value and a sharp decrease are used for the retention curve of the filters (Figure 17).

A linear elastic model is used for the mechanical behaviour with the same Young modulus and Poisson ration as for argillite. It allows avoiding the development of stresses concentration and traction strains at the contact between the filter and argillite. The porosity of the filters is provided by GRS and is needed in order to reproduce the correct porous volume of the injection system. The thermal characteristics are the same as for argillite.

Table 5 : Filter mechanical characteristics

Geomechanical characteri	Geomechanical characteristics		
Young elastic modulus [MPa]	E_0	4000	
Poisson ratio [-]	υ	0.3	
Biot's coefficient [-]	b	1	

Table 6 : Filter hydraulic characteristics						
Hydraulic characteristics		COX argillite				
Initial porosity [-]	ϕ_0	0.29				
Intrinsic permeability [m ²]	K _r	10-14				
Tortuosity [-]	τ	0.25				
Air entry pressure [kPa]	P_r	50				
van Genuchten retention parameter [-]	n	6				

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Thermal characteristics	COX argillite	
Thermal conductivity [W/(mK)]	λ	1.9
Volumetric heat capacity [J m ⁻³ .K ⁻¹]	$ ho C_p$	1007
Linear solid thermal expansion coefficient [K ⁻¹]	β_s	-0.001
Volumetric liquid thermal expansion coefficient [K ⁻¹]	β_w	4.37 10 ⁻⁴
Liquid dynamic viscosity thermal coefficient [K ⁻¹]	α_w	0.01

 Table 7 : Filter thermal characteristics



Figure 17 : Retention curve of the filter

4.4 Numerical results

Experimental results evidence that increase of gas permeability is obtained from the EDZ intensification stage (Figure 18). We introduce therefore in the embedded fracture model a threshold strain value higher than the maximal tensile strain obtained during the borehole excavation stage (Figure 19).

Table 8 : Embedded fracture model parameters					
Embedded fracture model ch	Embedded fracture model characteristics				
Fracture density parameter [-]	λ	1700			
Threshold strain [-]	\mathcal{E}_0	0.0194			



Figure 18 : Applied stresses and gas permeability evolution during consolidation, borehole excavation and EDZ intensification stages



Figure 19 : Inner and outer radial strains during consolidation, borehole excavation and EDZ intensification stages

4.4.1 Consolidation, borehole excavation and EDZ intensification

Figure 20 and Figure 21 show that the Van Eekelen elasto-plastic model for argillite, with a hardening of the friction angle allows the reproduction of the experimental radial strains. The inner radial strains are well produced, whilst the outer ones are weakly overestimated during the borehole excavation stage. It must be added that experimental measurements show that the outer radial strain are not exactly the same at the middle and the quarter of the cylinder height. A friction resistance of the load pistons at the ends of the sample can maybe explain the higher radial strains at the middle than at the ends of the samples. Our model does not reproduce such phenomena and give homogeneous deformation, because the contact between



the porous disk and the cylinder is assumed perfect and the mechanical characteristics of the porous disk (deformation moduli) are the same as for argillite, which avoid the development of stresses concentration at the ends of the cylinder.

For the embedded fracture model we have introduced a threshold strain of 1.94 % (Table 8). Aperture opening cannot be initiated before strains reach this tensile strain (corresponding to failure). Due to the mechanical loading radial tensile strains appear at the sample inner, which imply an increase of the vertical permeability. Permeability increase is obtained only during the EDZ intensification stage owing to the value of the threshold strain. At the end of the third stage a very small zone at the inner of the sample is damaged (Figure 22), but the vertical permeability value is three orders of magnitude higher than that before.



Figure 20 : Inner radial strain - Comparison between experimental and numerical results



Figure 21 : Outer radial strain (1/4 L) – Comparison between experimental and numerical results

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Figure 22 : Vertical intrinsic permeability at the end of the EDZ intensification stage

4.4.2 Water injection tests

The evolution of the experimental water volume shows an instantaneous increase at the beginning of the first water injection test (Figure 23). The same behaviour is observed at the beginning of the second injection test. This instantaneous increase is interpreted by an initial desaturation of the porous disks that are quickly resaturated at the onset of the water injection tests. An initial degree of saturation of 0.50 of the filters is therefore considered in the modelling, which corresponds to a capillary pressure of 52 kPa.

The permeability increase at the sample inner provided by the embedded fracture model allows the reproduction of the global evolution of the water volume through argillite (Figure 23). For long term predictions the water inflow at the steady state flow is nearly the same as the experimental one (about 3,3 cm³/d). That highlights the ability of the embedded fracture model to reproduce the global permeability increase of the whole sample. Nevertheless an accurate reproduction of the experimental water volume is not obtained, but the numerical results are strongly influenced by the initial desaturation of the filters (for which we don't know the retention behaviour). The comparison with the numerical water volume obtained with a constant permeability is also presented in Figure 23. It shows the underestimation of the water volume when damage of the hollow cylinder is not considered. Moreover the steady state flow is not exactly reaches in this case at the end of the water injection tests.

The porous disk influences also the water pressures measured at the top of the hollow cylinder. Figure 24 presents a comparison between the experimental and numerical water pressures at the ends of the sample. Instantaneous decrease of the pressures is obtained with the modelling during the shut-off periods, which does not allow the reproduction of the experimental measurements. This evolution is also strongly influenced by the retention curve used for the filters (Figure 17). It must be added that no water outflow is observed at the

bottom of the sample, because argillite remains partially saturated at the bottom of the hollow cylinder at the end of the water injection tests (Figure 25).

The experimental measurements show also an increase of the convergence of the borehole during the water injection tests (Figure 26), which cannot be reproduced by our mechanical model.



Figure 23 : Water volume injected during the injection tests – Comparison between experimental and numerical results



Figure 24 : Water pressures evolution at the top of the hollow cylinder during the injection tests

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Figure 25 : Water pressure at the end of the water injection tests



Figure 26 : Inner radial strain during water injection tests – Comparison between experimental and numerical results





Figure 27 : Outer radial strain during water injection tests – Comparison between experimental and numerical results

4.4.3 Heating and cooling steps

The experimental results show that the heating increases the water inflows (caused by the decrease of the water viscosity), but not significantly the permeability of the whole sample (Deliverable 7). Water outflows is also observed at the bottom of the sample (Figure 29), but the modelling underestimates the experimental measurements.

Our thermo-mechanical model dos not take into account any influence of the temperature on the mechanical characteristics of argillite, which does not allow the reproduction of thermoplastic strains during heating. Figure 30 and Figure 31 show that the inner and outer strains are underestimated by the modelling. Nevertheless using a negative thermal expansion coefficient for argillite allows the reproduction of the increase tendency of the outer radial strain at the beginning of the heating, as observed experimentally. This behaviour is characteristic of the normally consolidated soils.





Figure 28 : Water volume injected during heating and cooling stages (V and VI) – Comparison between experimental and numerical results



Figure 29 : Water volume expelled during heating and cooling stages (V and VI) – Comparison between experimental and numerical results







Figure 30 : Inner radial strain during heating and cooling stages (V and VI) – Comparison between experimental and numerical results



Figure 31 : Outer radial strain during heating and cooling stages (V and VI) – Comparison between experimental and numerical results

4.5 Conclusions

An elastoplastic model with a hardening of the friction angle provides a good reproduction of the experimental strains measured at the sample inner and outer during the different mechanical loading steps.

The embedded fracture model has been used for the modelling of the different steps. It allows the increase of the permeability assuming the development of preferential pathways in the



zones where tensile strains are developed. Aperture of discrete paths is the main variable that controls the permeability evolution. This model allows the reproduction of the permeability increase observed at the inner of the COX hollow cylinders submitted to mechanical load. Nevertheless the experimental results seem to be strongly influenced by the initial desaturation of the porous disk, which makes difficult an accurate reproduction of the injected water volume through the sample during the water hydraulic tests.

During the heating and the cooling stages, the modelling could reproduce the general tendency of the water inflows or outflows, but underestimate the experimental water volume. The thermo-mechanical model of the COX hollow cylinder does not take into account the influence of temperature on the mechanical characteristics, but argillite seems to behave as a normally consolidated rock with the development of compressive strains when the temperature increases. For long term predictions the modelling underestimates nevertheless the experimental radial strains, but the development of potential thermo-plasticity is not taken into account in the model.

5 Numerical results of GRS

GRS benchmark modelling was performed by using CODE-BRIGHT (version cdv3, 2004). The available constitutive models in the code were studied before starting the benchmark. Based on that, some of them were considered adequate for the consolidated claystone and adopted for the benchmark. The associated parameters were established on the basis of the previous test data (Deliverable 2) and the actual results obtained within WP3.1 (Deliverable 5) as well as from literature (Vaunat et al., 2003; 2004; 2009). Two EDZ-simulation tests BMT1 and BMT4 were modelled.

Considering the complex testing procedure and boundary conditions of the large hollow cylinder tests, coupled THM calculations were carried out by solving a set of balance equations of energy, solid mass, water mass, air mass and stress equilibrium with selected constitutive models. The main assumptions were made:

- 1. The COX clay rock is relatively isotropic and homogeneous because of the insignificant bedding planes;
- 2. Heat transport includes conduction (Fourier's law) through the porous medium, advection of liquid water and vapour flow;
- 3. Water transport is controlled by liquid water advection (Darcy's law), vapour diffusion in air (Fick's law), and liquid / gas phase changes (psychrometric law);
- 4. Gas migration is governed by advection (Darcy's law), dissolution in liquid (Henry's law) and the ideal gas law;
- 5. The damage-elastoplastic model developed by UPC for argillaceous rocks (Vaunat et al., 2003; 2004; 2009) is applied for description of the mechanical behaviour of the COX claystone.

Details of the formulations and applications of the applied balance equations and constitutive models are given in a number of UPC's publications (Gens et al., 2006; 2007; Vaunat et al., 2003; 2004; 2009). In this report, the main features of some adopted models and parameters are represented below.



5.1 Constitutive models and parameters

5.1.1 Mechanical model

A damage-elastoplastic model has been developed by Vaunat et al. (2003; 2004; 2009) for argillaceous rock which is considered as a composite material made of a clay matrix connected by bonds (Figure 32). The clay matrix behaves like a typical elastoplastic soil, while the bonds behave like a typical quasi-brittle material that can be represented by a damage elastic law. The stress - strain behaviour of the composite material is determined by coupling both responses of matrix and bonds under compatible conditions. The deformation of the composite material is the sum of the pore strain and the bond strain:

volumetric strain:
$$\varepsilon_v^M = \varepsilon_v + \varepsilon_v^b$$
 (10)

$$\varepsilon_q^M = \varepsilon_q + \varepsilon_q^b \tag{11}$$

where ε_v^M and ε_q^M are the matrix volumetric and shear strain (externally observed), ε_v and ε_q are the volumetric and shear strain between clay particles (pores), ε_v^b and ε_q^b are the volumetric and shear strain in bonds.



Figure 32 : Conceptual model of claystone as composite material with clay matrix and bonds

<u>Clay matrix</u> is considered as a ductile material governed by an elasto-plastic law using Hoek and Brown's criterion as yield surface. Inside the yield surface the matrix behaves elastically.

Elastic law:

$$d\sigma_{ij}^{M} = D_{ijkl}^{eM} \left(d\varepsilon_{kl}^{M} - \delta_{kl} \frac{ds}{K_{s}^{M}} - d\varepsilon_{kl}^{p} \right)$$
(12)

where σ_{ij}^{M} = stresses prevailing at clay particles contact

 D_{iikl}^{eM} = elastic stiffness matrix of the clay

 $d\varepsilon_{kl}^{M}$ = total strains of the clay matrix (equal to the external strains)

 K_s^M = bulk modulus against suction change ds

$$d\varepsilon_{kl}^{p}$$
 = plastic strains of the clay matrix

 δ_{kl} = Kronecker delta.

Assuming linear elasticity, the elastic stiffness D_{ijkl}^{eM} is determined by Young's modulus E^{M} and Poisson's ratio v^{M} of the clay matrix. Volumetric swelling or shrinking of the clay matrix is linearly related with suction change ds by the bulk modulus K_{s}^{M} .

Yield function (Hoek & Brown criterion):

$$F^{p} = \frac{4\sin^{2}(\theta^{M} - \pi/6)}{R_{c}^{M}} (J^{M})^{2} - \frac{2m^{M}\sin\theta^{M}}{\sqrt{3}} J^{M} - m^{M} (p^{M} + p_{t}^{M}) \ge 0$$
(13)

where p_t^M = tensile strength of the clay matrix (isostatic)

 R_c^M = uniaxial compressive strength of the clay matrix

 $m^{M} = R_{c}^{M} / p_{t}^{M}$ ratio defining the shape of the yield surface.

The uniaxial compressive strength R_c^M of the clay matrix increases with elevating suction (drying) by

$$R_{c}^{M}(s) = R_{c}^{M}(o) \left[\left(1 - r^{M} \right) \exp \left(-\beta^{M} s \right) + r^{M} \right]$$
(14)

where the coefficient r^{M} depicts the limit strength by $r^{M} = \lim_{s \to \infty} \left(\frac{R_{c}^{M}(s)}{R_{c}^{M}(0)} \right)$ and β^{M} defines the change rate of the strength R_{c}^{M} with suction *s*.

Plastic potential:

$$G^{p} = \frac{4\sin^{2}(\theta^{M} - \pi/6)}{R_{c}^{M}} (J^{M})^{2} - \frac{2m^{M}\sin\theta^{M}}{\sqrt{3}} J^{M} - \omega^{M}m^{M} (p^{M} + p_{t}^{M})$$
(15)

where ω^{M} is a parameter defining the non-associativity of the plastic flow: $\omega^{M} = 1$ when associated and $\omega^{M} = 0$ for zero dilatancy.

A hardening/softening law is introduced through the following dependency of the tensile strength on the plastic strain:

$$p_{t}^{M} = \frac{R_{c}^{M}}{m^{M}} \left[1 - \left(1 - \alpha^{M}\right) \frac{\max\left(\varepsilon_{1}^{pM}, \xi_{r}^{M}\right)}{\xi_{r}^{M}} \right]^{2}$$
(16)

where R_{c0}^{M} = uniaxial compressive strength of the intact clay

 $\epsilon_1^{pM} =$ major principal plastic strain

- ξ_r^M = accumulated major principal plastic strain at which the residual strength $\alpha^{M2} R_{c0}^M$ is reached
- α^{M} = brittleness parameter relating the intact and residual uniaxial compressive strength R_{c0}^{M} and R_{cres}^{M} , $\alpha^{M} = 1$ means perfect plasticity and $\alpha^{M} = 0$ indicates total degradation (residual strength $R_{cres}^{M} = 0$).

Visco-plastic strain:

Rate dependency is introduced as a visco-plastic mechanism. Plastic multiplier λ^{p} is expressed as a function of the distance between the current clay matrix stress point and inviscid plastic:

$$d\lambda^{p} = \frac{dt}{\eta^{M}} \left\langle F^{p} \right\rangle \tag{17}$$

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where dt is the time increment, η^{M} is the matrix viscosity and $\langle \rangle$ is the Macauley bracket. Inviscid plastic locus takes the form

$$\overline{F}^{p} = F^{p} - \frac{\eta^{M}}{dt} d\lambda^{p} \le 0$$
(18)

where F^{p} is the Hoek & Brown yield criterion (Eq. 13). The visco-plastic strains are computed as

$$d\varepsilon_{vp}^{M} = \frac{dt}{\eta^{M}} \frac{\partial G_{M}}{\partial p_{M}} \left\langle F^{p} \right\rangle \qquad d\varepsilon_{vq}^{M} = \frac{dt}{\eta^{M}} \frac{\partial G_{M}}{\partial q_{M}} \left\langle F^{p} \right\rangle$$
(19)

The plastic strains in Eq. 12 are replaced by the visco-plastic ones for cases of time dependency.

<u>Bonds</u> are considered as quasi-brittle material whose behaviour is represented by elastic law with damage. Bond damage or degradation occurs as the result of apparition of micro-fissures within the bonds, which reduces the surface on which stresses and strains are active. The operative stresses and strains acting on the reduced surface of solid bonds are related to stresses and strains averaged over the whole bond area by a damage parameter.

Elastic law:
$$d\sigma_{ij}^{b} = D_{ijkl}^{eb} \left(d\varepsilon_{kl}^{b} - d\varepsilon_{kl}^{d} \right)$$
(20)

where σ_{ii}^{b} = stresses inside bonds

 D_{ijkl}^{eb} = secant damaged elastic stiffness matrix of bonds $d\varepsilon_{kl}^{b}$ = strains of bonds $d\varepsilon_{kl}^{d}$ = damage strains.

The damaged elastic matrix is related to the undamaged elastic matrix tensor D_{iikl}^{ebo} by

$$D_{ijkl}^{eb} = (1-D)D_{ijkl}^{ebo} = e^{-L}D_{ijkl}^{ebo}$$
(21)

where D is a measure of damage of the material and equal to the ratio of bond fissures over the whole area of bonds, L is the damage variable related to D by $L = \ln(1/(1-D))$, and D_{ijkl}^{ebo} is defined by Young's modulus E^{bo} and Poisson's ratio v^{bo} of the undamaged bonds through the linear isotropic elasticity. The damage parameter D and variable L are explicitly related to the stiffness degradation by

$$D = 1 - \frac{K^{b}}{K^{bo}} = 1 - \frac{G^{b}}{G^{bo}} = 1 - \frac{E^{b}}{E^{bo}}$$
(22)

$$L = \ln \frac{K^{bo}}{K^{b}} = \ln \frac{G^{bo}}{G^{b}} = \ln \frac{E^{bo}}{E^{b}}$$
(23)

where K^{bo}, G^{bo}, E^{bo} and K^{b}, G^{b}, E^{b} are the bulk, shear and Young's modulus of the undamaged and damaged bonds, respectively. When D = 0 (L = 0), the material is intact and the bond stiffness is determined by K^{bo}, G^{bo}, E^{bo} . As D increases, cracks in bonds develop and the material stiffness decreases progressively. When D = 1 (L $\rightarrow \infty$) the bonds are fully damaged and the stiffness is eliminated.



Damage locus:

Current bond damage locus is defined in the stress space as a threshold of equal energy r^{b} , corresponding to the maximum energy input to the bond during its history

$$F^{d} = \frac{1}{2}\sigma^{b}_{ij}\varepsilon^{b}_{ij} - r^{b}(s)$$
⁽²⁴⁾

This condition draws an ellipse in the $p_b - q_b$ space. For a stress state moving inside the ellipse, no damage develops. When the ellipse is reached by the current stress state, damage occurs. The value of energy threshold depends on suction s

$$r_{o}^{b}(s) = r^{b}(0) + r_{0s}^{b}.s$$
 (25)

where $r^{b}(0) =$ damage threshold at zero suction (fully saturated)

 r_{0s}^{b} = parameter defining the change rate of damage locus with suction.

Damage rule:

Damage rule gives the evolution of damage strain $d\varepsilon_{kl}^d$ with damage variable L. This relation is constrained by the evolution of bond elastic modulus and takes the form

$$d\varepsilon_{kl}^{d} = \varepsilon_{ii}^{b} dL \tag{26}$$

Damage evolution law:

It defines the evolution of damage locus r^{b} with damage variable L. A simple linear expression is considered

$$r^b = r_o^b + r_1^b L \tag{27}$$

where r_o^b = value of energy threshold at which damage starts

 r_1^b = parameter defining the evolution rate of damage locus, as a function of suction $r_1^b = r_{10}^b + r_{11}^b \cdot s$ with parameters r_{10}^b and r_{11}^b .

Rate dependency is introduced by a delayed micro-cracking and uses the visco-damage formalism. The damage variable is expressed as a function of distance between the current bond stress point and the infinitely slow damage locus:

$$dL = \frac{dt}{\eta^b} \left\langle F^d \right\rangle \tag{28}$$

where η^{b} is the damage viscosity of bonds. Infinitely slow damage locus takes the form

$$\overline{F}^{d} = F^{d} - \frac{\eta^{o}}{dt} dL \le 0$$
⁽²⁹⁾

Coupling

Any load applied to an element of cemented material will distribute itself between the soil matrix and the bonds according to a ratio that depends on the geometric arrangement of both components. Following the principle of energy equivalence that establishes the equality between the energy of the composite material and the sum of energies for all components leads to the expressions of strains and stresses:

$$d\varepsilon_{ii}^{M} = d\varepsilon_{ii} + d\varepsilon_{ii}^{b} \tag{30}$$

$$\sigma_{ij} = (1 + \chi) \sigma_{ij}^{M} + \chi \sigma_{ij}^{b}$$
(31)

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with

$$\chi = \frac{\varepsilon_v^b}{\varepsilon_v} = \frac{\varepsilon_q^b}{\varepsilon_q} = \chi_0 \cdot \sqrt{1 - D} = \chi_0 \cdot \exp\left(-\frac{L}{2}\right)$$
(32)

where the local stresses σ_{ij}^{M} and σ_{ij}^{b} must be in equilibrium with the external stress σ_{ij} and the local strains ε_{ij} and ε_{ij}^{b} must be compatible with the external strains ε_{ij}^{M} . χ_{0} is a coupling parameter related to cement concentration, giving the relative importance of the bond- and matrix-behaviour in the overall response of the composite material. The structure parameter χ decreases as damage evolves inside the bonds. In case of fully damage $(D \rightarrow 1, L \rightarrow \infty)$, the rock behaves like the de-structured soil. In case of triaxial compression, the Hoek & Brown's yield function for the composite claystone can be expressed as

$$F^{p} = \frac{q^{2}}{(1+\chi)R_{c}^{M}} + \frac{m^{M}}{3}q - m^{M}p - (1+\chi)R_{c}^{M} \ge 0$$
(33)

Parameters

In total, there are 18 independent parameters in the model. They were determined on the basis of the test results data (Deliverable 2; 7) and from literature (Vaunat et al., 2003; 2004; 2009). All parameters are given as follows:

$E^{M} = 2000 MPa$	$v^{M} = 0.28$	$K_{s}^{M} = 30000 MPa$	$m^M = 3$	$R_c^M(o) = 17 MPa$
$r^{M} = 2.5$	$\beta^{\scriptscriptstyle M} = 0.02$	$\sigma^{M} = 0.25$	$\xi_r^M = 0.02$	$\alpha^{M} = 0.5$
$E^{bo} = 4500 MPa$	$v^{bo} = 0.28$	$r^b(o) = 0.7 MPa$	$r_{os}^{b} = 0.001$	$r_{10}^{b} = 0.04 MPa$
$r_{11}^b = 0.7$	$\eta^{\scriptscriptstyle M}=10^5$	$\chi_0 = 0.5$	$\eta^b = 10^5$	

It is to be pointed out that the respective parameters for the clay matrix and the bonds in the rock mass can hardly be identified independently. This may lead to some degrees of uncertainty with the parameters and thus may limit the application of the model.

Main features

The stress – strain behaviour modelled for the COX claystone is compared in Figure 33 with the test data obtained by GRS at temperatures of 26 °C and 90 °C. It can be seen that, while the measured stress – strain curves before yielding are reasonably represented by the model, the post-failure behaviour can not well be matched.





Figure 33 : Stress - strain behaviour of the COX claystone in comparison between model and data

The damage threshold of bonds, the yield locus of clay matrix, and the failure boundary of the saturated clay rock (s = 0) are depicted in p–q stress plane in Figure 34 together with the strength data obtained on the COX argillite. The bond damage threshold (Eq. 27) at s = 0 draws in the p–q plane an ellipse with the major axis of $\sqrt{2K^{bo}r^{b}(0)}$ and the minor axis of $\sqrt{2G^{bo}r^{b}(0)}$ for the in situ stress state at the depth of ~500 m in the URL Bure ($\sigma_1 = 16$ MPa, $\sigma_2 = \sigma_3 = 12$ MPa). When the stress state reaches the ellipse, damage of bonds occurs and develops with increasing stress beyond the locus. The lower limit of the rock strength is taken as the yield boundary of the clay matrix (Eq. 13). When this boundary is attained by current stress state, plastic deformation takes place. The mean curve of the peak strength data represents the failure envelope (Eq. 33) for the clay rock. The post-failure behaviour appears as the stress is over the failure envelope. Since the test data do not indicate significant impact of temperatures on the rock strength, the above mentioned boundaries may be applicable for the high temperatures up to 100 °C.



Figure 34 : Damage, yield and failure boundaries of the COX argillite

The strength of the clay matrix and thus the clay rock are dependent on water content. The effect of suction is taken into account in the model (Eq. 14). Figure 35 compares the calculated curves with the strength data obtained on COX and OPA samples with different water contents at confining stress of 10 MPa (Blümling et al., 2005). The strength decreases



with water content. The effect of water content on the strength is apparently well represented by the model.



Figure 35 : Dependency of the strength of the COX and OPA clay rocks on the water content

5.1.2 Hydraulic model

In highly-consolidated clay rocks, a very significant portion of the water content is adsorbed on mineral surfaces and may not be able to participate in advective transport under normallyencountered pressure gradients. However, the adsorbed water is able to move out thermodynamically from the pores at high external suction, and in contrast, external water can also be taken-up by clays. The process of de- and re-hydration is controlled by the relationship between suction and water content (water retention curve). For both COX and OPA clay rocks, the water retention curves were determined on unconstraint samples placed in desiccators at different values of relative humidity adjusted by means of salt solutions, as shown in Figure 36. Because of the negligible difference between the retention curves measured along the wetting and the drying paths, an average relationship between suction and degree of water saturation is established for each clay rock type, respectively, and can be expressed by the Van Genuchten model:

$$S = \frac{S_{l} - S_{lr}}{S_{ls} - S_{lr}} = \left[1 + \left(\frac{s}{P}\right)^{1/(1-\beta)}\right]^{-\beta}$$
(34)

where S_l , S_{lr} , S_{ls} , S are the actual, residual, maximum and effective saturation of liquid, respectively, $s = P_g - P_l$ is the suction, P is a material parameter, and β controls the shape of the water retention curve. In the modelling, the mean values of P = 28 MPa and β = 0.37 are taken.



Figure 36 : Water retention curves of COX and OPA clay rocks

The Kozeny's model is employed for the relationship of permeability k with porosity ϕ :

$$k = k_o \frac{\varphi^3}{(1-\varphi_0)^2} \frac{(1-\varphi_0)^2}{\varphi_0^3}$$
(35)

with the initial permeability value of $k_0 = 2 \cdot 10^{-20} \text{ m}^2$ at the initial porosity of $\varphi_0 = 15\%$ for the COX argillite (see Figure 37).



Figure 37 : Permeability relating with porosity for the COX clay rock

It is to be noted that this model may not be adequate for description of permeability changes induced by fracturing. Currently, GRS has investigated on permeability changes in relation with fracture closure in the frame of another GRS project (Zhang, 2010). Based on the lab tests by compression of fractured COX and OPA claystones as shown in Figure 38, Zhang proposed an exponential model for the fracture closure by increasing normal stress:

$$\Delta b = b_m \left[1 - \exp\left(-\alpha \sigma_n^{\ \beta} \right) \right] \tag{36}$$

where Δb is the aperture closure, b_m is the possible maximum aperture closure (equal to the initial aperture), σ_n is the normal stress, α and β are constants; and for the permeability change by fracture closure:

$$k = k_{matrix} + \frac{b_{eff}^3}{12s} = k_{matrix} + \frac{(b - b_c)^3}{12s}$$
(37)

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where b_c denotes a critical aperture, k_{matrix} is the permeability of the rock matrix. As the geometric fracture aperture b decreases with increasing normal stress to a very low magnitude, $b < b_c$, some parts of the fractures may be separated and isolated by more compacted areas thus eliminating geometric connectivity and hydraulic conductivity in the dead-end fractures. This means that the cubic law is limited within "macro-cracks", $b > b_c$. The Kozeny's model (Eq. 35) may be suitable for the permeability of matrix k_{matrix} .

This fracture closure – permeability model has not been used in the frame of this benchmark modelling before its implementation in CODE-BRIGHT.

In addition to the advective transport of water and air, vapour diffusion in air and the solubility of air in liquid water are controlled by Fick's law and Henry's law, respectively. The changes of liquid and gas phases are represented by the psychrometric law. Details of these models can be found in (CODE-BRIGHT, 2004) and are not represented herein.



Figure 38 : Relationships of fracture closure with normal stress and fracture permeability with fracture aperture

5.1.3 Thermal model

Heat transport is governed by conduction through the porous media and by advective flow of liquid water and vapour. Thermal conduction is expressed by Fourier's law:

$$i_c = -\lambda \nabla T \tag{38}$$

where ΔT is the temperature change and λ is the thermal conductivity. Because of stratification, argillaceous rocks usually exhibit thermal anisotropy. The thermal conductivity values measured on along the directions parallel ($\lambda_{//}$) and perpendicular (λ_{\perp}) to the bedding plane are: $\lambda_{//} / \lambda_{\perp} = 1.9 / 1.3 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$ for COX claystone and $\lambda_{//} / \lambda_{\perp} = 2.1 / 1.0 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$ for OPA clay (Deliverable 2). This anisotropic property may be not so significant for the clay rocks under the confining stresses and therefore is not considered in this modelling work. A mean value of $\lambda = (\lambda_{\perp} + 2 \cdot \lambda_{//})/3 = 1.7 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$ is adopted for both the rocks. A value of specific heat capacity $C_s = 800 \text{ J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$ is adapted for the solid phase, while for liquid water $C_l^w = 4184 \text{ J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$ and for water vapour $C_g^w = 1900 \text{ J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$ are taken into account.

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According to the data presented in Deliverable 2, the thermal expansion of the clay rocks is also characterized by anisotropy with different coefficient values, for instance, $\alpha_{//} = 1.2 \cdot 10^{-5}$ K⁻¹ parallel and $\alpha_{\perp} = 1.9 \cdot 10^{-5}$ K⁻¹ perpendicular to the bedding for COX claystone, yielding an average value of $\alpha_m = 1.6 \cdot 10^{-5}$ K⁻¹. In saturated condition, the thermal expansion of a porous medium is governed by the expansion of both the solid minerals and the pore water. Without considering the anisotropy, a linear thermal expansion coefficient for the saturated porous medium may be expressed by:

$$\alpha_m = \alpha_s \left(1 - \varphi \right) + \frac{\alpha_w}{3} \varphi \tag{39}$$

where φ is the porosity in the rock, and α_s , α_w , α_m are the expansion coefficients of the solid grains, the pore water, and the saturated rock mass, respectively. The expansion coefficient for clay minerals have a low value of $\alpha_s = 2 \cdot 10^{-6} \text{ K}^{-1}$ (Noynaert et al., 2000). Using $\alpha_w = 3.4 \cdot 10^{-4} \text{ K}^{-1}$ for water, the coefficient is calculated to $\alpha_m = 1.65 \cdot 10^{-5} \text{ K}^{-1}$ for $\varphi = 13\%$ and $\alpha_m = 1.75 \cdot 10^{-5} \text{ K}^{-1}$ for $\varphi = 15\%$. Because the expansion coefficient of the pore water is two orders of magnitude higher than that of the solid grains, the thermal expansion of saturated clay rocks is mainly dominated by the water expansion. Figure 39 compares the theoretic model with the data obtained on OPA samples (Zhang et al., 2007; 2008) and the averaged thermal expansion curve of the COX argillite. The comparison shows that: a) the thermal expansion behaviour is nearly the same for both the claystones; b) the measured data are well represented by the theoretic model for a porosity range of $\varphi = 13-15\%$; and c) the numerical calculation with CODE-BRIGHT gives a slight over-prediction. In case of unsaturated state, thermal contraction may take place under certain confining stresses, as predicted by the numerical modelling in Figure 40.



Figure 39 : Thermal expansion behaviour of COX and OPA claystones in comparison between model and data







Figure 40 : Thermal contraction and expansion of claystone in unsaturated and saturated states

5.2 Modelling results

5.2.1 Benchmark modelling BMT1

The EDZ-simulation test BMT1 was performed on a COX hollow cylinder (DIR2003-K4) of D/d/L= 280/100/525 mm at ambient temperature of 26 °C in four steps:

- i. <u>Initial state</u> at the same outer and inner borehole pressure of $\sigma_R = \sigma_r = 15$ MPa and axial stress of $\sigma_a = 17$ MPa;
- ii. <u>Borehole excavation</u> by decreasing the inner pressure down to $\sigma_r = 2.6$ MPa;
- iii. <u>Unloading</u> in radial direction down to $\sigma_R = 3$ MPa for 4 days;
- iv. Loading in axial direction to failure.

During the test, gas flow was recorded at injection pressure of 1.5 MPa at the bottom. This test was simulated in a hydro-mechanical coupling way using an axisymmetric model. Because the sample was initially not saturated at a degree of 82 %, the corresponding suction of s = 22 MPa is adapted as the initial condition in the sample. The modelling steps with application of the corresponding boundary conditions are illustrated in Figure 41.







Figure 41 : Geometry and boundary conditions for modelling of the hollow cylinder test BMT1

The modelling results are compared with the test data in terms of time evolution of the applied temperature, confining stresses and gas injection pressure in Figure 42, the resulting displacements in Figure 43, changes of the stress state in Figure 44, and variations of the porosity and the permeability near the borehole wall in Figure 45, respectively.

From Figure 43 one can recognise that the short-term deformations induced by the stress changes are reasonably represented by the model, comparing with the recorded data of axial and outer radial displacements. The time-dependent deformation can not be captured because the model allows the visco-plastic deformation only after yielding.

Figure 44 indicates that after the borehole excavation by reducing the inner borehole pressure from $\Box r = 15$ to 2 MPa, the deviatoric stress near the borehole wall increases largely but below the yield criterion. Far from the wall the deviatoric stresses are much lower. Further increase of the axial stress during the last loading phase, however, leads the stress rising at all points in the hollow cylinder. In the calculation, an upper limit of the loading was encountered, at which the computation ceased. This computed maximum stress of $\Box y = 22$ MPa is lower than the realistic value of 27 MPa. Due to the limitation, the failure and the post-failure behaviour could not be modelled.







Figure 42 : Applied boundary conditions of temperature, stress and gas pressure



Figure 43 : Comparison of deformations between modelling results and test data





Figure 44 : Calculated stress paths at typical points in the large hollow cylinder

According to the Kozeny's model adopted for the modelling, the permeability change in the damaged zone near the borehole wall is calculated based on the modelled porosity at that location and compared with the recorded data in Figure 46. It is obvious that the permeability – porosity model is not able to capture the dramatic increase in the permeability due to fracturing. Obviously, adequate models are needed for description of such a percolation flow during the fracturing process.



Figure 45 : Calculated permeability variations in comparison with the measured data

5.2.2 Benchmark modelling BMT4

The EDZ-simulation test BMT4 was performed on a COX hollow cylinder (DIR1004-EST27312) of D/d/L= 280/100/460 mm. The test layout and the pictures of the sample before and after testing are shown in Figure 11. The test procedure involved six phases with respective boundary conditions:





- i. <u>Initial state</u> at the same outer and inner borehole pressure of $\sigma_R = \sigma_r = 15$ MPa and at fixed axial strain ($\Delta \epsilon_a = 0$);
- ii. <u>Borehole excavation</u> by reducing the borehole pressure down to $\sigma_r = 1.0$ MPa;
- iii. <u>EDZ-intensification</u> by increasing the external radial load till gas breaking through;
- iv. <u>Water injection</u> to the top of the fractured sample at pressures of 0.5 to 0.3 MPa for 17 days;
- v. <u>Heating</u> by increasing the temperature from 29 °C to 74 °C at the outer surface during 3 days and kept constant for 19 days;
- vi. <u>Cooling</u> down by reducing the temperature to the initial level of 29 °C over 3 days and kept for 18 days.

Considering the complex testing procedure and conditions, coupled THM calculations were carried out. The initial porosity of 15.8 % and saturation degree of 90 % (suction s = 10 MPa) are taken into account. An axisymmetric model is adopted for the hollow cylinder (Figure 46). The realized test procedure with the above mentioned steps is simulated by applying the corresponding conditions to the model. Figure 47 illustrates the applied boundary stresses and temperatures in comparison with the data.

The following boundary conditions are applied: (1) instead of the fixed axial strain, the recorded axial stress of 1.7 MPa is applied in the model within the first three steps (I-III) because the poor control of the axial strain and possible weak contacts between the load pistons and the end faces of the sample; (2) the gas migration test during the first three steps (I-III) is not simulated by keeping the gas pressure atmosphere; (3) the temperature measured at the inner borehole wall is applied as a boundary condition because some amounts of heat lost from the sample ends; and (4) various values of the intrinsic permeability between 4·10-20 and $5\cdot10-18$ m2 are examined by comparing the water flow and pressure with the measured data.





Figure 46 : Geometry and boundary conditions for modelling of the hollow cylinder test BMT4



Figure 47 : Applied temperatures and stresses in comparison between model and data

First, the modelled deformations due to the borehole excavation and the EDZ intensification (steps I-III) are compared with the measurements. Figure 48 shows that the deformations at the measuring points and the borehole convergence due to the borehole excavation ($\sigma_r = 15 \rightarrow 1$ MPa) can be reasonably revealed by the model, confirming the elastic parameters. After that, the calculated deformations remain constant without continuation with time as observed



in the test, because the stress state after borehole excavation is still below the yield criterion. Further increasing the external load in radial direction resulted in a large convergence of the borehole and fracturing in the sample at $\sigma_R = 24$ MPa, which was detected by gas flow during the test. However, this failure stress is not matched by the modelling because the computation ceased at $\sigma_R = 17$ MPa. As mentioned before, the failure and the post-failure behaviour could not be modelled. Inevitably, for next modelling steps the outer radial stress is reduced to 15 MPa.



Figure 48 : Calculated and measured mechanical behaviour of COX hollow cylinder – (a) applied stresses and permeability change by fracturing – (b) response of deformation to loading

Figure 49 indicates that, after the borehole excavation, the deviatoric stress near the borehole wall increases subsequently over the yield boundaries of the bonds, clay matrix and the composite argillite at suction of zero (saturated) and the initial suction of 10 MPa

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(unsaturated). The claystone near the borehole wall is more damaged than the inside where only the bonds are damaged but the clay matrix does not yield.



Figure 49 : (a) Stress evolution calculated for typical points in the cylinder in comparison with the yield boundaries of bonds, clay matrix, and the argillite and (b) damage distribution at external radial load of 17 MPa

After damaging, the water injection (IV), heating (V) and cooling (VI) phases followed at fixed axial strain $\Delta \epsilon_v = 0$, and constant outer / inner radial stress of $\sigma_R = 15$ MPa / $\sigma_r = 1$ MPa. In the modelling, different permeability values of $4 \cdot 10^{-20}$ and $5 \cdot 10^{-18}$ m² are accepted to fit the observed water inflow and outflow as well as the water back-pressure at the inlet side. Figure 50 compares the calculated and observed water inlet pressure pin and outlet pressure pout, while the modelled water inflow Qin and outflow Qout are compared with the measurements in Figure 51. During the water injection, the inlet was closed several times to examine response of the water back-pressure. From Figure 50 one can see that the modelled inlet pressure evolution with $k = 4 \cdot 10^{-20} \text{ m}^2$ agrees well with the data. However, the corresponding water inflow and outflow are significantly underestimated (Figure 51a). In contrast, the water flow rates (slop of the flux – time curve) can be well represented with the high permeability of k =5.10⁻¹⁸ m² (Figure 51b), but the corresponding water back-pressure calculated is much lower than that observed (Figure 50). Obviously, these modelled hydraulic parameters are not consistent with each other and also disagree with the measurements. This may suggest that the applied hydraulic models being validated for homogeneous porous materials are not adequate for strongly-fractured clay rocks. Additionally, a great amount of the water inflow at the beginning was recorded in the test, probably filling the space of interconnected fractures. This observation is also not revealed by the modelling with use of the hydraulic models for undamaged materials. Moreover, the deformation and borehole convergence after fracturing can also not be matched by the modelling (Figure 52). The calculated thermal deformations during the heating and cooling phases are rather small compared with the measured data.

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Figure 50 : Calculated and observed water pressures at inlet/outlet before, during and after heating



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Figure 51 : Calculated and observed water inflow and outflow before, during and after heating (a) calculated water inflow at $k = 4 \cdot 10^{-20} m^2 - (b)$ calculated water inflow at $k = 5 \cdot 10^{-18} m^2$



Figure 52 : Calculated and observed deformations before, during and after heating

5.3 Discussion and conclusion

In the GRS benchmark modelling, the capabilities of the THM constitutive models in CODE-BRIGHT (cdv3), particularly the damage-elastoplastic model for argillaceous rocks, have been examined by comparison with the results of the large hollow cylinder tests on the COX claystone in regard to the development and recovery of the EDZ around HLW disposal boreholes. The results indicate that:



- The short-term deformation behaviour of the hollow cylinders is reasonably represented by the model with indication of micro-damage evolution, but the post-failure behaviour could not be modelled due to earlier stop of the computation.
- The drastic increase in permeability by fracturing and the permeability decrease by recompaction of the fractures can not be captured by the Kozeny's permeability – porosity relationship for porous media without fractures.
- The observed water inflow into the fractured claystone is significantly underestimated by the modelling even though the real permeability value of the fractured claystone is used.
- The significant responses of deformation in the damaged claystone to heating and cooling are weakly revealed by the modelling.

Generally speaking, the THM behaviour of damaged claystones can not reasonably be approached by the constitutive models for continuum porous media without involving effects of discontinuities. From our knowledge, the behaviour of damaged claystones is not yet well characterized and understood. Further research work is obviously necessary to improve the constitutive models for the prediction of the development and recovery of the EDZ and to enhance the certainty of the long-term performance and safety assessments of HLW repositories in argillaceous formations.

6 Conclusions and perspectives

Thermo-hydro-mechanical modelling of the COX hollow cylinder tests has been performed by ULg and GRS. Additional hydro-mechanical couplings have been used in order to reproduce the increase of the axial permeability by fracturing:

- A coupling between the permeability and the tensile strains (ULg). This embedded fracture model assumes that aperture controls the fracture permeability through a cubic relationship.
- A coupling between the permeability and the porosity through the Kozeny relationship (GRS).

Numerical results show that the embedded fracture model allows the reproduction of the permeability increase of the damaged sample, whilst the Kozeny relationship is not sufficient to reproduce the drastic increase of the permeability. Nevertheless the experimental results seems to be strongly influenced by the initial desaturation of the porous disk, which modifies the injected water volume during the water injection tests and complicates an accurate reproduction of the numerical results.

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