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1 Introduction

In all nuclear power generating countries, spent nuclear fuel and/or long lived radioactive-waste management is an important environmental issue today. Disposal in deep clay geological formations is one of the promising options to dispose of these wastes. An important item for the long-term safety of underground disposal is the proper evaluation of the Damaged Zone (DZ) in the clay host rock. The DZ is first initiated during the repository construction. Its behaviour is a dynamic problem that depends on the changing conditions during the open-drift period, the initial closure period and the entire heating-cooling cycle of the decaying waste. Other factors concern the even longer-term issues of chemical reactions and biological activities.

In recent years, there have been intense efforts to evaluate the extent and properties of the Excavation Damaged Zone (EDZ), the DZ initiated during the repository construction, involving field, laboratory, and theoretical studies (as in the recently terminated EC project SELFRAc). Performance assessment models for different repository designs in different clay formations have demonstrated that even for rather unfavourable EDZ conditions the overall performance of the repository system is not adversely affected and that dose rates remain well below regulatory guidelines.

The influence of the temperature on the clay host rock has also been studied in previous research projects. The THM characterization was mainly performed on samples in surface laboratory and from small/medium scale in-situ heater tests. At the same time, different THM models and numerical codes were developed to better understand the THM processes. However, the influence of the thermal load generated by the radioactive waste on the performance of the disposal system has only been studied at a limited scale of time and space compared to a real repository. This aspect is particularly important since the early transient THM (Thermo-Hydro-Mechanical) perturbation might be the most severe impact the repository system will undergo on a large spatial scale and in a relatively short period of time. Assessing the consequence of the thermal transient on the performance of the disposal system will be the main objective of the proposed TIMODAZ project. Even the full THMC (Thermo-Hydro-Mechanical-Chemical) coupling aspect will be studied, the effect of temperature on the chemistry will be investigated in a more limited extent. The TIMODAZ project will focus on the significance of THM processes, in the context of the safety case. Especially the combined effect of the EDZ and the thermal impact on the host rocks around a radioactive waste disposal. The influence of the temperature increase on the EDZ evolution as well as the possible additional damage created by the thermal load will be investigated.

The present report gives a synthesis of the relevant works previously performed on the three investigated clays (Boom Clay, Opalinus Clay and Callovian Oxfordian Argillite) in surface laboratories and in in-situ facilities. It comprises a database and a reference document to optimise the testing procedures of the laboratory experiments and the in-situ experiments to be performed in the present project.

The first part of the report points out the main issues related to the thermal impact, which should reflect the viewpoints of end users. The second part is devoted to the state of the art for each investigated clay, including the main characteristics of each clay, the available THM characterisation, the related chemical aspects and the current development of the constitutive models. For each clay the report provides a discussion in order to:

- delineate the most important temperature-dependent material properties
- define the most important coupled processes and parameters
- assess the effect of discrete fractures and fracture connectivity on the effective hydraulic
properties, to determine the importance of chemical impact

- derive/evaluate the most appropriate conceptual models and numerical codes as well as to notice the remaining uncertainties on the THM properties of the clays

A detailed version of the Deliverable 2 is annexed to the report (technical annex 1).

2 Main issues related to the thermal impact

The disposal of heat emitting radioactive waste will induce disturbances in the host rock. The impact of the thermal load is particularly important since it will affect the temperature and the stress in the host rock to a large spatial extent (depending on the repository design) around the repository.

The disturbances can be of different types and are often coupled: thermal (T), hydraulic (H), mechanical (M) and chemical (C). The THMC responses will highly depend on the initial and the boundary conditions imposed by the repository design, as for example:

- the hydraulic boundary conditions around the waste imposed by the repository design
- the pore pressures reached around the disposal gallery before the waste disposal
- the mechanical conditions imposed by the lining
- etcetera

The overpressure generated in the host rock by the temperature rising depends highly on the hydraulic boundary conditions of the disposal gallery. This will in turn be controlled by the hydraulic properties of the seal closing the disposal gallery and by the saturation of the engineered components reached before the disposal of the waste. The thermal induced pore pressure build-up will be much more pronounced if a rather impermeable hydraulic boundary condition is assumed (as revealed by the scoping calculations, see technical annex 2). The impermeable boundary condition constitutes therefore a more critical situation for the host rock.

During the open drift period, pore water will flow from the host rock towards and into the disposal tunnels. Depending on the different national concepts and especially on regulatory guidelines with respect to monitoring and reversibility, such open drift phases could range from one month to a few years. On the one hand, the long term drainage of the disposal gallery will enhance the hydromechanical coupling due to the pore pressure drop and induce contracting strains that are able to create additional plastic deformation and/or damage (micro-macro) and thus increase the DZ that may have been limited by tunnel support. On the other hand, this may constitute, from a purely thermohydromechanical point of view, a favourable factor (less thermal induced pore pressure build-up) for the safety of the repository system. Meanwhile, the open drift will be ventilated and suction (possibly partial de-saturation) could evolve in the rock close to the tunnel wall. This suction could improve the hydro-mechanical properties of the rock (increase the permeability and increase the shearing strength). However, the excess desaturation may evoke additional damage through tensile failure and will affect the THMC coupled responses of the repository system (oxidation, etc.). The long term drainage also favourises the sealing process as observed in Boom Clay around the URL HADES.

Consequently, the maximum thermal source term is not the only issue to be considered when assessing the thermal impact of heat emitting waste. Other design issues controlling the hydraulic conditions of the repository system are also important to be taken into account.

Hereafter more specific issues related to the three considered clays (Boom Clay, Opalinus Clay and Callovo-Oxfordain Argilite) are given.
2.1 Boom Clay

2.1.1 Temperature evolution in the Host Rock in the Belgian repository designs

In the Belgian disposal system for the vitrified High Level radioactive Waste and Spent Fuel, the Boom Clay host-rock is the main barrier for the long term isolation in the normal evolution scenario. The waste packages will be disposed of in a network of horizontal galleries in the Boom Clay host formation.

The safety function of the host rock is delaying and spreading the radionuclide release. The Boom Clay will slow down the migration of radionuclides towards the biosphere allowing radioactive decay within the disposal system. In order to prevent any alteration of the favourable physico-chemical properties of the repository components and those of the host rock, a criterion for the admissible maximum temperature in the different parts of the disposal system was established. In particular, the maximum temperature in the host rock must be kept below 100°C (NIROND 2001-05). A sufficiently long cooling time of the radioactive waste (intermediate storage), a suitable canister and gallery spacing are necessary.

NIRAS/ONDRAF is now considering three alternative designs (NIROND 2003-01):

- the Supercontainer (SC)
- the Borehole
- the Sleeve

Based on a multi criteria analysis, the Supercontainer design was selected as the preferred option (NIROND 2004-03). However, NIRAS/ONDRAF considers the two other options as possible alternatives.

The Supercontainer design for vitrified waste considers disposal of two vitrified Cogema canisters in a carbon steel overpack, surrounded by a concrete buffer (see Figure 2.1). The heat produced by the Supercontainers will increase the temperature in the near field, in the Boom Clay host formation and even in the aquifers during several hundred of years.

The Supercontainer design for spent fuel is very similar to the design mentioned above but in this case four assemblies of spent fuel UOX (or one assembly of MOX) will be placed in a carbon steel container instead of a common overpack. The maximum heat flux (W/gallery length) produced by the Supercontainer for spent fuel is very comparable to the case of vitrified waste (about 240W/m) but the thermal period will extent to several thousand of years.

Different calculations have been made to assess the maximum temperatures in the engineered barriers and the Boom Clay for different cooling periods and the different waste types (vitrified waste, UOX and MOX), considering the Supercontainer designs (Weetjens & al. 2005). The disposal gallery spacing is about 50m for the galleries with vitrified waste while it is extended to about 120m for the galleries with spent fuels. This repository geometry (i.e. the gallery spacing) implies that, for the same cooling period, the maximum temperatures in the Boom Clay will be slightly higher (10% up to 15%) for spent fuel than for vitrified waste (Figure 2.2). For an OPC concrete buffer and a cooling period of 50 years, the maximum calculated temperature for vitrified

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1 The supercontainers for spent fuels have a length of about 6 m instead of 4 m for the supercontainer for vitrified waste.
2 t=0 is defined as the time when the waste is produced in its final form, i.e. vitrification of the reprocessing waste and unloading from the reactor for the spent fuel.
waste at the interface Boom Clay/liner is 65°C (ΔT = 49°C) and 74°C (ΔT = 58°C) in the case of spent fuel.

Figure 2.1: ONDRAF/NIRAS reference design (anno 2006) for vitrified waste (above) and spent fuels (below)
Figure 2.2: Maximum temperatures in Boom Clay for the supercontainer design for (above) spent fuel (50y cooling, 120m gallery spacing) and for (below) vitrified waste (50y cooling, 50m gallery spacing)

It is worth to note that the above calculations were based on the actual knowledge on the thermal properties of the Boom Clay on which uncertainty still exists. Especially the thermal conductivity will largely affect the final geometry of the repository (especially the gallery spacing).

2.1.2 Thermal effects on the host rock

A good comprehension of the inter-related processes in the Boom Clay around the repository is an essential element of confidence building to assess to what extent the favourable properties of this clay are, temporally or permanently, altered according to the safety function. These favourable properties are the low permeability, good sorption and retention capacity for radionuclides, the slow diffusive transport capability combined with the absence of preferential migration pathways for solutes and the sealing capacities.

The construction of the disposal infrastructure and the repository components (RC) will induce disturbances in the Boom Clay. The time and spatial evolution of the THMC disturbances around a disposal gallery are schematically represented on Figure 2.3.

Different sources of disturbance can be distinguished:

- disturbances created by the construction of the disposal infrastructure and by the operational phase: these disturbances will affect the hydro-mechanical conditions of the Boom Clay and concern the whole thickness of Boom Clay
- disturbances created by the large scale thermal load generated by the waste: these disturbances can affect a) the hydro-mechanical conditions of the Boom Clay at short term (0 to 500 years for the vitrified waste and 0 to 2000 years for the spent fuel) and concern the whole thickness of Boom Clay; b) the diffusion coefficient c) the chemical conditions in the near field, which could induce changes in the transport properties. However disturbances b) and c) are expected to be very limited for the considered temperatures and temperature gradients
- disturbances created by the chemical interactions with the repository components: these disturbances will be mainly limited to the near field and concern the long term (several thousand of years)
- disturbances created by the radiation of the waste: these disturbances can affect the near field when the thickness of the repository components surrounding the waste is small (this is the case for the borehole design, which consists in inserting the waste package directly into the lined borehole). The CERBERUS experiment demonstrated that the extent of these disturbances can expected to be
limited taking (Noynaert & al., 2000). Simple radiolysis calculations lead to a similar conclusion
Consequently the early THM perturbation created by the excavation, the operational phase and the
thermal load might be the most severe transient that the repository will undergo on a large spatial
scale and in a relatively short period of time. Given an identical thermal flux, the temperature
profiles around the disposal galleries will be very similar independently of the considered design
and are mainly determined by the thermal properties of the Boom Clay under saturated condition.
The repository design can significantly influence the disturbances in the Boom Clay. The major
affecting factors are the HM conditions prevailing the heating phase: the pore water pressure and
stress profiles in the Boom Clay, the saturation degree of the repository components and the
hydraulic boundary conditions imposed by the repository design. These factors will have a direct
impact on the maximum pore water pressure build-up reached during the heating phase. For
example, the longer the drainage phase before the disposal of the waste, the lower the maximum
core pressure during the heating phase.

![Figure 2.3: Time and spatial evolution of the disturbed zone (dZ) around a disposal gallery](image)

**2.1.3 Thermal impact on the geochemical aspects**
The temperature increase can also affect the chemistry of the host rock. Recent experimental work
in collaboration with l'Institut Français de Pétrole (IFP) has shown the quick release of CO₂ from
Boom Clay kerogen, even at a moderate temperature increase. H₂S release is also expected but to a
smaller extent. This rising temperature will likely cause changes in clay mineralogy and pore water
chemistry. These geochemical perturbations could have a potential impact on the integrity and the
performance of Boom Clay as a geological barrier. Therefore they demand a further investigation.

**2.1.4 Thermal impact on the lining stability**
The thermal load can also affect the stability of the disposal gallery lining. Calculations show that
the temperature increase can induce high stresses in the lining. The use of compressive materials
between the concrete lining blocks could be a solution to limit these stresses. This issue is particularly important when the retrievability of the waste is considered.

2.2 Opalinus Clay

2.2.1 Near field temperature evolution in the Swiss repository design
The design of a possible geological repository for high-level radioactive waste that has been used to demonstrate the feasibility of such a repository at a potential site in NE Switzerland (Nagra 2002a) is based on a multiple barrier concept. Canisters containing radioactive waste are emplaced into tunnels drilled into the Opalinus Clay. The tunnels are backfilled with a mixture of bentonite and sand (Figure 2.4). In order to maintain the favourable chemical properties of the backfill material the peak temperature of a predefined part of the bentonite will be kept sufficiently low to prevent significant mineralogical or chemical alteration of the material. This is ensured by a sufficiently long intermediate storage time of the radioactive waste, an appropriate canister loading (mixing of MOX and UO2 spent fuel elements) and a suitable canister spacing. These requirements for the backfill material also limit the thermal load on the surrounding rock.

Numerical simulations show that with an intermediate storage time of 40 years these requirements can be met (Nagra 2002b). The canisters, which have an average initial heat output of 1500 W, reach a peak temperature shortly after backfilling of 150 degree on their outsides (Figure 2.5). The temperature field in the surrounding bentonite material and the host rock depend strongly on the water content of the backfill material. This water content is controlled by the water flow rates towards the repository which are in turn limited by the permeability of the Opalinus Clay. Resaturation is expected to take a few hundred years. In the unsaturated case the bentonite has a low thermal conductivity and the temperature at the point midway between the spent fuel canisters and the bentonite / host rock interface will reach a maximum of 110 °C. Host rock temperatures remain below 90 °C in the base case. Rapid saturation of the near field occurs within decades and would lead to significantly lower temperatures (10 to 20 °C lower at the mid-bentonite position).

The strong dependence of near field temperatures on bentonite thermal conductivity leads to some uncertainty in temperatures within the bentonite because groundwater inflow rates are uncertain. Smaller uncertainties in predicted temperatures (approximately 10 °C) arise from uncertainty in the values of thermal conductivity assumed for the host rock. In any case, there is relatively little uncertainty regarding the maximum projected temperatures at the bentonite-canister interface since the maximum temperature is reached within only 10 years, i.e. when this region is still dry.
2.2.2 Thermal effects on the host rock in the near field

In indurated clays several heat sensitive processes may affect the state and the properties of the tunnel nearfield. These are for example damage caused by temperature induced stresses (crack growth), increased pore pressures, chemical and mineralogical changes in the host rock that affect its barrier function.

Investigations at the Aspo URL and the Canadian URL show that thermally induced damage on a micro scale is detectable in crystalline rock by acoustic emission (AE) monitoring. Analysis of AE
time series shows that the damage accumulation depends mainly on (1) thermal gradients over time and (2) minimum stress (e.g. Read et al. 1997). Similar dependencies can be expected for indurated clays but the strong hydromechanical coupling introduces some additional complexities.

Thermal expansion of fluids is generally by an order of magnitude larger than that of solids. As a result fluid saturated porous rocks like the Opalinus Clay show a pore pressure increase during heating (Wileveau, 2005). The increased pore pressure reduces the effective stresses and may destabilize critically loaded regions around excavations and enlarge the damaged zone. Similar to crystalline rocks, the temporal and spatial gradients of heating are important. If the nearfield is already desaturated or drainage from the heated and pressurized region is possible and operates at similar rates as the heating, the pore pressure built-up may be considerably reduced. However, both lab data and field experiments relating pore pressures and heating rate in the Opalinus Clay are scarce. This highlights the need for new laboratory and field investigations of THM coupling in the Opalinus Clay.

Thermally assisted weakening of the Opalinus Clay has been postulated in a few studies. Tests with samples at natural water content show that the short term strength is significantly reduced by heating. In contrast, creep rates do not differ much between room temperature and 80 °C. This may indicate that the increase of the pore pressure plays a more important role for the strength reduction than the temperature assisted growth of defects.

Chemical or mineralogical changes in the Opalinus Clay due to heating in the nearfield are unlikely. Possible effects would include (1) maturation of organic material that leads to the production of carbohydrates or changes in the pore water chemistry, (2) the transition of smectite to illite in the composite clay minerals that leads to an embrittlement of the material and a partial loss of the swelling capacity, (3) an acceleration of oxidation reactions ensuing from a change in porosity and pore water chemistry, (4) the re-adjustment of chemical equilibrium reactions. However, experimental data, natural analogues and chemical model calculations show that heating of 85 to 95 °C for a few hundred years is insufficient to induce any significant impact by the above mechanisms (Mazurek 2002).

In the context of the entire repository system the potential for damage in the tunnel nearfield due to heating is considerably reduced. In the Swiss concept of a high level waste repository the nearfield will be desaturated during the excavation and operation of the tunnels. The resaturation is limited by the permeability of the host rock and will take several hundred years. This has several consequences. On the one hand the bentonite buffer will retain its low thermal conductivity throughout the rise of the canister temperatures in the first decades. Consequently the heating of the host rock will be slow, thus decreasing the likelihood of any thermal damage. On the other hand pore pressures that reduce the effective stresses cannot increase while the rock is not re-saturated. Hence, desaturation of the nearfield and thermal isolation of the canisters by the bentonite material protect the nearfield host rock from excessive thermal damage.

### 2.2.3 Impact of thermal damage in the tunnel nearfield onto performance assessment

In order to assess the importance of the host rock properties in the vicinity of the underground excavations the entire repository system has to be taken into account. Such an evaluation has been done in a performance assessment of the Swiss repository concept (Nagra 2002a). In this study all relevant components and properties of the repository system have been included and their performance has been evaluated in terms of the calculated radiation exposure for an individual of the most affected group living in the surface environment.

It shows that for rock masses with low hydraulic conductivity and no natural water-conducting
features, the flow through the EDZ is mainly limited by the inflow from the undisturbed rock into the tunnels and partly by the effectiveness of the seals (Nagra 2002a). Even without seals, the flow along tunnels levels off at hypothetical effective conductivities of the EDZ of about $10^{-8}$ m/s, implying that higher conductivities would not result in an increase in flow through the repository. But flow is not the only parameter that controls transport and radionuclide release from a repository. The retention capacities of the buffer and the host rock are at least equally important. It has been shown that, especially in the case of long emplacement tunnels (long distance between radionuclide source and the end of the tunnel), radionuclides will be released from the EDZ into the intact host rock by matrix diffusion. Smith et al. (2004) conducted a sensitivity study to evaluate the effect of EDZ conductivity on dose for a repository in Opalinus Clay. Figure 2.6 shows that even for the hypothetical case of an EDZ conductivity of $10^{-8}$ m/s (flow levels off at this value, see above) the dose stays well below the regulatory guideline.

2.3 Callovo-Oxfordian Clay

2.3.1 Near field temperature evolution in the French repository designs

The inventory of French radwaste contains exothermal packages: mainly high level vitrified wastes and to a lesser extent some intermediate level long-live (IL) wastes (and of course spent fuel if it were sent to the disposal).

The HL waste disposal cell is a dead-end tunnel (700 mm in diameter, 40 m long) with a steel casing as lining (see Figure 2.7).
Figure 2.7: HL wastes cell while in operating configuration (up) and after sealing (down)

For IL wastes, the disposal cell is a dead-end horizontal tunnel with a useable length of 250 m and an excavated diameter of 12 m (see Figure 2.8).

The waste package emplacement in the repository induces a gradual but transient increase in temperature from the packages to the geological environment.

Figure 2.8: IL wastes disposal cell while in operation (foreground of the image) and after sealing (background of the image)

The chosen geologic formation in France is a thick layer of Callovo-Oxfordian argillites. Numerical simulations show that the temperature field linked to the thermal load is rapidly uniform in and around the disposal cell (from a few hundred to a thousand years). The temperature in the argillites reaches 90 °C in the first tens of years and remains in the order of 80 to 50 °C during the resaturation of the EBS. A few meters away from the repository, the thermal profiles in the Callovo-Oxfordian show a rapid decrease in the temperature (weaker slope of the temperature profile) and the temperature does not exceed 60 °C. At the roof of the Callovo-Oxfordian, it reaches a maximum
of 35 °C after about 1 000 years and descends again to less than 30 °C after about 10 000 years. Between 50 000 and 100 000 years are required to return to the geothermal temperature.

This thermal load affects the hydraulic, chemical or mechanical processes that govern the repository evolution, notably corrosion phenomena and release and transport of solutes.

In order to reduce impact of the heating the repository is subdivided in zones 250 m apart from each other. At this distance the thermal effects are negligible and the temperature is limited to 90 °C in the bulk of the host rock. As a consequence the main issues related to the thermal impact are limited to the near field\textsuperscript{3}. In the far field (i.e. beyond the Callovo-Oxfordian formation) the stress increase due to the thermal loading is lower than 1 MPa. This cannot lead to a fracturing of the limestone overburden, but only to a very small uplift (some dm) above the disposal due to the thermal dilation of the rocks.

2.3.2 Thermal Effects on the hydro-mechanical behaviour of the disposal cells

The Callovo-Oxfordian argillites are characterized by strong water/mineral interactions due to its petrofabric. Free pore water probably only exists if the pore opening is larger than approximately 5 to10 nm. Therefore the part of porosity occupied by bound water is estimated to make up 40 % of the total porosity.

The thermal cycle has different transient effects on the pore water:
- decreasing the viscosity of the water
- increasing the pore pressure
- weakening the bound of absorbed water on the external surface of clay particles (dipole-dipole and Van der Waals type interactions).

This is however only possible when water saturation and temperature rise are concomitant. This concomitance does not exist in exothermic IL waste disposal cells or their access drifts subjected to thermal load, because the temperature rise timescale (about a decade in the IL waste disposal cells and a few centuries in the access drifts) is much shorter than the time required to return to saturation inside these structures (Figure 2.9).

In the high level vitrified waste disposal cells the argillites are close to saturation after cell closure and during the thermal phase. A thermal load-induced hydraulic overpressure may thus be produced in the argillites around the disposal cells over several meters. It causes a divergent water flow because the overpressure is at its maximum at the disposal cell walls (4 MPa in ca. ten years). This overpressure lasts for a few centuries at the most. The created flow decreases more rapidly, within a few decades, as the temperature in the argillites evens out. Rises in temperature generate deformations and stresses in the repository components and argillites (Figure 2.10). The evolution

\textsuperscript{3} Following the definition given by « dossier 2005 », the near field refers to "the part of the geological disposal system of the radwastes including the Host Rock in the immediate surroundings, where the thermal, hydraulic, mechanical and chemical disturbances are induced by the presence of the wastes" - "Partie d'une installation de stockage géologique de déchets radioactifs, y compris la roche d'accueil en environnement immédiat, qui est généralement le siège de perturbations thermiques, hydrauliques, mécaniques et chimiques induites par la présence du stockage."

It’s worthwhile to note that the limit between near field and far field is not precisely defined. The near field is not only limited to the EDZ, but corresponds to a zone subjected to several sorts of perturbation that is able to modify the radionuclide migration and retention parameters. In the case of argilitte, the hydric and chemical perturbations, as well as the modification of the transport properties are quasi limited to the EDZ. However, thermal field (temperature) as well as the hydraulic field (pore pressure) may be disturbed farther, but they only have a limited impact on the nuclides migration (comments from Patrick Lebon).
of the mechanical behaviour of the repository engineered structures and surrounding argillites is then coupled to temperature evolutions in and around the engineered structures.

The thermal effect on pore water causes (i) developing stresses within the argillites and (ii) accelerating the argillite creep. Consequently the convergence of the cell reaches 1.7 to 2.1 % of the excavation radius after a few years. It contributes to a gradual reduction of the gaps between the lining and the argillites at the disposal cell wall. 50 to 60 % of the initial gaps are closed at this time and all gaps are closed after ca. 100 to 150 years. Thermo-mechanical interactions between neighbouring disposal cells induce a slightly anisotropic fractured zone up and down the disposal cell, extending less than 0.1 times the cell radius (Su & Barnichon, 2005).

When the gaps between the argillites and the lining are filled, the total convergence of the argillites reaches 2.8 to 3.3 %. During these deformations the EDZ extents around the disposal cells: a fractured zone up to ca. 0.4 times the radius of the disposal cell (about 0.15 m) and a microfissured zone progressing up to ca. 1.4 times the radius of the disposal cell (about 0.50 m). A rapid installation of the swelling clay plug limits the convergence of the argillites and the evolution of the EDZ. The argillite creep rate is stabilised when thermal paroxysm is reached.

Hydraulic and thermal experiments conducted *in-situ* at Bure (TER experiment) and Mont-Terri (HE-D experiment) show strong thermo-hydro-mechanical couplings. The values of THM coupling parameters for argillites are the main input data when modelling of the mechanical behaviour of the argillites and components inside the cells during the thermal phase of the repository. Given the knowledge acquired in “Dossier 2005” (see Site reference document, Volume 2) the key questions to be addressed by the R&D program are:

- the reduction of the uncertainty in the THM coupling parameters that determines
- the induced interstitial overpressure, especially the coefficient of thermal expansion $\alpha$ and the coefficient of differential thermal expansion $\alpha_m$
- the impact of this interstitial overpressure on damage (what is the threshold above which fissuring occurs?; is there a temperature effect on the rupture and damage thresholds?)
a better understanding of the relationship between temperature and creep rate in argillites

To reach these objectives, additional tests will be performed under saturated conditions at temperatures lower than or equal to 90 °C. Furthermore some tests are performed at temperatures between 90 and 120°C to identify the major aspects of argillite behaviour at the limit of the repository operating domain and to obtain data for analysing hypothetical failure cases.

1. EDZ evolution with the temperature

![Diagram of EDZ evolution with temperature](image)

- After excavation no fractured zone, isotropic microfissured zone
- During temperature increase slightly extended fractured zone up and down, increased elliptic microfissured zone

2. EDZ evolution with the convergence

![Diagram of EDZ evolution with convergence](image)

- Gap total closure
- Initial state

Figure 2.10: Effect of a temperature rise on the evolution of the EDZ and the deferred convergence around a vitrified waste disposal cell (hypothesis of maximum gaps)

2.3.3 Thermal Impact on the conditions of solute transfer

The overpressure developed around the exothermic waste cells provides higher gradients than the ones naturally occurring. The high thermal gradients in the near-field imply a significant Soret effect on solute transfer. Thermal load also increases the diffusion coefficient and permeability to water (Coelho, 2005).

However, according to the very slow corrosion rate of the steel overpack (a few microns per year),
the period of the maximal thermal load persistence is much shorter than the leak tightness period of
the waste package (e.g. a few centuries compared with 4000 years). Beyond 4000 years, the
temperature rapidly decreases and is between 25 and 30 °C after approximately 10000 years. It has
no effect on the transfer of radionuclides released by the vitrified waste. Furthermore, the hydraulic
overpressure caused by the thermal load would not overlap the overpressures created by the
hydrogen because it will have disappeared by the time the latter becomes significant. Nonetheless
diffusion remains the dominant process. The relationship between temperature and anion effective
diffusion coefficients is empirical and must be better understood. A same approach will be
developed for cation diffusion.

2.3.4 Thermal impact on geochemical processes

Changes in degradation processes of waste package and overpack

During the thermal period, the corrosion kinetics under anoxic conditions are increased by a factor
of 4 at 90 °C and a factor of 2 at 60 °C compared with those at the natural geothermal temperature
of 22 °C. Given the decrease in temperature in the disposal cells after a few decades, the effects of
the thermal load on the corrosion of the vitrified waste overpack are limited.

The dissolution kinetics of vitrified packages is controlled by the chemical composition of the glass
and by the thermal and chemical conditions of the water in contact with the glass. The αβγ self-
irradiation processes which begin from the moment that the vitrified packages are manufactured, do
not influence the dissolution kinetics of the glasses, mainly because of the high self-healing ability
of the glass matrix (Andra, 2005). In vitrified waste disposal cells the water comes into contact with
the glass at least beyond 4 000 years. By then the temperature has dropped below 50 °C and
dissolution kinetics are not significantly altered (Bauer, 2005).

Evolution of swelling clay and argillite properties

In the swelling clay heating can cause (i) precipitation of gypsum, (ii) dissolution of quartz, (iii)
illitisation of smectite. But the quantity of quartz is small in swelling clays (< 3 %) (Andra, 2005g,
Tome 1) and the available potassium in argillites is in very small concentration. The temperatures
reached in disposal cells during the first thousand years (between 85 °C and 55 °C in contact with
the containers) are insufficient to allow illitisation of the swelling clay plug in its mass⁴. Geochemical changes remain localised at the interface with the overpack. Modelling estimates the
extent of the illitisation process into the plug to be less than a centimetre (Michau, 2005). It is
accompanied by iron/clay disturbance developing in swelling clay in contact with the overpack. The
reaction processes are only really effective when the plug is re-saturated (after about a hundred
years) and are more intense at higher temperatures. Thus, the iron/clay disturbance develops mainly
when favourable temperature and saturation conditions occur simultaneously, i.e. during the first
thousand years. It develops more slowly after the thermal transient. The influence of iron/clay
disturbance on illitisation has not been assessed so far, but is almost certainly negligible due to the
mechanisms involved in the two disturbances.

The physico-chemical interactions between the Callovo-Oxfordian argillites and the repository
materials are interface phenomena whose extent is limited to the initial EDZ.

It has been demonstrated that the temperature increase in the near field close to the exothermic
waste disposal cells should not have any mineralogical consequences. The chemistry of the

⁴ Numerous studies highlight the fact that illitisation process in sedimentary basins only starts at temperatures above 80
°C and does not become significant below 100 °C, as long as there is a potassium source
interstitial fluid also changes very little (Altmann & Jacquot, 2005; Cathelineau & Mosser, 1998). The iterative approach, with coupling between modelling and URL experiments on the pore water chemical composition, should ultimately weigh up if there is a need to precise the understanding of the regulatory mechanisms, notably of the influence of organic matter on fluid/rock equilibria and on speciation of elements in solution (in particular radionuclides). A main issue is to determine the type of “groupements fonctionnels” and their actual concentration, to assess their influence during the thermal load.

As for the swelling clay plug, the iron/argillite disturbance develops essentially during the thermal period. Beyond this period, it evolves very slowly. Furthermore, it ceases after several thousand years with the total corrosion of the metal components involved. It can therefore be considered that, over a million years, the extent of the disturbance remains close to that achieved at the end of the thermal period.

The research programme aims at (i) determining the enthalpy and hydration energy to model the chemical changes with temperature and (ii) measuring the relation between ion exchange constants and temperature taking into account the solubility variations of mineral phases.

Significant experience has been gained concerning the chemical retention properties of swelling clays. The influence of temperature on sorption equilibriums will be studied for temperatures until 100 °C to precise material reactivity with temperature (interaction with iron and alkaline fluids). Other effects (dissolution/precipitation processes, solute/surface interactions) will be examined to release the design constraints linked to the temperature (tight leak period). For that purpose thermodynamic data (e.g. the equilibrium constants for solids) and kinetic data (e.g. the dissolution/precipitation kinetic constants) will be measured for the clay minerals at low temperature (below 120 °C).

3 Terminology

Will be defined later in the project.

4 State of the art for Boom Clay

The present state of the art in the THMC behaviour of Boom Clay relies mainly on the data from in-situ integrated tests including the short/long term observations/measurements performed in the underground research facility (URF) HADES, constructed in the middle level of Boom Clay formation at 223 m depth in Mol, and laboratory tests/analysis on the samples taken from the HADES. The geochemistry of the Boom Clay has been studied in general at the different boreholes drilled in Boom Clay formation in different regions. The composition of the Boom Clay and its pore water chemistry have been studied more into detail on the boreholes drilled from HADES and associated piezometers.

4.1 Main characteristics

The Boom Clay formation is a marine sediment of tertiary, Rupelian age (30 My). At the Mol-Dessel nuclear site, the Boom Clay lies 190-290 m below ground level. The Boom Clay layer is almost horizontal (it dips 1-2% towards the NE) and water bearing sand layers are situated above and below it. The underground water level is situated more or less at the ground surface. The total vertical stress and pore water pressure at the level of HADES are respectively some 4.5 and 2.2 MPa. There remain, however, open questions about the in-situ stress state tensor. The K₀ value (ratio of horizontal to vertical effective stresses) was determined by laboratory methods and in-situ
investigations. The in-situ investigations from HADES by means of Pressuremeter, Dilatometer, Self Boring Pressuremeter (SBP), Hydrofracturing tests, borehole breakouts analysis and back-analysis of the stresses in the liner gave some scattered $K_0$ values (0.3-0.9). Laboratory investigations indicated values for $K_0$ between 0.5 and 0.8. Deeper investigation of this subject is therefore necessary: a new set of in-situ tests including SBP and Hydrofracturing tests in different directions is planned in 2007 (Bernier et al., 2007). The ambient temperature in the HADES is about 16 °C.

4.1.1 Mineralogy and pore water chemistry

The reference mineralogical composition of the Boom Clay is given in Table 4.1. The mineralogical composition is very homogeneous in the vertical profile of the Boom Clay from qualitative point of view. However, significant variations exist in the quantitative mineralogy, which is related to different grain-size distributions in silt-dominated and clay-dominated layers. In the studied profile the total non-clay content varies from 41 to 77 wt% while the total clay content is in the range of 23 to 59 wt%.

Table 4.1: The quantitative mineralogical composition of the Boom Clay at the reference site in Mol. All values are expressed as weight % and should be considered as indicative

<table>
<thead>
<tr>
<th>Clay minerals</th>
<th>23-59 %</th>
<th>5-15 %</th>
<th>35-50 %</th>
<th>1-4 %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kaolinite</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2:1 clays and micas</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Vermiculite/chlorite</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Non-clay minerals</td>
<td>41-77 %</td>
<td>23-57 %</td>
<td>6-11 %</td>
<td>1-5 %</td>
</tr>
<tr>
<td>Quartz</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>K-feldspar</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Na-plagioclase</td>
<td>0-3 %</td>
<td>1-5 %</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Carbonates</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pyrite</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Organic matter</td>
<td>1-5 %</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The present-day mineral assemblage of the Boom Clay is considered to represent more or less the mineral assemblage of the Boom Clay shortly after deposition (30 My ago). No evidence of important mineral transformations is found in the Boom Clay. Nevertheless, several diagenetic products are recognized, the most important being pyrite and carbonates, the latter forming septarian carbonate concretions. These are the result of early-diagenetic processes taking place in the shallow burial environment. Since then, the mineralogy of the Boom Clay probably remained the same.

The pore water composition was determined from squeezing and leaching of clay cores and in-situ from MORPHEUS and R13U piezometers in HADES. The reference Boom Clay pore water composition and the measured MORPHEUS pore water composition are given in Table 4.2. Vertical variations in pore water composition are present, but are very small. The only remarkable difference was found in the chlorine concentration in the pore water which was 10-20 mg/l above the HADES URF and 20-30 mg/l below the HADES URF.
### Table 4.2: The reference Boom Clay pore water composition and the measured MORPHEUS water composition.
The major ion concentrations of the reference water are calculated by cation exchange and mineral dissolution reactions that are calibrated against the measured composition.

<table>
<thead>
<tr>
<th>Composition</th>
<th>Reference Water</th>
<th>MORPHEUS Water -217~ -235 m TAW</th>
</tr>
</thead>
<tbody>
<tr>
<td>mg/l</td>
<td>mmol/l</td>
<td>mg/l</td>
</tr>
<tr>
<td>Na</td>
<td>359</td>
<td>348-431</td>
</tr>
<tr>
<td>K</td>
<td>7.2</td>
<td>6.7-8.3</td>
</tr>
<tr>
<td>Ca</td>
<td>2.0</td>
<td>1.5-2.9</td>
</tr>
<tr>
<td>Mg</td>
<td>1.6</td>
<td>1.3-2.6</td>
</tr>
<tr>
<td>Fe</td>
<td>0.2</td>
<td>0.10-0.68</td>
</tr>
<tr>
<td>Si</td>
<td>3.4</td>
<td>4.2-5.5</td>
</tr>
<tr>
<td>Al</td>
<td>0.6E-3</td>
<td>0.03-0.06</td>
</tr>
<tr>
<td>HCO₃⁻</td>
<td>878.9</td>
<td>173-206</td>
</tr>
<tr>
<td>TIC (mg C/l)</td>
<td>181.3</td>
<td>14.4</td>
</tr>
<tr>
<td>Cl</td>
<td>26</td>
<td>24-30</td>
</tr>
<tr>
<td>total S</td>
<td>0.77</td>
<td>na</td>
</tr>
<tr>
<td>SO₄²⁻</td>
<td>2.2</td>
<td>0.63-2.31</td>
</tr>
<tr>
<td>HPO₄²⁻</td>
<td>na</td>
<td>na</td>
</tr>
<tr>
<td>NO₃⁻</td>
<td>~0.4</td>
<td>6.5E-3-0.02</td>
</tr>
<tr>
<td>F</td>
<td>2.6-3.3</td>
<td>0.7-0.8</td>
</tr>
<tr>
<td>Br</td>
<td>~0.6</td>
<td>7.5E-3</td>
</tr>
<tr>
<td>B</td>
<td>~7</td>
<td>0.6</td>
</tr>
<tr>
<td>DOC (mg C/l)</td>
<td></td>
<td>120-200</td>
</tr>
<tr>
<td>Cs</td>
<td>&lt;0.5 (µg/l)</td>
<td>&lt;4E-9 (M)</td>
</tr>
<tr>
<td>Sr</td>
<td>46-90 (µg/l)</td>
<td>5-10 E-7 (M)</td>
</tr>
<tr>
<td>U</td>
<td>0.3-1.2 (µg/l)</td>
<td>1-5 E-9 (M)</td>
</tr>
<tr>
<td>pH</td>
<td>8.5</td>
<td>na</td>
</tr>
<tr>
<td>pCO₂ (atm)</td>
<td>10⁻².62</td>
<td>na</td>
</tr>
<tr>
<td>Eₜ (mV)</td>
<td>-274</td>
<td>na</td>
</tr>
<tr>
<td>temperature (°C)</td>
<td>16</td>
<td>na</td>
</tr>
<tr>
<td>conductivity (µS.cm⁻¹)</td>
<td>0.016</td>
<td>1700</td>
</tr>
</tbody>
</table>

### 4.1.2 Basic thermo - hydro - geomechanical properties of Boom Clay

The basic geotechnical and hydraulic properties of the Boom Clay are listed in Table 4.3, which indicates that the Boom Clay, at its saturated state, is a plastic, low permeable clay.

The actual knowledge on the thermal properties is summarised in Table 4.4. The value of the thermal conductivity given by the SAFIR2 report (NIROND 2001-05) is quite different from that obtained by the in-situ tests ATLAS I-II and in Lab (Djeran, et al. 1992). This parameter value as well as its anisotropy are being investigated in the framework of ATLAS III test. The uncertainty on...
the thermal dilation coefficient is not excluded, since the results of laboratory tests (heating test, dilato) present dispersion. Actually, many factors may influence the result, for example, the heating rate (Horseman, 1987, Djeran, et al. 1992).

<table>
<thead>
<tr>
<th>Table 4.3: Hydraulic and Physical characteristics of Boom Clay</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
</tr>
<tr>
<td>Water content</td>
</tr>
<tr>
<td>Plastic limit</td>
</tr>
<tr>
<td>Liquid limit</td>
</tr>
<tr>
<td>Plasticity index</td>
</tr>
<tr>
<td>Porosity</td>
</tr>
<tr>
<td>Hydraulic conductivity</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>Water bulk modulus</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 4.4: Thermal characteristics of Boom Clay</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal conductivity</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>Volumetric heat capacity</td>
</tr>
<tr>
<td>Linear thermal dilation coef. (drained condition)</td>
</tr>
</tbody>
</table>

### 4.2 THM characterization in lab

During the construction of the URF HADES, numerous Boom Clay samples in form of blocks or cores were taken and served for the different campaigns of laboratory tests. These were piloted in two main directions:

- **Short term THM behaviour:**
  - The elastoplastic *hydro-mechanical* behaviour in “saturated” condition and ambient temperature;
  - The *thermal* effects on the hydro-mechanical behaviour at saturated state.

- **The time related** behaviour at ambient and elevated temperature in “saturated” condition. It is worthwhile to note that, until now, the majority of laboratory tests on Boom Clay were carried out in a “supposed to be saturated” condition. The work on the thermo-hydro-mechanical behaviour of natural Boom Clay at unsaturated or partially saturated state is very limited.

Most laboratory tests were odometer and triaxial tests on cylinder samples. Some hollow cylinder tests and thick tube tests were realised in different projects.

Recently, more attention was paid to the evaluation of both mechanical and transport properties in the Excavation Disturbed Zone around the underground storage gallery. The perturbation of the excavation may induce a significant increase of the permeability, related to diffuse and/or localised crack proliferation in the material (Process A). Self-healing properties of clays can in turn reduce the permeability with time (Process B). In the recent EC project SELFRAC (Bernier, et al. 2006), additional laboratory tests were realised to characterise Processes A and B. Triaxial tests, isotropic tests and biaxial tests as well as hollow cylinder tests on both damaged and undamaged samples...
(with or without artificial fractures) were performed at different stress states and different hydraulic boundary conditions. During the tests, the permeability was monitored to obtain the correlation between the diffuse and localised plastic strain and permeability as well as the self-sealing capacity.

Permeability tests on initially fractured core samples are being performed also. Some of these tests are followed up by means of non destructive microfocus X-ray computer tomography (µCT) to analyse the evolution of the density of the sample. Consequently, these µCT analyses can confirm if there is a closure of the fractures during the permeability tests.

Detailed test programs and corresponding results obtained in different projects are given in the technical annex I. This report provides a global view on the THM characteristics of Boom Clay derived from these lab tests. The range of some important (constitutive) parameters will be given and the associated uncertainties will be highlighted.

4.2.1 Short term HM behaviour

4.2.1.1 Stress – strain responses under deviatoric stress states

Triaxial tests revealed that the Boom Clay is characterized by the following behaviour:

- a highly non-linear stress-strain response. Although there is some scatter in the results, laboratory tests showed a very clear trend of stiffness variation with strain level: its tangent stiffness at 0.01% deformation may be one order of magnitude bigger than that at 1% deformation
- softening at large deformation. The magnitude depends on the hydromechanical boundary conditions and stress paths subjected
- the progressive transition of elasto-visco-plasticity and elastic limit is very small. The visco-plastic deformation appear at very small deformation, as illustrated by Figure 4.1
- the stiffness (Young’s modulus) increases with stress level (preconsolidation pressure) as illustrated by Figure 4.1 and Figure 4.2
- the stiffness (Young’s modulus) decreases with accumulated irreversible deformation (Figure 4.1, Figure 4.4)
- shear band leading to the failure of the specimen may be developed under certain conditions (overconsolidated, high shearing rate, etc.).
Figure 4.1: Undrained triaxial test with loading-unloading cycles (P=10 MPa) (Rousset, 1988)

Figure 4.2: Stress/strain curves for specimens isotropically consolidated at various pressures in the range 0.89 to 5.42 MPa (Horseman et al., 1987)

Figure 4.3: Shear tests on samples consolidated at different effective isotropic stress: 0.4 MPa (BC11, BC08), 2 MPa (BC18), 2.3 MPa (BC07, BC12) (Coll, 2005)
4.2.1.2 Stress - strain responses under isotropic and/or odometric conditions

Odometer tests and isotropic consolidation tests reveal the following characteristics:
- strong non linear elasticity as most of clayey soils
- anisotropic behaviour as illustrated by Figure 4.5. The anisotropy seems to decrease with increasing stress (the ratio of lateral to vertical strain decreases)
4.2.1.3 Mechanical parameters deduced from triaxial and odometer/isotropic consolidation tests

By lumping all test results together, the basic mechanical parameters (shearing strength as well as Cam-clay elasto-plastic parameters) can be obtained (Table 4.5).

Table 4.5: Mechanical parameters from triaxial and consolidation tests

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Drained</th>
<th>Undrained</th>
</tr>
</thead>
<tbody>
<tr>
<td>Friction angle</td>
<td>18-25°</td>
<td>2-4°</td>
</tr>
<tr>
<td>Cohesion</td>
<td>≈ 0.3 MPa</td>
<td>0.5-1.3 MPa</td>
</tr>
<tr>
<td>Drained Young's modulus</td>
<td>E*** 0.3 MPa</td>
<td>0.3 MPa</td>
</tr>
<tr>
<td>Preconsolidation pressure</td>
<td>( p'_0 \approx 5 - 6 ) MPa</td>
<td></td>
</tr>
<tr>
<td>Overconsolidated ratio</td>
<td>OCR** 2.05 - 2.64</td>
<td></td>
</tr>
<tr>
<td>Slope of the elastic line</td>
<td>( \kappa \approx 0.13-0.178 )</td>
<td></td>
</tr>
<tr>
<td>Slope of the normal consolidation line</td>
<td>( \lambda )</td>
<td></td>
</tr>
</tbody>
</table>

* average out over a range of mean effective stress 2.5 to 4 MPa
** for the Boom Clay at the level of HADES.
*** As mentioned above, the Boom Clay presents very high non-linear stress-strain responses. The Young's modulus can be measured in different ways: secant or tangent at different deformations, by unloading responses, etc. Quite divergent values were quoted. The value given in the table relies on the unloading responses of some lab tests and estimations from the analysis and interpretation of the in-situ measurements made during the excavation of the test drift (Mair et al. 1992).

4.2.1.4 Hydraulic conductivity variation during consolidation and shearing

Odometer/isotropic consolidation test results revealed clearly that the hydraulic conductivity decreases with increasing effective stresses as shown by Figure 4.6.

Figure 4.6: Hydraulic conductivity plotted against the vertical effective stress (adapted from Horsemann et al., 1987)

Evolution of the hydraulic conductivity during shearing phase has been investigated in the frame of the EC SELFRAC project (Bernier, et al. 200). Triaxial tests (Coll, 2005) showed that:

- when the mechanical behaviour is contractant (ductile), the hydraulic conductivity decreases slightly due to the contractance of the pore space during the shearing phase
- when the mechanical behaviour is characterized by the development of shear bands leading to the failure of the specimen. The stress-strain \( q_{\text{axial}} \) curves show a peak and the specimen exhibits dilatancy. In this case, the permeability is not influenced neither by the onset of
localisation and the propagation of shear bands nor by the dilatancy before the peak stress (Figure 4.7). We can note that to detect an important increase of the permeability, the porosity of the specimen (bulk porosity or discontinuities) has to change significantly. Moreover, the discontinuities (if they exist) have to be interconnected to each other and to the hydraulic pore pressure lines. In the tests realised, the shear bands observed were very thin indicating a low change of the bulk porosity. They were not always propagating from one to the other end of the specimen and, due to their slope, they were not always connected with the pore pressure lines of the system.

Figure 4.7: Evolution of hydraulic conductivity during shearing phase (Coll, 2005)

- by plotting all measurements obtained during triaxial tests against the effective mean stress, same relationship as that obtained from consolidation tests was obtained (Figure 4.8). In fact, it is the change in porosity that controls the variation of the hydraulic conductivity (Figure 4.9).

Figure 4.8: Evolution of hydraulic conductivity against mean effective stresses obtained from triaxial tests (Coll, 2005)
4.2.1.5 Swelling pressure of Boom Clay
Considering its clay mineralogy and its overconsolidated state, the Boom Clay is likely to exhibit capacity for swelling. The maximum value for the swelling pressures obtained by Horseman et al. (Horseman et al. 1987) is about 0.92 MPa. Recent laboratory tests (Coll, 2003; Le, 2006) revealed that the procedure to determine the swelling pressure is delicate as it highly depends on the suction state of the sample. This matter is under investigation in the frame of the PhDs of Le and Alanice devoted to the THM behaviour of the Boom Clay (Le, 2006; Alanice 2007).

4.2.2 Temperature effects on the short term HM behaviour
Particular attention has been paid to the thermomechanical behaviour of Boom Clay (Baldi et al., 1988, 1991; Sultan, 1997, Sultan, et al. 2001, Delage et al. 2004). Temperature effects on the short term hydromechanical behaviour have been investigated in temperature controlled isotropic and triaxial cells. Different test paths have been included in the tests, mainly:

- thermal consolidation tests
- heating/cooling under constant load at different OCR
- isotropic compression at different constant temperatures
- shearing tests at different temperatures
- heating at different hydraulic conditions: drained and undrained

Generally, the effect of heat on the Boom Clay behaviour is characterized by non-linearity and irreversibility affecting the HM properties. Following major aspects may be pointed out from lab tests.

4.2.2.1 Temperature effect on the preconsolidation pressure
The temperature effect on the preconsolidation pressure was studied through a series of isotropic compression tests at different constant temperatures. All samples were initially isotropically loaded to 4 MPa and subsequently heated to 100 °C. Finally these samples are brought to temperatures of respectively 23, 40, 70 and 100 °C after which they are all isothermally loaded (Sultan, 1997, Sultan, et al. 2002). The test results are given in Figure 4.10 which shows that the yielding points at different temperatures are aligned in a log p'-T plane, the preconsolidation pressure decreases with
increasing temperature according to an exponential function.

4.2.2.2 Thermal volume changes at different OCRs

Heating/cooling tests under different constant loads showed clearly that the thermal induced volume changes of Boom Clay depends highly on the over consolidation ratio OCR as shown by Figure 4.11.

For highly overconsolidated samples, heating first induces volumetric dilation strain until a certain temperature then exhibits compaction. This thermal dilation/compaction behaviour of the soil depends on the OCR values as well as on the imposed temperature change (Figure 4.11). The temperature at which the dilatation/compaction transition occurs increases with increasing OCR.
However, the slope of the volumetric strain curve in the cooling stage is independent of the applied mean effective stress. The cooling slope is parallel to the slope of the dilation heating phase. This thermal induced volumetric strain behaviour has been observed for Boom Clay by Baldi (Baldi, et al. 1991) and for other kind of clayey soils (Sultan, et al. 2002, Laloui, et al. 2003).

4.2.2.3 Temperature effect on the shearing strength

The following temperature effects on deviatoric behaviour of Boom Clay are observed (Djeran, et al. 1992, Sultan, 1997, Baldi 1989, De Bruyn, 1999):

- temperature decreases the shearing strength
- temperature decreases the Young's modulus at small deformation

However, quantitative conclusions cannot be drawn due to the limited number of test and dispersion of the test results.

4.2.2.4 Dissipation of thermal induced pore pressure: Thermal consolidation

In order to investigate the thermal induced pore pressure dissipation pattern in Boom Clay, a series of thermal consolidation tests were performed on natural Boom Clay by Sultan (1997) and Baldi et al. (1987). Figure 4.12 shows the consolidation curves of a Boom Clay sample (saturated and consolidated to OCR = 2) for a range of temperature within which the sample exhibits thermal contraction. The shapes of the curves are similar to that of standard consolidation curves, the volume decrease is related to thermal induced excess pore pressure dissipation (Delage et al., 2004).

![Figure 4.12: Thermal consolidation curves (Delage et al., 2004)](image)

The variation of the consolidation coefficient \(C_v\) and permeability \(K_w\) in function of temperature is given in Figure 4.13. The slight variation in \(C_v\) and \(K_w\) is related to two simultaneous, but opposite effects: with increasing temperature the permeability increases (due to water viscosity decreasing), but this effect is compensated by a decrease in void ratio (thermal contraction).
4.2.2.5 Temperature effect on permeability

Due to the complex thermal volumetric strain, the change in permeability due to heating results in general from two coupled effects: a change in water viscosity and in porosity. In order to decouple these two effects, a series of permeability tests at different temperatures and different stresses has been performed by Delage et al. (2004). The test paths and results are given in Figure 4.14. Figure 4.14 reveals that, when the temperature effect on the water viscosity is decoupled by back calculation of test results, the intrinsic permeability $K$ depends only on its porosity and not on the thermo-mechanical path previously followed. It can thus be concluded that the temperature effect on the permeability $k$ mainly result from the variation of the water viscosity.

![Figure 4.14: Results of permeability tests at various temperatures and stresses; a) in terms of permeability $k$ b) in terms of intrinsic permeability $K$ (Delage et al., 2000)](image)

4.2.3 Time related THM behaviour

The time related behaviour is related to two processes: dissipation of pore water pressure and viscosity of the solid skeleton. A clear distinction between them by means of lab test is difficult due to the very low permeability of the Boom Clay.

A set of laboratory tests was nevertheless carried out (Rousset, 1988, Dejaran, 1994):

- drained and undrained triaxial creep tests to distinguish the time related behaviour due to the
hydraulic diffusion (drained tests) from that due to the viscosity of solid skeleton (undrained tests)

- odometer creep tests and triaxial drained creep tests at different temperatures
- thick tube creep tests

Quantitative conclusions are still difficult to draw. The test results present dispersion because of numerous factors. The tested samples present inhomogeneity in terms of water content and saturation degree and not all tests were carried out properly (loading rate too high, test duration not long enough, etcetera).

Figure 4.15 shows two triaxial creep tests at different constant deviatoric stresses. The first was performed in drained conditions (D), the second in undrained conditions (ND). The importance of the consolidation due to pore water dissipation in the delayed deformation was put in evidence by the first loading in the drained test. The importance of the delayed deformation due to the viscosity of the skeleton can be observed in the undrained test and more specifically in the creep in the last load step (Djeran et al., 1994).

A creep rate, in the order of 4-5 $10^{-5}$/h, was obtained for the tested time duration (order of months). The tests revealed a very low creep threshold, namely in the order of 0.5 MPa of the deviatoric stress.

![Creep Rate Graph](image)

**Figure 4.15: Creep at 20 °C – Drained (D) and Undrained (ND) (Djeran et al., 1994)**

Figure 4.16 represents undrained creep tests realised at 100 °C on two different samples. Compared to the curve ND on Figure 4.15, it can be seen that the temperature increases sensibly the viscosity of the material (creep rate) and decreases the creep threshold.
4.2.4 Sealing/healing behaviour

The fast self-sealing capacity of Boom Clay has been clearly demonstrated with permeability tests in permeameter and isostatic cells and visualised by means of μCT. Figure 4.17 shows the μCT images of an artificially fractured clay sample. Figure 4.17a shows the sample shortly after the artificial fracture was created and before saturation of the sample. Figure 4.17 b gives an image of the sample after 4.5 hours of hydraulic conductivity measurement. The closure of the fracture due to the saturation of the sample was evidenced. Sealing was confirmed by measuring the hydraulic conductivity measurement of the sample (Figure 4.18) which was of the same order of magnitude as the undisturbed value (~10^{-12} m/s).

![Figure 4.17: μCT images of an artificially fractured clay sample (30.3 mm high, 38 mm in diameter). Figure "a" was taken after the artificial fracture was created. Figure "b" was taken after 4.5 hours of hydraulic conductivity measurement.](image-url)
4.2.5 Main remarks on the performed laboratory works

Laboratory investigation allowed to get a global view on the THM behaviour of Boom Clay. **Quantitative** conclusions are however difficult to draw at actual stage. Actually, although a lot of work was performed on Boom Clay, there is a lack of coherent and systematic THM characterization program due to:

- **the inhomogeneity** of the samples. Moreover, the origin of this inhomogeneity is unclear and there is no sensitive analysis to study its influence on the THM behaviour of the Boom Clay.

- **the tests results** present a big **dispersion**. Indeed, the tests were realised in different laboratories, with different test equipments, following different test procedures, different protocols, etc.

- **Although all samples were initially assumed saturated**, the saturation state of the samples is not always clear. A lot of factors like the sampling procedure, the sample conservation and the unpacking can provoke the **desaturation** of the samples. A small lack of saturation can alter the hydro-mechanical response of the clay and hinders the interpretation of test results and parameters determination.

Besides, following aspects need to be investigated:

- **Anisotropy** : The anisotropy of the Boom Clay was revealed in several projects but this is not enough investigated to quantitatively evaluate this aspect

- Combined effects of **temperature** and **suction** (desaturation) on the short/long term HM behaviour

**4.3 THM characterization in-situ**

A detailed presentation of all in-situ experiments performed in HADES can be found in the technical annex 1. In general, the in-situ THM characterisation program can be summarised in terms of:

- short term HM responses around the gallery mainly based on in-situ measurements during the construction of gallery, drilling of boreholes or wells for THM testing
- long term HM responses around the gallery based on the long term monitoring around the gallery and in the liner (Mine-by test, convergence of the test drift front, pressure on the liner, etc.)
- short/long term THM responses: on the basis of in-situ experiments: ATLAS, CERBERUS, CACTUS, etc.
- interaction EBS and Host Rock: BACCHUS, RESAEAL, etc.

4.3.1 Short term HM responses

4.3.1.1 Excavation HM responses
When studying the short term hydromechanical response around excavations, it is important to have a sound knowledge of the excavation parameters and the boundary conditions. This was achieved by the use of a tunnelling machine during the construction of the connecting gallery and the installation of a comprehensive instrumentation programme within the CLIP EX (Clay Instrumentation Program for the Extension of an Underground Research Laboratory) project (Bernier et al., 2002). Although a lot of in-situ measurements exist, the present report concentrates on the measurements obtained within this project. Prior to the drilling of this tunnel, a series of instrumented boreholes A, B, C, D, and E (Figure 4.19) were established. This set of instrumentation allowed the monitoring of the pore pressures, total stresses and displacements around the excavation and ahead of the excavation front.

The tunnelling machine was composed of a 2.3 m long shield, a road-header for the excavation of the rock and a bird-wing erector system for the installation of the lining (Figure 4.20). The shield was equipped with a cutting head to ensure a smooth excavation profile. This excavation technique achieved good control of the initial excavated diameter and hence provided a good baseline for subsequent convergence measurements. This is quite important for the correct interpretation of the measurements. The total radial convergence during construction was limited to 90 mm. This value is the sum of the instantaneous radial convergence ahead of the excavated front (45 mm) and the radial convergence occurring between the excavated front and the last installed lining segment (45 mm). Because of the very low permeability of the Boom Clay formation and the quite high excavation rate (about 3m/day), the response of the host formation to the excavation can considered to be undrained. Therefore it was possible to clearly dissociate the instantaneous response from the delayed effects.

During the excavation of the connecting gallery, all piezometers installed ahead of the excavation front registered a similar regular evolution of the pore water pressure with the approach of the excavation front: a progressive increase followed by a sharp drop as the excavation front approached very closely (Figure 4.21). The pressure response and mechanical displacement were strongly coupled as shown by Figure 4.22, which indicates the strong HM coupling behaviour of Boom Clay. Note that the pressure and displacement become steady as the excavation front passed due to the emplacement of a stiff lining support following the tunnelling machine.
Figure 4.19: CLIPEX instrumentation program (Bernier et al., 2007)

Figure 4.20: The tunnel machine used for the connecting gallery

Figure 4.21: Pore pressure evolution of piezometer B2; the filters 1-6 are located at 30-20 m distance of the Test Drift face.
4.3.1.2 Excavation Damaged Zone (EDZ)

Evidences of fractures induced by the excavation have been gathered during the construction of the connecting gallery. The systematic observations of the front and the sidewalls allowed to determine the fracture pattern in the surrounding formation (Figure 4.24). The orientation of the encountered fractures is consistent along most of the excavation. Because of the strong hydromechanical coupling, the development of fractures was also evidenced through the pore water pressure measurements. Indeed, the high decompression of the formation near the excavation face generated pore water suction (negative pore pressure) as shown in Figure 4.25. The suction created at about 3 meters ahead of the excavation front was followed by an abrupt recovery up to the atmospheric pressure as the front was coming closer. This sudden re-equilibrium with the atmospheric pressure indicated the opening of fractures in the formation ahead of the excavation front up to a distance of about 2 to 3 meters along the gallery axis. It is worth to note that the range of the sensors is limited:

Figure 4.22: pore pressure (u) and vertical displacement (δv) in borehole E2 and E1, the sensors shown are located at ~15 m from axis of the second shaft

An unexpectedly extended disturbed zone (both hydraulic and mechanical) due to excavation was observed. As shown in Figure 4.23, the pore pressure and displacement sensors began to register a regular variation when the excavation front was still more than 60 metres (i.e. 12.5 tunnel diameters) distant. This far-field behaviour remains difficult to explain and constitutes an important issue for the proper understanding of the hydromechanical behaviour of the Boom Clay.

After excavation, the pore pressure distribution around the gallery was anisotropic. This anisotropy depends on both the anisotropy of the stress state and the anisotropy of the hydraulic conductivity (Bernier et al., 2003).

Figure 4.23: Far field reaction to excavation
a) Pore pressure b) displacement (Bernier et al., 2003)
they can only measure absolute pressures as low as 0 MPa. This corresponds to a suction of ~0.1 MPa. The actual suction was without doubt larger.

The fracturation pattern consists of two conjugated fracture planes: one in the upper part, dipping towards the excavation direction (north); the other in the lower part, dipping towards the opposite direction (south). The distance between the fractures is a few decimetres, and they originate at about 6 metres ahead of the front. Nevertheless pre-existing fractures were not observed at the Mol site, it is impossible to prove their absence. Two cored borings performed shortly after the construction of the connecting gallery to assess the radial extent of the fractures revealed the presence of fractures up to about 1 metre into the clay.

![Observed fracture pattern around the connecting gallery (vertical cross-section).](image)

**Figure 4.24: Observed fracture pattern around the connecting gallery (vertical cross-section).**

![Evidences of the development of fractures in borehole A2 (absolute pore pressures measured ahead of the excavation face).](image)

**Figure 4.25: Evidences of the development of fractures in borehole A2 (absolute pore pressures measured ahead of the excavation face).**

### 4.3.2 Long term HM responses

The Boom Clay is characterized by an elasto-visco-plastic behaviour. Viscosity of the skeleton (creep, relaxation, etc.) and pore water pressure dissipation imply long term effects around underground excavations. Long term in-situ measurements deliver an important data-base for the constitutive modelling of the Boom Clay.

Figure 4.26 shows the best estimate of the time evolution of the total stresses around the gallery measured by self-boring pressuremeter tests in horizontal boreholes at two different periods. The values are likely to be more representative of the vertical component of the in-situ stress. Between the two tests, the total stress close to the gallery wall appears to have risen, indicating stress build-
up (re-equilibrium) around the excavation. The total stress seems to be influenced up to at least 6-8 m into the host rock. The obtained value in the far field (5-5.5 MPa) is somewhat higher than the initial in-situ stress. This may be due to data interpretation or it may be a consequence of the excavation of the gallery. Further tests using a deeper borehole are necessary to get a more accurate interpretation of these likely higher values.

Strain gauges were embedded in the lining segments of the connecting gallery to monitor the stresses in the lining and the pressures exerted on it by the host rock (Figure 4.27). The continual increasing of the external pressure on the linings of the gallery by the Boom Clay embodies the time-related behaviour of the Boom Clay through hydraulic diffusion processes and the viscosity of the skeleton.

![Figure 4.26: Total (vertical) stress evolution based upon two series of self-boring pressuremeter tests conducted from the connecting gallery in 2002 and 2004.](image)

![Figure 4.27: Time related behaviour: outside pressure exerted on the lining (Bernier et al., 2003).](image)

The convergence of the Test-Drift has been measured over a period of 19 years. Figure 4.28 shows the diameter reductions of 4 sections from the central part of the Test Drift. The decrease of the lining diameter was fastest during the first year after the construction. The rate of convergence has progressively slowed since the initial excavation but convergence is still continuing, currently (some 18 years after construction) at a rate of about 0.5 mm/year. Since the measurements started, the diameter was reduced by ca. 60 mm.
Figure 4.28: Diameter reduction at four sections located in the central part of the Test Drift

Figure 4.29 shows the results of the piezometers installed in vertical and horizontal boreholes around the Test Drift. The pore pressures are expressed as a percentage of the undisturbed in-situ pore pressure. The Test Drift lining is considered to be very permeable compared to the Boom Clay. Some 2.5 years after the excavation, pressures measured in horizontal boreholes are relatively higher than those in vertical boreholes, but this relation is reversed in time. The HdZ profiles are likely dominated in the short-term by the anisotropy of the initial stress state (undrained instantaneous response) and in the long-term by the anisotropy of the hydraulic conductivity.

Figure 4.30 shows the results of the hydraulic conductivity measurements around the connecting gallery at different periods (Bastiaens et al., 2006). The hydraulic conductivity was determined at several filters on a horizontal and a vertical (downward) multi-port piezometer. The tests performed were single point steady state measurements. An increase of the hydraulic conductivity is observed up to about 6-8 m from the lining. Values of ~6 x 10^{-12} m/s and ~4 x 10^{-12} m/s were obtained outside the influenced zone, respectively on the vertical (downward) and the horizontal piezometer. The time evolution of the hydraulic conductivity in the vicinity of the gallery clearly indicated the time dependent coupled hydromechanical behaviour of the Boom Clay.

The increase of the hydraulic conductivity around the gallery is attributed to the lower effective stress in this zone. Fractures do not play an important role in this case (cf. sealing). Almost all
measurements were performed further than 1 m into the host rock and thus well beyond the fractured zone (Bernier et al., 2006).

**Figure 4.30: Hydraulic conductivity (k) around the connecting gallery (Bernier et al., 2006)**

### 4.3.3 Self sealing/healing behaviour

The radial extent of the fractured zone around the gallery is about 1 m (Figure 4.24) in which the pore pressure should be in equilibrium with the atmospheric pressure if the fractures are not sealed. The pore pressure evolution around the connecting gallery was measured. The results of December the 6th 2004, i.e. about 2 years and 9 months after gallery construction, are presented on Figure 4.31. The pore pressure could be measured as little as 40 cm into the host rock. This indicates that any fracture network existing beyond a few decimetres into the host rock (at most) is sealed. Moreover, since no packers are used, the filters are sealed off by natural convergence of the borehole walls around the instrument. This result confirms that the Boom Clay has important sealing properties.

**Figure 4.31: Overview of pore pressure measurements around the connecting gallery on the 6th of December 2004, expressed as a percentage of the original undisturbed value at each filter location (Bernier et al., 2006)**

### 4.3.4 Thermal-Hydro-Mechanical (THM) responses

The in-situ THM responses of the Boom Clay were studied in different in-situ tests (see technical annex 1) among which ATLAS I-II delivers the most information on the host rock. Since its design includes alone the Host Rock, no EBS intervenes and the thermal loading is thus applied directly on the Boom Clay (Figure 4.32). Measurements of the temperature, the total stress and the pore
pressure distributions in the clay mass around the heater were made. A first heating phase started in July 1993 with a power of 900 W up to late 1995, a second phase of heating was carried on in doubling the power to 1800 W. In May 1997, after almost 1 year of supplementary heating, ATLAS was cooled down (Jeffries, 1995). This long period of measurement (5 years of heating and several years of cooling) allows to study the long term THM behaviour of the Boom Clay.

Figure 4.32: General layout of the ATLAS experiment (De Bruyn & Labat, 2002)

The evolution in time of the total pressure $\sigma$, the pore pressure $u$ and the temperature $T$ is shown in Figure 4.33.

Figure 4.33: Evolution in time of the total pressure, the pore pressure and the temperature; a) ring 93 – b) ring 85 (adapted from De Bruyn & Labat, 2002)

During the first heating phase heating induces:

- an increase in total stress $\sigma$. This increase stabilises while the temperature still increases. In the case of ATLAS, the maximum total stress is obtained after 1 year of heating. The decrease after 2 more years of constant heating remains limited (0.1 MPa)
- a rapid increase in pore pressure $u$, followed by a slight decrease when the rate of the temperature increase slows down. The decrease, caused by dissipation, amounts 0.2 MPa and is larger than for $\sigma$. Apparently, the hydraulic characteristic time of Boom Clay is smaller than the thermal one.
Despite the fact that the second temperature increase is in the same range as in the first heating phase, the behaviour of total and pore pressures is quite different. The increase in the total stress and the pore pressure is faster (2 to 3 months), their maximum occurs almost simultaneously and is followed by a marked decrease which is significantly larger than in the first phase due to the higher pressure gradient.

During cooling, a large and rapid decrease of pore pressure is observed together with a total pressure decrease. This behaviour is just opposed to what has been recorded in the first heating phase. After having reached a minimum, the pore pressure and the total pressure increase again to the value recorded before the first heating phase. The total stress reaches its initial value before the pore pressure which was still slowly increasing in 2002 (De Bruyn & Labat, 2002).

4.3.5 Remarks on the in-situ THM characterisation

When studying the THM responses, it is important to have a sound knowledge of the boundary conditions and initial states of the formation. Comprehensive and sufficient instrumentation is necessary. The excavation of the connecting gallery (CLIPEX) provided a valuable database for the validation of the (to be) developed constitutive laws.

The in-situ experiments realised in the URL provided a valuable database for the calibration and validation of the (to be) developed models. A lot of THM in-situ responses of Boom Clay were observed in several in-situ tests (ATLAS, CACTUS, BACCHUS, PHEBUS, CERBERUS).

However, a global examination of the performed in-situ tests revealed that many tests were conceived for observing THM phenomena and not for calibrating the models. Moreover, in most of the tests, there is a lack of information on the in-situ deformation, saturation and in-situ stresses. Despite extensive testing, there is still considerable uncertainty regarding the anisotropy of the stress profile around the gallery. More extensive site characterization tests are therefore needed.

4.4 Modelling

The modelling development works included two parts: building the constitutive laws and the validations – simulations – predictions. They were carried out in parallel with the laboratory and in-situ test programs.

4.4.1 Constitutive laws

A global view on the constitutive laws that have been considered/developed for Boom Clay in different projects can be found in technical annex 1. Principal constitutive laws can be cited here:

- saturated elastoplastic models at ambient temperature (p'-q plan)
  - Mohr-Coulomb (MC) and modified Cam-Clay models (MCC)
  - Dafalias-Kaliakin and "Two bubbles" models
  - Sultan's anisotropic model

Most used models simulating the excavation of the gallery are MC and MMC for which the parameters are available for Boom Clay.

- unsaturated elastoplastic model at ambient temperature (p-q-s space)
  - Barcelona Basic Model, which was mainly used to model the BACCHUS and RESEAL tests. The unsaturated parameters of Boom Clay were calibrated by matching the in-situ measurements
saturated thermo-elastoplastic models (p'-q-T space)
  - Hueckel and Borsetto (1990) and Hueckel and Baldi (1990) model
  - Sultan's model
These three models are mainly applied to model the laboratory tests performed at different temperatures. They can account for the observed thermal plasticity behaviour of Boom Clay, especially the thermal contraction/dilation behaviour.

saturated thermo-elasto-visco-plastic models
The first viscoplasticity model was developed by Rousset based on a series of undrained test results performed on Boom Clay. The model was developed in terms of "total stress" and not "effective stress". In other words, the effect of water is not taken into account. This model was later on extended to "effective stress" in the framework of the ONDRAF-G3S contract. At the same time, the temperature effect on the viscosity was introduced in the model via the dependence of the viscosity parameters and hardening parameters on the temperature.

4.4.2 Simulations of connecting gallery excavation
In the framework of the CLIPEX project, numerical simulation of the HM responses during the excavation was performed. The simulation was performed in the framework of the soil mechanics for saturated porous media taking into account the hydromechanical coupling. The Boom Clay behaviour was represented by the classical elasto-perfect plasticity Mohr-Coulomb model. Typical numerical results are given in Figure 4.34, Figure 4.35 and Figure 4.36.

a) ahead of the excavation front: Borehole A2 (installed horizontally along the axis of the gallery)

b) radial profile

Figure 4.34: Pore water pressure evolution (comparison between numerical predictions and in-situ measurements)
measurements) (Li et al., 2006)

It can be seen that the Mohr-Coulomb model agrees well with the general tendency of the in-situ measurements. But, it cannot produce the extended HdZ (Figure 4.34a) and underestimates the variation of the pore pressure at near field (Figure 4.34b) (Li et al., 2006).

Modelled total axial displacement agrees with the in-situ measurements (Figure 4.35). But again, the far-field behaviour was not reproduced numerically, since the sensors react very late compared to the in-situ measurements (Li et al., 2006).

The measurements of the instantaneous radial convergence of the clay through the little holes in the shield indicated that the shield was in contact with the clay at its rear, over a distance of about one third to one half of its total length. They agreed very well with the modelled convergence (Figure 4.36).

The numerical simulation of the excavation of the vertical well for the Cactus test with the Cam clay and Druker-Prager models (Picard, 1994) did underestimate the radial variation of the pore pressure around the excavation.

The mechanisms of this large distance HM response need further investigation.

![Figure 4.35: Axial convergence (Bernier et al., 2007)](image)

![Figure 4.36: Instantaneous radial convergence prediction](image)

### 4.4.3 Modelling of the In-situ heating tests: ATLAS and CACTUS

Figure 4.37 shows the temperature simulation results observed in the CACTUS (detail is given in technical annex 1) and ATLAS test. Both simulations considered only the heat transfer by isotropic conduction. The configuration of both tests indicate that the measured temperature evolution reflect more horizontal thermal conductivity (parallel to bedding). From an inspection of the two simulations we note the existence of the uncertainty on the thermal conductivity (\(\lambda_{\parallel}\)) of the Boom.

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Coupled THM modelling of the ATLAS test revealed that the obtained numerical HM responses during heating phase depends highly on their initial state prior to heating, which is however difficult to model at this moment.

Coupled THM simulation of the CACTUS carried out by Picard suggested that the thermal plasticity behaviour observed in Lab is less important in in-situ CACTUS test (Picard 1994). The conclusion should be considered with caution, since the thermal plasticity observed in Lab does not only depend on the initial stress state but also on the imposed temperature range. The effective stress state and temperature reached in the host rock around CACTUS may be such that thermal plasticity did not appear.

### 4.4.4 Remarks on the THM modelling

Modelling of connecting gallery excavation revealed the necessity to enhance the knowledge and modelling capacity for the short term HM responses of the Boom Clay. The unpredictable large extended HdZ needs more investigation.

From point of view of constitutive model development, the HM coupling parameters, the progressive transition of elastoplasticity, the viscosity of the skeleton, the EDZ including the fracturation and degradation of the material (decreasing of E, cohesion, etc. in function of the irreversible deformation for example), the suction effects, the anisotropy of the Boom Clay, etc. need to be included in the modelling. The viscosity of skeleton should then be incorporated.

From numerical point of view, the effect of the hydraulic boundary condition around the gallery (ventilation) needs to be analysed.

In terms of THM responses modelling, the thermal-plasticity models developed by Sultan, Baldi and Laloui are worthwhile to be validated with the help of in-situ tests (CACTUS, ATLAS, PRACLAY, etc.).

### 4.5 Related chemical aspects – Geochemical perturbation in the Boom Clay

The present-day mineral assemblage of the Boom Clay is considered to represent more or less the mineral assemblage of the Boom Clay shortly after deposition (30Ma ago). No evidence of
important mineral transformations is found in the Boom Clay.

The radiochemical study of the Boom Clay, in particular the application of uranium-thorium series disequilibrium studies, indicates that, in general, the Boom Clay is in a state of secular radioactive equilibrium. This means that the Boom Clay can be considered as a stable geological system.

The geochemical perturbations of the Boom Clay occur, e.g. as a result of the engineering activities related to the construction of the shafts and galleries. During the excavation, the Boom Clay becomes inevitably oxidized. The cement, commonly used for the lining, as waste matrix and as a component in the recent Belgian super-container design, is known to emanate hyperalkline fluids after saturation. These high-pH solutions will interact with the Boom Clay and will alter its geochemical characteristics. Additional perturbations are expected after the disposal of the HLW generating heat and radiation. Correspondingly, the most important geochemical perturbations include oxidation, the alkaline plume and heat/radiation effects.

4.5.1 Oxidation

In-situ experiments have been performed in the Test Drift (ventilated for ~20 years) and the Connecting Gallery (ventilated during ~4 years) of the in HADES URL to assess the extent and degree of oxidation induced by the excavation and ventilation of the Boom Clay. Within this scope, two N₂ drillings were performed to avoid any additional oxidation caused by drilling and piezometers with filters at different depths from the concrete/clay interface were installed. The pore water chemistry was analysed to study the extent of the oxidation in the Boom Clay in both galleries. Furthermore the mineralogy was studied on micro-scale from cutting edges taken from the Test Drift and the Connecting Gallery. Meanwhile, a conceptual model of oxidation was developed (Van Geet et al., 2006). The experimental and modelling data suggest that oxidation of the host rock is limited to about 1m, even after 20 years. The scoping calculations are rather conservative since only pure transport and no reactive transport (oxygen sink) has been taken into account.

4.5.2 Alkaline plume

All available information suggests that the expected impact of an alkaline plume on the Boom Clay as a repository formation is limited. Laboratory experiments and modelling indicate that an alkaline plume disturbed zone in the Boom Clay is about 2.5 meters at maximum (Wang et al., 2007). This range is in good agreement with the conclusions from studies on similar type of clays in France and Switzerland.

4.5.3 Heat/Radiation

Heating can modify the structure and composition of clay minerals and organic matter, which are considered to be the most active constituents of the clayey barriers from the radionuclide retardation point of view. The alteration of smectite to illite as a response to the increasing thermal gradient is the most extensively studied mineral reaction occurring in buried sediments. Smectite illitization represents one of the greatest concerns with respect to the long-term stability of the clay barriers as it might significantly influence the chemical and physical evolution of the near field by controlling the water release and overpressure and affects the chemical budget of elements such as Si, Ca, Na and K.

An in-situ heater test has been performed in HADES URL within the framework of the CERBERUS project (Noynaert et al., 2000). The CERBERUS (Control Experiment with Radiation of the Belgian Repository for Underground Storage) aimed to simulate the combined effects of heat and radiation on the near field of a HLW repository. For this purpose, a ⁶⁰Co-source was installed with the
activity of 397 TBq and 6 heating elements with a nominal power of 500W each. The effect of heat on the pore-water chemistry was followed in the near field of the CERBERUS test with the aid of piezometers. The Boom Clay samples selected for the mineralogical characterization were either irradiated and heated (100-120°C/0.1-11MGy) or just heated (50-120°C/0MGy). The results of the pore water chemistry study showed that after a short period of oxidation (reflected in the increase of sulphates and a pH drop), the chemical parameters of the pore water chemistry have been re-established. Fluids remained Na-HCO₃ type with a pH close to the neutrality and a reducing redox potential (-280 mV). The heating/irradiating of the Boom Clay samples for 5 years did not induce any significant changes in either clay or non-clay mineralogy.

The Boom Clay contains a substantial amount (average value around 3 wt %) of organic matter. From this organic matter, over 90% corresponds to kerogen. The study on the thermal stability of the kerogen isolated from Boom Clay showed that kerogen can already undergo a significant degradation under mild to moderate thermal stresses. This degradation mainly releases oxygen-containing compounds, especially CO₂, and monocarboxylic acids (weak quantity compared to the total CO₂ production, but important compared to organic acids naturally present in the Boom Clay pore water). One understands here the temperature/time couples typically relevant for the present repository design (80°C for decades or hundreds of years depending on the type of waste). The release of oxygen-containing compounds from Boom Clay, especially CO₂ and carboxylic acids may significantly disturb the geochemistry in the near field of the radioactive waste. This physico-chemical disturbance of the clay-water system may result from changes in pCO₂, in acidification of the pore water, in dissolution of carbonate minerals, in cation exchange, in modification of pore water ionic strength and from changes in clay surface properties and radionuclide complexation.

Finally, the radiation is known to induce structural defects in clay minerals, which are accompanied by changes in cation exchange capacity, specific surface area, sorption capacity, mineral solubility, etc. Important to note is that due to the current Supercontainer design in Belgium, the radiation effects on the mineral stability of the Boom Clay can be neglected. The radiation from supercontainer is very low corresponding to a dose of 25 µSv/h. The radiation on the contact with the host rock will be further decreased by the backfill and the concrete lining.

4.6 Discussion

The review on the past work (laboratory and in-situ tests as well as model development) on the THM behaviour of natural Boom Clay allowed to identify the main uncertainties on this behaviour. The important issues for the future research in terms of THM behaviour as well as the constitutive study are equally identified.

4.6.1 Uncertainties

The analysis of the existing laboratory tests pointed out the following general aspects that imply the uncertainties on the past test results and consequently on the parameters derived:

- The samples for the tests present a strong inhomogeneity. The origin of this inhomogeneity is unclear. Very little of sensitivity analysis to study its influence on the THM behaviour of Boom Clay was performed
- The initial state of the tested samples. The on-going study by CERMES in the frame of a PhD thesis on the thermal mechanical behaviour of natural Boom Clay reveals that the tested samples present an initial matrix suction. This suction is induced by the decompression of the massif followed by the gallery excavation (for block samples) or sampling procedure. Additional matrix suction can occur due to some water loss during the long-term storage of
the samples. Taking this initial suction in the tested samples into account during the tests certainly influences the test results. A proper test protocol needs to be defined to account for the impact of this initial suction of samples. Moreover, the ageing of the samples also influences the test results

- The test procedures and test boundary conditions. The obtained test results present large dispersion. This uncertainty in test results evidently induces uncertainties on the observed behaviour and on the derived parameters. Indeed, recent laboratory research reveals that the test procedures, test boundary conditions, etc. have an important effect on the test results. This implies the need for a consistent, systematic test program on natural Boom Clay.

Concerning the modelling development, following aspects are put in evidence:

- numerical simulations of the excavation of the connecting gallery revealed that the principal uncertainty concerns the capacity to model the extended excavation disturbed zone (EdZ), especially the HdZ. There is need to enhance the knowledge and modelling capacity for the short term HM responses of the Boom Clay.
- The modelling of the heating tests revealed that still big uncertainty exists on the value of the thermal conductivity and its anisotropic characteristic.
- In terms of THM constitutive laws development, the thermal-plasticity models developed by Sultan, Baldi and Laloui are applied to model some lab tests, but these models have to be validated by in-situ tests (CACTUS, ATLAS, etc.). The application of these models in a large scale in-situ test would allow to assess the importance of the thermal plasticity of Boom Clay generally observed in Laboratory.
- More efforts should be made to get a relevant elasto-visco-plastic constitutive model for the Boom Clay. The long term measurements around HADES should provide a valuable database to build, calibrate and validate this EVP model.
- Finally, the unsaturation/suction effects on the THM coupling processes/behaviour need more investigations for Boom clay. The recent constitutive laws developed in the frame of generalised effective stress concept (Bishop’s effective stress concept) would be worthwhile to be validated with the help of new lab tests and in situ tests for Boom clay. For example, the unsaturated thermo-mechanical constitutive model ACMEG-TS developed by EPFL would offer great perspective for modelling the THM coupling process in Boom clay (Laloui, et al. 2006).

Concretely, the following aspects of the Boom Clay need to be reviewed:

**THM characteristics:**

- the thermal conductivity as well as its anisotropy
- the anisotropy of the properties, especially the Young's modulus
- the swelling pressure

**THM coupling processes:**

- the variation of the thermal conductivity with temperature as well as the saturation
- the modification of the stiffness (Young's modulus) and strength (internal friction angle and cohesion) induced by temperature
- the temperature effects on the evolution of the EDZ as well as on the sealing/healing
processes in the EDZ

- the occurrence and eventual pattern of additional damage/failure induced by temperature variations: more laboratory tests under well controlled boundary conditions
- creep rates (viscosity related parameters) as well as its (their) dependence on the temperature
- suction related THM behaviour: experimental information concerning unsaturated THM behaviour of natural Boom Clay is very limited. Therefore there is a need to examine more systematically the combined effects of temperature and partial saturation on the hydro-mechanical behaviour of natural Boom Clay under controlled conditions. Basic questions concerning its sensitivity to thermal impact under quasi-undrained conditions, its thermal sensitivity to the enhancement of creep and anisotropy effects remain largely unanswered.

All these aspects constitute the main objective of the present TIMODAZ project. Specific laboratory tests will be performed. In particular, the effects of the temperature on damaged clay as well as on the clay properties will be investigated. Special attention will be addressed to the study of the eventual creation of irreversible damage. These tests include the study of desaturation / resaturation processes on ambient and at different temperatures. These laboratory tests will provide the necessary data for the numerical models to be used in TIMODAZ.

4.6.2 The most important temperature-dependent material properties

The following temperature-dependent material properties are considered to be important:

- the temperature induced variation in hydraulic conductivity
- the temperature induced variation in thermal conductivity
- the temperature induced stiffness and strength modification
- the temperature dependence of creep rates
- the thermal sensibility on anisotropy

4.6.3 The most important coupled processes and parameters

Short term HM coupling:

Strongly hydromechanical coupling processes have been put in evidence during the excavation of the connecting gallery and by the long term in-situ measurements. The dependence of the permeability on the irreversible deformation is an important parameter for the short term HM coupling behaviour.

Long term HM coupling:

The low permeability nature of the Boom Clay implies that the long term coupling behaviour deals with the superposition of at least two mechanisms: creep and consolidation, which are difficult to differentiate. An important issue is to perform tests at a very low loading rate and the creep tests in the very long term.

THM coupling:

The heat transport is mainly by conduction due to the extremely low hydraulic conductivity of the clay. The effect of coupling HM processes to heat transport can be considered very weak. Conversely, the thermal conditions strongly influence the hydro-mechanical processes. The most important parameters are the relative importance of the characteristic time length of mechanical
processes and the relative importance of fluid and thermal diffusion processes.

The new laboratory tests and in-situ tests performed within the TIMODAZ project will allow to increase the knowledge on these processes and parameters.

4.6.4 Effect of discrete fractures and fracture connectivity on the effective hydraulic properties

The majority of the in-situ measurements on the hydraulic conductivity of the Boom Clay around HADES were made beyond the extent of excavation induced fractures (ca. 1 m radially). However, the available results around the excavation only show a limited increase of the hydraulic conductivity of about one order of magnitude (Bastiaens et al., 2007). Furthermore, in-situ measurements around the HADES indicate that no interconnected fracture network is present beyond (at most) some decimetres into the clay host rock. These results were confirmed by laboratory experiments (Coll, 2005). Moreover, the hydraulic conductivity of (artificially) fractured Boom Clay samples was measured and the measured hydraulic conductivity turned out to be comparable to undisturbed clay (within the same order of magnitude). Finally, the sealing process was visualised by μCT imaging. In conclusion, the influence of excavation induced fractures in Boom Clay on the hydraulic conductivity is limited due to sealing phenomena. These phenomena were evidenced in previous laboratory tests as well as in in-situ experiments.

The thermal impact on sealing will be studied within the scope of the TIMODAZ project.

4.6.5 Importance of chemical impact

Based on literature review, the expected temperature increase in the near field of the PRACLAY gallery should not have a significant impact on the geochemical stability of the Boom Clay. However, the generated heat may become important when it is coupled to geochemical perturbations, e.g. the oxidation and the alkaline plume. The oxidation and alkaline plume perturbations will take place in the near field of the PRACLAY gallery and, when coupled to an increased temperature, may trigger irreversible changes in the host rock properties. These changes might have both positive and negative effects on the self-sealing and radionuclide retention of the clay.

In the TIMODAZ project, some laboratory tests dealing with sealing/healing process will be complemented with a radionuclide migration test to evaluate any possible relict of a preferential migration along the sealed fracture. Different chemical conditions will be considered: a chemically undisturbed, an oxidised and an alkaline environment. Mineralogical analyses will be performed and linked to hydromechanical observations.

4.6.6 Derive the most appropriate conceptual models and evaluate the most appropriate numerical code

Based on the discussion above, it is thought that the most appropriate conceptual models would include:

- an EVP-damage model that can properly take into account the transition of the elasto-viscoplastic properties, anisotropy, the degradation of the mechanical properties (Young's modulus, cohesion, etc.), etc.
- the fracture development: localization, shear band, etc.
- sealing processes
the temperature effect on all processes
the suction effect on THM behaviour

An appropriate numerical code should allow to take into account all important THM coupling processes.

The new lab tests to be performed in the TIMODAZ project, the short and long term measurements around HADES and the new in-situ test (ATLAS III) should provide a good database allowing to establish an appropriate concept model.

The modelling work together with the results of the lab and the in-situ tests should allow the validation of the numerical code to be used.
5 State of the art for the Opalinus clay

5.1 Main characteristics

5.1.1 Geological setting

The Opalinus Clay was deposited some 180 million years ago by the sedimentation of fine clay, quartz and carbonate particles in a shallow marine environment. It is part of a thick sequence of Mesozoic and Tertiary sediments in the Molasse Basin (Figure 5.1), which overly Palaeozoic sediments and crystalline basement rocks. The overlying Tertiary sediments thicken considerably towards the Alpine Front. The Mesozoic sediments containing the Opalinus Clay are of uniform thickness over several kilometres, almost flat-lying (dipping gently to the south east) below the Molasse Basin and in NE Switzerland and little affected by faulting. Miocene Deformation has affected this sedimentary pile in the Jura Mountains that form an arc shaped foreland fold-and-thrust belt around the Molasse basin to the south.

Figure 5.1: Schematic geological profiles from NW to SE through the sedimentary rocks of NE Switzerland (Nagra, 2002c)

The Opalinus Clay reached a burial depth of about 1000 m during the Cretaceous (about 65 to 120 million years ago). During its burial and compaction history it has experienced maximum temperatures of about 85 °C. The present temperature of the Opalinus Clay at 650 m at the Benken drill site is 38 °C. Detailed geological information is given in technical annex 1.

5.1.2 Mineralogy and porewater chemistry of the Opalinus Clay

The average mineralogical composition of the host rock is presented in Table 5.1. The presence of pyrite and siderite, which show no signs of oxidation, indicate the reducing nature and the high redox-buffering capacity of the Opalinus Clay. The mineralogy in shear zones does not differ from that of the rock matrix (Nagra, 2002c).

Due to its marine origin, the porewater of the Opalinus Clay is relatively saline and sodiumchloride dominated. The so-called reference porewater chemistry for Opalinus Clay is given in Table 5.2. It corresponds to the most probable water composition based on current understanding. The pH conditions are expected to be near-neutral but the uncertainties are rather large mainly because the
partial pressure of CO$_2$ cannot precisely be determined. Bounding pH values of 6.9 to 8.2 have been proposed (Pearson, 2002). Redox conditions are reducing as evidenced by the large amounts of unoxidised pyrite and siderite. From mineralogical observations, Eh measurements performed at Mont Terri and geochemical modelling, redox potentials of about -170 mV (SHE) for the reference water and bounding values of about -140 to -240 mV were derived. The derivation is based on the assumption of thermodynamic equilibrium between pyrite, sulphate and siderite.

### Table 5.1: Average mineralogy of the Opalinus Clay (Nagra 2002c)

<table>
<thead>
<tr>
<th>Mineral</th>
<th>wt % (average)</th>
<th>Standard deviation (1σ)wt%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Illite</td>
<td>18</td>
<td>6</td>
</tr>
<tr>
<td>Kaolinite</td>
<td>17</td>
<td>6</td>
</tr>
<tr>
<td>Illite/smectite mixed layer</td>
<td>14</td>
<td>4</td>
</tr>
<tr>
<td>Chlorite</td>
<td>5</td>
<td>2</td>
</tr>
<tr>
<td>Quartz</td>
<td>20</td>
<td>5</td>
</tr>
<tr>
<td>Calcite</td>
<td>16</td>
<td>10</td>
</tr>
<tr>
<td>Dolomite/ankerite</td>
<td>1</td>
<td>0.4</td>
</tr>
<tr>
<td>Siderite</td>
<td>4</td>
<td>2.4</td>
</tr>
<tr>
<td>Feldspar</td>
<td>3</td>
<td>1.3</td>
</tr>
<tr>
<td>Pyrite</td>
<td>1.1</td>
<td>1</td>
</tr>
<tr>
<td>Organic carbon</td>
<td>0.6</td>
<td>0.3</td>
</tr>
</tbody>
</table>

### Table 5.2: Reference water chemistry of the Opalinus Clay at the Benken site (Pearson, 2002)

<table>
<thead>
<tr>
<th>pH</th>
<th>7.24</th>
</tr>
</thead>
<tbody>
<tr>
<td>Eh [V]</td>
<td>-0.167</td>
</tr>
<tr>
<td>temperature [°C]</td>
<td>25.0</td>
</tr>
<tr>
<td>log pCO$_2$</td>
<td>-2.2</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>concentrations [mol L$^{-1}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO$_2$(tot)</td>
</tr>
<tr>
<td>Na</td>
</tr>
<tr>
<td>K</td>
</tr>
<tr>
<td>Mg</td>
</tr>
<tr>
<td>Ca</td>
</tr>
<tr>
<td>Sr</td>
</tr>
<tr>
<td>Si(VI)</td>
</tr>
<tr>
<td>Si(III)</td>
</tr>
<tr>
<td>F</td>
</tr>
<tr>
<td>Cl</td>
</tr>
<tr>
<td>Br</td>
</tr>
<tr>
<td>Fe(II)</td>
</tr>
<tr>
<td>Mn</td>
</tr>
<tr>
<td>Si</td>
</tr>
</tbody>
</table>

* The temperature refers to the model water composition of Pearson (2002); the actual temperature of the formation at 650 m at Benken is 38 °C

### 5.2 THM characterization in lab

The current knowledge on the THM properties of the Opalinus Clay relies on data from two different sites in Switzerland. Laboratory and in-situ testing in the frame of TIMODAZ will be done with the Mont Terri variant of the Opalinus Clay. Hence, in the following, we focus on the properties of the Mont Terri material.
5.2.1 Mechanical properties

5.2.1.1 Temperature effect on the short term behaviour

The influence of temperature on the short term behaviour becomes visible in relatively rapid triaxial shear experiments. These have been performed in true triaxial and conventional triaxial tests (Schnier, 2005; Göbel et al., 2006, Zhang et al., in prep.). The experiments by GRS show a significant decrease of the failure strength along the bedding planes with increasing temperature (Figure 5.4). Tests parallel to bedding by Schnier (2005) indicate only a very minor decrease in failure strength (Figure 5.3). Finally the true triaxial tests in the frame of the HE experiment (Göbel et al., 2006) may indicate that failure strength normal to bedding and parallel to bedding even increases with temperature (Figure 5.2).

Figure 5.2: Failure strength in true triaxial tests at 25°C and at 80°C (Göbel et al., 2006). Samples are stronger parallel to bedding than normal to bedding and strengthen with increasing temperature.

Figure 5.3: Linear fit of strength values in p-q plot for loading parallel to bedding. Fitted coefficients for a linear Mohr-Coulomb criterion are given in the legend. Note that the failure strength decrease at 80°C largely depends on the two samples tested at higher confining stresses (Schnier, 2005).
Figure 5.4: Triaxial tests on Opalinus Clay performed at 40° to bedding. Samples were first isotropically loaded, then heated to the desired temperatures and subsequently tested at a constant strain rate of $10^{-7}$s (Zhang et al., in prep.)

5.2.1.2 Long term deformation: creep rates

In the example shown in Figure 5.5, the sample is first loaded with an uniaxial stress of 0.74 MPa at 24 °C and 30 % relative humidity. Upon loading, the sample did not contract but expand. Subsequent heating steps (28 °C and 38 °C) each resulted in initial expansion followed by contraction. Surprisingly, creep rates at 38 °C appear to be lower than at 28 °C. When the temperature was decreased and the humidity increased to 85% the sample expanded again at half the contraction rate of 38 °C and 30 % relative humidity. Heating to 58 °C re-started contraction. A subsequent increase in loading at the same temperature also increases the creep rates. However, inspection of the deformation curve shows that it is unsure if stationary creep was reached during the first loading phases (Figure 5.5). Finally, the sample was cooled to 23 °C at a constant load of 5.6 MPa. The cooling reduced the deformation rates to extremely low values.

Figure 5.5: Uniaxial creep test at elevated temperatures and different loads (Zhang et al., in prep)
The complex evolution of the deformation rates cannot be explained by conventional temperature activated rock creep mechanisms (crack propagation, dislocation creep) alone. It has been suggested that the free and the adsorbed pore water play a key role in the process. Heating reduces the viscosity of the water and thus increases its mobility in the pores. Drainage of the sample interior and the resulting volume reduction may thus be temperature assisted. However, the drainage will ultimately increase the grain contact area and in that way increase the shear resistance within the rock. It can be interpreted from the test that at least at relatively low stress levels the temperature mainly affects the pore water that in turn controls the deformation.

5.2.2 Thermal properties

5.2.2.1 Thermal conductivity

The thermal conductivity was measured in the frame of the HE-D and HE experiments. The values are listed in Table 5.3. LAEGO measured the thermal diffusivity normal and parallel to the bedding at 20 and 80 °C. This resulted in a thermal diffusivity of $8.22 \times 10^{-7}$ m$^2$/s to $9.27 \times 10^{-7}$ m$^2$/s parallel to bedding and $4.13 \times 10^{-7}$ m$^2$/s to $5.32 \times 10^{-7}$ m$^2$/s parallel to bedding, whereby the values at 80 °C were $10^{-7}$ m$^2$/s, lower than at room temperature. The resulting conductivities (see Table 5.3) have an anisotropy factor of about 2. It should be noted that the samples for the two orientations were prepared from two different cores taken several meters apart. The tests by DBE were performed normal and oblique to the bedding (Figure 5.6). The values show no significant temperature dependence and an anisotropy factor of about 2. The measurements also indicate that thermal conductivity is independent of the confining pressure between 0.8 and 7 MPa.

![Figure 5.6: Thermal conductivity measurements by DBE (Wilveau, 2005)](image)

5.2.2.2 Specific heat

Specific heat measurements are listed in Table 5.3. Measurements from different laboratories show that the pore water loss has a profound effect on the heat capacity of the rock (Figure 5.7).
5.2.2.3 Thermal expansion

The available thermal expansion measurements for the Opalinus Clay are listed in Table 5.3. The measurements show a wide range, mainly due to variable test conditions (containment, drainage, etc.) and possibly also variable sample quality (desaturation and disturbance). Drying of the sample at rising temperatures resulted in generally smaller values for thermal expansion as shown by Figure 5.8. The anisotropy factor obtained by the DBE tests reaches a value of 10. However, most other tests suggest that it is in the range of 1.5 to 3.

It must be noted that these data need careful consideration as the subsequent THM modelling in the frame of the HE-D experiment showed that the observed deformations require significantly higher values for thermal expansions.

5.2.2.2.3 Thermal expansion

The available thermal expansion measurements for the Opalinus Clay are listed in Table 5.3. The measurements show a wide range, mainly due to variable test conditions (containment, drainage, etc.) and possibly also variable sample quality (desaturation and disturbance). Drying of the sample at rising temperatures resulted in generally smaller values for thermal expansion as shown by Figure 5.8. The anisotropy factor obtained by the DBE tests reaches a value of 10. However, most other tests suggest that it is in the range of 1.5 to 3.

It must be noted that these data need careful consideration as the subsequent THM modelling in the frame of the HE-D experiment showed that the observed deformations require significantly higher values for thermal expansions.

Figure 5.8: Thermal expansion by DBE (Wileveau, 2005), showing the effect of pore water loss at higher temperatures
## Table 5.3: Thermal and thermomechanical properties of the Opalinus Clay

<table>
<thead>
<tr>
<th>Property</th>
<th>angle to bedding</th>
<th>Source</th>
<th>Value</th>
<th>Unit</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Termal conductivity $\lambda$</td>
<td>0</td>
<td>DBE</td>
<td>1.60</td>
<td>W/mK</td>
<td></td>
</tr>
<tr>
<td></td>
<td>90</td>
<td>DBE</td>
<td>0.75</td>
<td>W/mK</td>
<td></td>
</tr>
<tr>
<td></td>
<td>45</td>
<td>DBE</td>
<td>1.55</td>
<td>W/mK</td>
<td>carbonate layer</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>LAEGO</td>
<td>2.26</td>
<td>W/mK</td>
<td>20°C</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>LAEGO</td>
<td>2.29</td>
<td>W/mK</td>
<td>20°C</td>
</tr>
<tr>
<td></td>
<td>90</td>
<td>LAEGO</td>
<td>1.17</td>
<td>W/mK</td>
<td>20°C</td>
</tr>
<tr>
<td></td>
<td>90</td>
<td>LAEGO</td>
<td>1.21</td>
<td>W/mK</td>
<td>20°C</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>LAEGO</td>
<td>2.40</td>
<td>W/mK</td>
<td>80°C</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>LAEGO</td>
<td>2.45</td>
<td>W/mK</td>
<td>80°C</td>
</tr>
<tr>
<td>Specific heat $C_p$</td>
<td>0</td>
<td>LAEGO</td>
<td>2.22</td>
<td>W/mK</td>
<td>80°C</td>
</tr>
<tr>
<td></td>
<td>90</td>
<td>DBE</td>
<td>1230</td>
<td>J/kgK</td>
<td>20°C</td>
</tr>
<tr>
<td></td>
<td>90</td>
<td>DBE</td>
<td>1360</td>
<td>J/kgK</td>
<td>20°C</td>
</tr>
<tr>
<td></td>
<td>90</td>
<td>DBE</td>
<td>1140</td>
<td>J/kgK</td>
<td>20°C</td>
</tr>
<tr>
<td></td>
<td>90</td>
<td>DBE</td>
<td>1390</td>
<td>J/kgK</td>
<td>140°C</td>
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<tr>
<td></td>
<td>90</td>
<td>LEAGO</td>
<td>852</td>
<td>J/kgK</td>
<td>20°C, dry</td>
</tr>
<tr>
<td></td>
<td>90</td>
<td>LEAGO</td>
<td>912</td>
<td>J/kgK</td>
<td>20°C, dry</td>
</tr>
<tr>
<td></td>
<td>90</td>
<td>LEAGO</td>
<td>994</td>
<td>J/kgK</td>
<td>80°C, dry</td>
</tr>
<tr>
<td></td>
<td>90</td>
<td>LEAGO</td>
<td>1078</td>
<td>J/kgK</td>
<td>80°C, dry</td>
</tr>
<tr>
<td>Thermal expansion $\alpha$</td>
<td>45</td>
<td>DBE</td>
<td>2.00E-05</td>
<td>1/°C</td>
<td>Unconfined, wrapped, heating path</td>
</tr>
<tr>
<td></td>
<td>90</td>
<td>DBE</td>
<td>1.40E-05</td>
<td>1/°C</td>
<td>Unconfined, wrapped, cooling path</td>
</tr>
<tr>
<td></td>
<td>45</td>
<td>DBE</td>
<td>1.00E-05</td>
<td>1/°C</td>
<td>Unconfined, wrapped, heating path</td>
</tr>
<tr>
<td></td>
<td>90</td>
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<td>Unconfined</td>
</tr>
<tr>
<td></td>
<td>45</td>
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<td>1.00E-05</td>
<td>1/°C</td>
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</tr>
<tr>
<td></td>
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<td></td>
<td>45</td>
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<tr>
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<td>45</td>
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</tr>
<tr>
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<td>1/°C</td>
<td>Heating path, mean stress 15 MPa</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>BGR</td>
<td>1.1E-05</td>
<td>1/°C</td>
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<tr>
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<td>1/°C</td>
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</tr>
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<td>Unconfined dilatometer</td>
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<td>1/°C</td>
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<tr>
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<td>2.1E-05</td>
<td>1/°C</td>
<td>Heating path, mean stress 15 MPa</td>
</tr>
<tr>
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<td>3.90E-06</td>
<td>1/°C</td>
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<td>1/°C</td>
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<td>GRS</td>
<td>1.70E-05</td>
<td>1/°C</td>
<td>weak temperature dependence</td>
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</table>

### 5.3 THM characterization in-situ – Experiment and modelling

#### 5.3.1 HE experiment

The description of the HE experiment was slightly shortened and modified from the final report of the experiment published by the EC. Details can be found in the original version (Göbel et al., 2006). The objective of the HE experiment was to improve the understanding of the coupled thermo-hydro-mechanical (THM) processes in a host rock-buffer system, based on experimental observations and numerical modelling. To achieve the defined objectives, the experiment was
accompanied by an extensive program of continuous monitoring, numerical modelling of the coupled thermo-hydro-mechanical processes and experimental investigations on-site and in laboratories and. Finally, the experiment was dismantled to provide laboratory samples of post-heating buffer and host rock material.

The HE experiment was performed at the Mont Terri Rock Laboratory in a niche excavated for this purpose in the shaly facies of the Opalinus Clay formation. A central vertical borehole (BHE-0) 300 mm in diameter and 7.5 m long was drilled in the niche floor. Heat-producing waste was simulated by a heater element with 10 cm diameter, held at a constant surface temperature of 100 °C. The 2 m long heater element was placed in the vertical borehole at a depth of 4 to 6 m. It was embedded in a barrier of ring-shaped compacted bentonite blocks with an outer diameter of 30 cm and a dry density of 1.8 g/cm³. A total of 19 boreholes were drilled in the niche floor for instrumentation purposes (Figure 5.9). Sensors for measuring the most relevant rock parameters, such as temperature, humidity, stress state, pore pressure, displacement and electric resistivity, as well as devices for determining gas and water release were installed in the boreholes. To simulate the long-term behaviour and because of the absence of free water in the Mont Terri Rock Laboratory, an artificial hydration system was installed to accelerate the saturation process in the buffer prior to the heating phase (Figure 5.10).

The water used was synthetic experimental water, which is chemically similar to the water in the Opalinus Clay formation. The artificial saturation lasted for 35 months before the begin of the heating phase.
heating phase (duration 18 months). Evolution of applied power (W BHE-0) and temperatures in BHE-0 versus time is given in Figure 5.11.

\[ \text{Figure 5.11: Evolution of the applied power (W BHE-0) and temperatures in BHE-0 versus time (numbers indicate depth of sensor in the vertical borehole, e.g. 0500 meaning 5 m)} \]

5.3.1.1 Monitoring results
The pore pressure sensors show a pressure build-up at the beginning of the heating, followed by a slow decrease and then a sharp pressure drop after the heating has stopped (Figure 5.12). The curves also differ in the size of their maxima, etc. Measurements of the relative humidity (capacity sensors) showed no conclusive results and were probably perturbed by the heating.

The angle variations registered by the inclinometers were very small (Figure 5.13). The maximum displacement was about 5.5 mm (measured a few days after the end of the heating; at 4,50 m depth in the inclinometer). After heating phase, the displacements decreased slightly. The measured values are more than one order of magnitude larger than the results of the computer simulations.

\[ \text{Figure 5.12: Evolution of pressure in boreholes BHE-19 and BHE-20. Depth of sensors: /1 = 3.5 m, /2 = 5 m = mid-heater, /3 = 6.5 m, /4 = 8 m)} \]
Hydraulic conductivities were measured before and after the heating period in boreholes close to the heater borehole (Bühler et al., 2006). Figure 5.14 shows the measured conductivities of Opalinus Clay as a function of depth. The post-heating saturated hydraulic conductivity is estimated to be $K_s = 5 \times 10^{-11}$ m/s. Assuming saturated conditions in the deeper parts of the borehole, the pre-heating hydraulic conductivity is $K_s = 1 \times 10^{-12}$ m/s. Although there is no strong indication that the hydraulic conductivity has really changed due to the heating, as the temperatures at a distance of 0.65 cm from the heater borehole did not exceed 50 °C and as nothing indicates a decrease in saturation. In comparison, Gaucher et al. (2003) report hydraulic conductivities in the Opalinus Clay of

Matrix rock: 1 \times 10^{-13} to 5 \times 10^{-13} m/s  
EDZ: 4 \times 10^{-12} to 8 \times 10^{-8} m/s  

The conductivities measured in the boreholes are similar to the values for the EDZ. This suggests that the heating may have influenced the hydraulic conductivity.
be found because the temperatures were too low (Kaufhold & Emmerich, 2006). Regarding heat-induced changes in bentonite and particularly in Opalinus Clay, future heater experiments should consider the use of a different test configuration to get more representative repository conditions, i.e. higher temperatures on the clay.

5.3.1.3 Modelling of the HE experiment
The near-field model comprises the most important technical features of the engineered barrier. It includes all sequences in the history of the test, beginning with the excavation of the HE niche. Modelling the initial phases of the experiment is of vital importance as they control the initial stress state and the pore pressure for the subsequent phases. The far-field model deals with the THM interactions in the host rock only.

HE Experiment: near-field modelling
The initial model for the near-field of the HE experiment was axisymmetric.

The mechanical behaviour of the host rock has been modelled by the mechanical constitutive law proposed by Vaunat & Gens (2003). Opalinus Clay is considered as a composite material made of a clay matrix interlocked by bonds. The bond response is modelled by a damage model proposed by Carol et al. (2001), while the clay matrix can be represented by any model usually used to characterize a clay soil. In the case of Opalinus Clay, which has a low porosity (13.7 %), a Hoek-Brown criterion associated with a linear-elastic law was used. Applying the compatibility and equilibrium equations between bond, matrix and external strains and stresses, the material response was derived. More information on the THM parameters used for the modelling are given in technical annex 1.

A comparison with monitoring results shows that the evolution of the stress state and the pore pressures during niche excavation and borehole drilling could be reproduced well.

During the hydration phase, the high initial suction of bentonite induced an unsaturated state in the surrounding rock, reaching a maximum at a radial distance of 0.70 m. The desaturation and subsequent resaturation took place in approximately 200 days. The hydration of the bentonite generated high swelling pressures, reaching a maximum value of 14 MPa in the rock close to the interface.

The bentonite swelling pressure produced significant changes in the stress state in the surrounding rock, affecting a zone of 1 m diameter. Plastic strains were produced in a narrow zone of the rock (thickness of 0.05 m) adjacent to the bentonite-rock interface. The post-dismantling analysis showed that the in-situ behaviour was different (see section on bentonite).

Modelled temperatures during the heating phase are close to measured values (Figure 5.15). The increase in the pore pressure and the subsequent dissipation measured during heating are well reproduced by the model (Figure 5.16). The magnitude of the pore pressure increase is controlled by the rate of the temperature increase, the rock permeability, the rock porosity, the rock stiffness and the geometry of the experiment. The heating phase generates a transient change in the total and effective stresses. Successive heating extends the annular zone of the plastic strain to a maximum thickness of 0.08 m. The latter could not be confirmed in-situ.

The cooling phase induces a reduction in the pore pressure. The magnitude of this reduction depends on the rate of the temperature decrease. The pore pressure reaches a stable state after approximately 250 days of cooling. Cooling implies a transient change in the total and effective stresses. On the long term, the steady state stresses do not seem to be affected by the heating and
To better represent the mechanical behaviour of the Opalinus Clay, an anisotropic elasto-viscoplastic model was applied. A lot of material parameters were taken from tests performed on the Opalinus Clay as part of the HE experiment. These parameters are given in the technical annex 1.

Significant differences between the isotropic and the anisotropic models have been found in:

- the direction and intensity of displacements
- the stress distribution
- the plastic zone developed

**HE-Experiment: Far-field model**

A THM-version of the MEHRLIN code was developed by adding the thermal reaction. Verification and testing showed that the overall observed behaviour of the measurements with respect to TH-processes could be well reproduced by an axisymmetric model. The thermal parameters obtained by numerical fitting to in-situ observations correspond well with the values measured on samples in the laboratory (see technical annex 1). Based on the data available, the work was not conclusive with regard to the simulation of mechanical effects: it was found that the volume of rock undergoing a rise in temperature by more than a few degrees was relatively small. The pore-water pressure rise
due to heating was important, as expected in the low-permeability Opalinus Clay. The induced changes in effective stress are equally important and can, at least for low effective stress conditions, not be ignored as these lower stresses can affect the mechanical stability (where applicable). Moreover, volumetric rock deformations and/or damage will influence the rock permeability and might create preferential features (fractures) that affect the integrity of the barrier. This aspect can be of key importance for design purposes, i.e. the back-fill material and geometry, as well as the maximum permissible heat load.

A reasonable fit with the measured temperature curves is obtained. The differences between measured and calculated values amounts a few 1/10 K assuming isotropic conditions and using the following parameters for the Opalinus Clay:

- **Intrinsic permeability**: \(8 \times 10^{-19} \text{ m}^2\)
- **Thermal conductivity**: 2.1 W/m/K
- **Heat capacity**: 920 J/kg/K

These values represent a best guess lying in an acceptable range of values presented in the literature.

The calculated pressure level is very sensitive not only to the rock permeability but also to the thermal parameters of the rock. A reasonable fit (Figure 5.17) could be achieved using a standard thermal expansion coefficient and a permeability of \(8 \times 10^{-19} \text{ m}^2\). Compared to undisturbed values for the Opalinus Clay (less than \(2 \times 10^{-20} \text{ m}^2\)), this permeability value is very large. This can indicate that the swelling of the bentonite buffer might have induced fractures in the Opalinus Clay during the resaturation of the bentonite. It is worth noting that this value is only slightly higher than the fitted value obtained by means of hydraulic tests in boreholes BHE-19 and BHE-20 (less than \(2 \times 10^{-19} \text{ m}^2\), see monitoring section). Therefore, the Opalinus Clay formation might be disturbed within this area.

The porewater pressures were, according to the calculations, significantly influenced by the heating. Considerable pore pressures developed even in regions that were only slightly affected by the rise in temperature. After the temperature reached a steady state, the overpressures dissipated due to flow within the Opalinus Clay. However, the porewater pressures did not drop back to their original level during the heater test duration, but levelled off to a more or less constant value. The early pore pressure increases reach up to 10 MPa. The rock permeability is a major parameter influencing the level of overpressure reached because of the heating as well as the porewater pressure dissipation.

Based on the results obtained, it seems that changes in effective stress due to pore pressure rise are the dominant mechanical effect, with changes in mechanical properties due to temperature effects or thermal plastification probably being very limited. Local changes in the stress field reach several MPa. As the effective stress reduction due to pressure variations is isotropic, this could potentially...
lead to strong mechanical effects and classic plastification under conditions which are characterized by a very anisotropic in-situ stress field and/or in cases of a generally low effective stress level compared to pore pressure changes. No direct comparison between the displacements measured and simulated could be made within this study, as the displacement measurements started (at least) at the beginning of the hydration process of the bentonite (prior to the heating phase) and no change in the evolution could be observed when the heater was switched on. In any case, displacements related to heating seem to be small and less than one millimetre, which is confirmed by the simulations.

5.3.2 HE-D experiment
The in-situ experiment HE-D aimed to investigate the coupled THM behaviour of the Opalinus Clay. The HE-D experiment was carried out in the homogenous shaly facies in the gallery 98 close to the MI niche in order to have access from two sides to the main experimental region (Figure 5.18).

![Figure 5.18: Top view of the HE-D test showing the overall borehole layout (Wileveau et al., 2005)](image)

5.3.2.1 Test procedure
A two element heated packer system was placed in the centre of the experiment. The heater elements were in direct contact with the host rock. Their diameter was 30 cm and each system included a 2 m long packer element. The total length of the system was 6.2 m. The heat output and the pressure onto the rock were fully controlled. 24 peripheral boreholes were drilled and instrumented with 110 sensors to record the reaction of the rock-water system to the heating.
The course of the test is presented by Figure 5.19, from which several events are reflected (detail is given in technical annex 1)

![Figure 5.19: Heating power and pressure of packer no. 1 after start of HE-D experiment on April, 6th 2004 (Zhang et al., in prep.)](image)

5.3.2.2 Results

Temperature recordings are depicted in Figure 5.20 and Figure 5.21 along with the radial distance of the sensors to the heater system.

![Figure 5.20: Temperatures above the heater number 1](image)
Figure 5.21: Temperatures below the heater number 2

Prior to heating the rock temperature was between 14 and 19 °C, clearly showing higher values close to the MI niche. Temperature variations in the rock showed correlations with the temperature variations in the Niche up to 7 m into the rock. These variations were also discernable in the pore pressure measurements.

The observed differences between the arrays above heater 1 and below heater 2 can possibly be attributed to the anisotropy of the rock.

The power interruption in December 2004 did only decrease the temperatures in the sensors below heater number 2. The other sensors remained largely unaffected.

Pore pressure measurements are shown in Figure 5.22, Figure 5.23 and Figure 5.24. During the pre-heating phase the pore pressures remained low in the array above heater number 1. In the second array below heater 2 the pore pressure equilibrated to approximately 0.8 to 1.2 MPa. These were also affected by the drilling of the heater borehole. In the closest borehole D14 a slight increase before the passing of the borehole face and a sharp overpressure peak of around 150 kPa is followed by a steep drop of 450 kPa. Subsequently the pressure slowly recovered. The reactions of the more distant boreholes are similar but the magnitudes are smaller.

Upon the start of heating the pore pressure decreased in sensors D8, D14 and D15. However, it re-increased soon afterwards and surpassed initial values within a few hours. The reason for the initial decrease of the pressures remains unclear. All other sensors showed increases upon pressurization and the start of the heating of the two central packers.

Temporary pressure drops in D08, D15 and D16 at the beginning of phase 2 remain unexplained while pressure drops in D14 and D15 on July 24, 2004 are related to the loss of heater packer pressure. Close to the MI niche (D07, D13; data of D12 are unreliable) the pressures were only slightly changed by the heating.

After the end of the heating phase on 13th March 2005 brief peaks were observed in the pressure sensors D08, D09, D15, D16 and D17, similar to the power failure event on 15th December 2004. This was followed by a smooth decrease in all pressure sensors to almost atmospheric pressures except for sensors D11 and D17 which were situated far away from the surrounding galleries.
Figure 5.22: Pore pressure changes during drilling of the central heater borehole. Note short overpressure pulse prior to the drop. The distance to the heater borehole is smallest for D14 and largest for D16, lateral positions are identical.

Figure 5.23: Pore pressure values in the sensors above heater number 1

Figure 5.24: Pore pressure values in the sensors below heater number 2
A deformation of the rock mass surrounding the heater borehole was measured as an axial extension in three subhorizontal or horizontal boreholes: normal to the heater, towards the centre (BHE-D6, Figure 5.27), normal to the heater but passing slightly below its centre (BHE-D5, Figure 5.26) and oblique towards the centre (BHE-D4, Figure 5.25).

The deformation time-series for the 3 extensometers are plotted as the difference between the fixed heads in the adjacent galleries and the base points in the rock. The oblique extensometer BHE-D4 records contractional deformation increments immediately after each increase in heating power, while later its axial direction keeps extending.

In the borehole BHE-D5 that passed below the heater only extension was measured. The deformation rates increased at the beginning of the two heating steps. After the heater has been shut down, the deformations were reversed. Close to the heater contraction surpassed the initial state.

Deformations in the borehole BHE-D6 were much larger than in the other boreholes. It has been speculated that the shotcrete layer bearing the headplate was detached from the rock during the experiment. This is in line with the observed opening of visible cracks in the MI niche during the excavation of the gallery 04 that took place at the end of the first heating phase (Wileveau, 2005).

Pulse injection tests performed with mini-packer systems after the end of the HE-D experiment were used to investigate whether heating affects the permeability of the Opalinus Clay. It shows that the hydraulic conductivities are in the range of the undisturbed rock. However no test results are reported from the time prior to heating. Hence, these results require verification (Andra in prep.).

Figure 5.25: Axial deformation between the headplate and fixed points in the borehole BHE-D4

Figure 5.26: Axial deformation between the headplate and fixed points in the borehole BHE-D5
5.3.2.3 Modelling of the HE-D experiment

The multitude of data that resulted from the HE-D test was analysed using various kinds of models. The results are reported in the modelling section. It shows that even with heavily instrumented tests like the HE-D, obtained modelling results depend on modelling technology, modelling skills and modelling assumptions. All of which have some inherent range and/or uncertainty.

Thermal modelling of the HE-D experiment

CEA constructed a 3D thermal model of the niche including the temperature sensors. The thermal properties of the Opalinus Clay were determined by back-analysis based on the first three months of 1st phase measurement. It was assumed that the Opalinus Clay is an orthotropic rock with a 40° dip. The mechanical impact of the borehole (disturbance) is not taken into account and the clay is considered to be fully water saturated.

It showed that to fit the overall thermal behaviour of the experiment another parameter (called $\alpha$) was required to account for a lower effective heat output of the heaters. At the current stage, this corrective coefficient does not have a well-identified physical sense.

Subsequent sensitivity analysis showed that there is no unique selection to $\alpha$ and the values for the thermal conductivity of the Opalinus Clay. During the parameter-optimisation phase through the inversion method, both verification models ($\lambda_l = 2.03 \text{ W/m·K}, \lambda_t = 1.03 \text{ W/m·K}, \alpha = 0.77$ for the first, and $\lambda_l = 2.74 \text{ W/m·K}, \lambda_t = 1.29 \text{ W/m·K}, \alpha = 0.99$ for the second) fully reproduce the entire set of in-situ temperature measurements (Figure 5.28). The reason for the loss in power of the heater that $\alpha$ accounts for may be in the heater system itself or in the EDZ, but remains unclear at the moment.
Various modelling approaches were used in a first interpretation stage of the HE-D experiment to model the system behaviour over the initial 200 days (Wileveau, 2005). The modelling approaches by GRS, DBE and UPC are summarized in Table 5.4.

**Table 5.4: Summary of model approaches for the HE-D experiment by GRS, UPC and DBE**

<table>
<thead>
<tr>
<th>Team</th>
<th>Code</th>
<th>Digital Model</th>
<th>Assumptions</th>
</tr>
</thead>
</table>
| UPC  | CODE BRIGHT   | Axissymmetric 2D geometry         | • Saturated THM Model  
• Elastic  
• Elasticity E=6.3 GPa and permeability K=5E-13m/s adjusted to results of drilling operations BHE-D0  
• No thermal or mechanical anisotropy  
• Initial pressures adjusted to measured values: 0.9 MPa  
• 20% decrease in heating power  
• Average thermal conductivity \( \lambda = 1.5 \text{ Wm}^{-1}\text{K}^{-1} \)  
• Average thermal expansion \( \alpha = 2.6 \times 10^{-5} \text{ °C}^{-1} \)  
• Solid grain expansion coefficient \( \alpha_s = 9.6 \times 10^{-6} \text{ °C}^{-1} \)  
• Thermal expansion coefficient of water \( \alpha_w = 3.4 \times 10^{-4} \text{ °C}^{-1} \) |
| GRS  | CODE BRIGHT   | Plane 2-D and axissymmetric 2-D geometry | • Saturated THM Model  
• Elastoplastic model, E = 3.4 GPa  
• No thermal or mechanical anisotropy  
• Initial pressures before drilling of heater borehole adjusted to 2D calculation: 1 MPa  
• Average thermal conductivity \( \lambda = 1.7 \text{ Wm}^{-1}\text{K}^{-1} \)  
• Average thermal expansion \( \alpha = 2.0 \times 10^{-5} \text{ °C}^{-1} \)  
• Solid grains linear expansion coefficient \( \alpha_s = 2.0 \times 10^{-6} \text{ °C}^{-1} \)  
• Fitted thermal expansion coefficient of water \( \alpha_w = 2.0 \times 10^{-4} \text{ °C}^{-1} \) |
| DBE  | FLAC3D        | 3-D model                         | • Saturated THM Model  
• Elastoplastic model (Drucker-Prager)  
• Thermal anisotropy  
• No mechanical anisotropy  
• Fitted thermal parameters: \( \lambda_v = 1.7 \text{ Wm}^{-1}\text{K}^{-1} \), \( \lambda_s = 0.8 \text{ Wm}^{-1}\text{K}^{-1} \)  
• Adjusted permeability K=5E-13m/s with initial pressure distribution  
• Thermal expansion coefficient of the matrix \( \alpha = 1.5 \times 10^{-5} \text{ °C}^{-1} \)  
• Thermal expansion of solid grains \( \alpha_s = 9.0 \times 10^{-6} \text{ °C}^{-1} \) |
The comparison of the model results with the measured data (Figure 5.29 to Figure 5.33) shows that the coupled models were able to reproduce quite accurately the thermal field of the experiment including the anisotropy of the rock properties. However, it proved to be more difficult to match the hydraulics and the mechanical response of the system.

Figure 5.29: Model – field data comparison for sensor BHE-D3

Figure 5.30: Model – field data comparison for pore pressure sensor BHE-D3-Pre 1
Figure 5.31: Model – field data comparison for pore pressure sensor BHE-D14-Pre 1.

Figure 5.32: Model – field data comparison for extensometer BHE-D4-PT5

Figure 5.33: Model – field data comparison for extensometer BHE-D4-PT5
Preliminary conclusions of the modelling results have been presented by Wilevau (2005):

**Temperature**

A detailed analysis of all the modelling results suggests that a reasonable combination of the parameters for the thermal modelling appears to be:

- $\lambda_{\text{normal}} = 2.1 \ \text{W/m·K}$
- $C_p = 860 \ \text{J/kg·K}$ at dry state and 20 °C.

**Hydraulic pressure**

Pore water pressures are adjusted to the hydraulic-pressure values measured at each point at the beginning of the heating process. The modelling results of the four teams are qualitatively correct. An overpressure phase is followed by a decrease of pressure. The peak values are correctly matched in BHE-D3 at around 4 MPa. The results confirm the relative consistency of the THM-coupling parameters, such as permeability, thermal-expansion coefficient, Biot’s coefficient, etc.

**Deformation**

For the points being studied, the observed axial deformation trend of the installed extensometers is reproduced by the models: a compression phase followed by an extension phase occurring more or less rapidly according to the remoteness of the heat source. It should be noted that the data are consistent with the DBE model that uses a ten times higher thermal expansion than the LAEGO model. Generally speaking, the deformations appear not to be consistent with the lab determinations of the thermal expansion. This may indicate that the geometry and mechanical boundary conditions of the HE-D experiment including the access drifts and the MI niche are not well represented in the model. The thermo-mechanical deformations of the massif are affected by those structures and are difficult to model through simplified models.

### 5.4 Chemical aspects related to heating of the host rock

Significant chemical effects of heating in the host rock are not expected. Possible effects of heating are listed in the Table 5.5.

<table>
<thead>
<tr>
<th>Process</th>
<th>Possible Consequences</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maturation of organic material</td>
<td>Production of gas, modification of pore water chemistry</td>
</tr>
<tr>
<td>Transformation of smectite to illite in</td>
<td>Loss of swelling capacity, embrittlement</td>
</tr>
<tr>
<td>composite clay minerals, cementation with SiO2</td>
<td></td>
</tr>
<tr>
<td>Acceleration of oxidation</td>
<td>Mineral reactions, Modification of porosity and pore water chemistry</td>
</tr>
<tr>
<td>Re-adjustment of geochemical equilibrium</td>
<td>Modification of porosity and pore water chemistry</td>
</tr>
<tr>
<td>reactions</td>
<td></td>
</tr>
</tbody>
</table>

An in-depth literature study of natural analogues and experimental data shows that none of these effects is rapid enough to produce measurable effects within the thermal phase of the waste that spans a few hundred years (Mazurek, 2002). For instance the maturation of organic material is mainly controlled by the Temperature-Time-Interval (TTI) that the rock experiences (Elie &
Landais; 2000). A brief comparison shows that the TTI of the thermal phase of the waste is 40 to 80 times smaller than the TTI of the geological burial. Hence the effect can be neglected. Similar reasoning applies for the illitization of the smectite layers. It has been pointed out in the basin analysis by Leu et al. (2001) that the Opalinus Clay has experienced 85° for at least 20 Ma in NE Switzerland. Investigations of the clay minerals show that smectite is still present in the rock (Mazurek 1998). This confirms numerical modelling results which show that the kinetics of the smectite-illite transformation are very slow and significant effects require Millions of years of heating.

5.5 Discussion

5.5.1 Uncertainty

Generally, large uncertainty on the experimentally derived parameters for the rock exists. For example, the anisotropy factor for thermal expansion varies between 1 and 10. Due to the small number of samples it is not always clear whether the large range of parameters represent natural variability, differences in test procedures or sample quality (sample disturbance by drilling, storage, subsampling, testing).

Modelling of the HE-D shows that the 3D models can be fitted to the observed temperature field by reducing the heat output to 80% and by adjusting the two parameters for the thermal conductivity normal and parallel to bedding. This is the case because thermal properties in intact rock are only weakly dependent on the mechanical and hydraulic state (pore pressures) of the model.

However, the modelling of strongly coupled processes involve larger uncertainties. Pore pressures generally show a poorer fit to the observed values and the deformations are even worse. The reason for this observation may be manifold. The values applied for THM coupling may be incorrect or they may have systematic spatial variations which are not accounted for in the models (e.g. an EDZ has not been implemented). Moreover, the real boundary conditions may not be well represented in the model and the concepts for THM coupling may be inadequate. For example the HM coupling in the fractured EDZ may be different from the continuum of the intact rock. This highlights the need for parameters from the damaged region around excavations that can be used for modelling. However, such experiments will have to bear in mind fracture network properties, scale and homogenisation issues both in the experiments as in the models.

More tests with thoughtful chosen boundary conditions are needed. As one simple example, thermal expansion could be tested at different heating rates under drained boundary conditions.

5.5.2 The most important temperature-dependent material properties

Some important parameters of the rock appear to be strongly temperature dependent. For example the temperature dependence of the strength is significant. However, the nature of the temperature dependence is little understood. It is not clear if the lower strength and the moderately higher creep rates at higher temperatures result from temperature sensitive deformation processes (e.g. crack growth) or from increased pore pressures and consequently reduced effective stresses.

5.5.3 The most important coupled processes and parameters

In the intact rock the temperature induced pore pressure rise (thermal diffusivity vs. hydraulic diffusivity) has to be considered. However, the database for modelling such phenomena is insufficient and more experiments are required. Specific tests are required to study the impact of the heating range on the pore pressure.
Furthermore the temperature dependence of the strength is an important issue. It is desirable to have more data on creep rates and strength limits at elevated temperatures and to investigate the influence of the temperature on the properties of the existing faults.

Long term evolution of the tunnel near-field will be controlled by the complex interaction of resaturation, backfill behaviour (swelling) and time-dependent deformation mechanisms in the host rock. All of these may be sensitive to elevated temperatures during the thermal phase of the radioactive waste. Important issues in the host rock EDZ appear to be the time and temperature dependence of fracture self-sealing and the thermally induced growth of fractures. It should be noted however that experimental test layouts should respect repository concepts. For example, during most of the thermal phase the near-field will be desaturated. Hence, the properties of the desaturated material should be determined under the influence of heat.

5.5.4 Effect of discrete fractures and fracture connectivity on the effective hydraulic properties

The major changes in the hydraulic properties of the host rock in the near-field of excavations in the Opalinus Clay (Martin and Lanyon et al., 2004; Marschall, 2004) are mostly a result of localized deformation i.e. the formation of fractures. Hence, the importance of the fractures, namely their geometry, their distribution and their interconnectivity cannot be overemphasized. In contrast, fractures only play a small role for the intact rock. The hydraulic properties of tectonic faults have been shown to be indistinguishable from the intact rock. So within the host rock they can even be neglected in terms of hydraulic properties.

5.5.5 Importance of chemical impact

For the Opalinus Clay chemical effects of heating can be neglected. All possible effects are too slow to have a significant impact on the host rock.

5.5.6 Derive the most appropriate conceptual models and evaluate the most appropriate numerical code

Beyond the EDZ in the intact rock, the continuum assumption holds and any anisotropic elastic FE code will be able to model the coupled processes quite adequately. The HE-D experiment shows that elastic modelling as done by UPC (Wileveau, 2005) can account for the general deformation trends. Things may be different in the vicinity of excavations. Here, fracture generation due to strain localisation has a large impact on the hydromechanical properties and thus need to be included in the modelling. Continuum models have a poor record of doing so. Hence, scale issues need to be taken into account.

6 State of the art for Callovo-Oxfordian argillite

6.1 Main characteristics

6.1.1 Geological setting

The Meuse/Haute-Marne site is located in Eastern France, on the boundary between the Meuse and Haute-Marne departments. Geologically, it is part of the eastern region of the Paris Basin. In this region, the Paris Basin is composed of alternating sedimentary layers (predominantly argillaceous) and limestone layers, deposited in a stable marine environment during the Jurassic, between 165 and 135 million years ago. These layers have a simple and regular geometric structure, slightly dipping
towards the northwest (1.5 to 2 degrees) in accordance with the general structure of the Paris Basin (bowl-shaped structured centred in the Paris area).

Within the sedimentary sequence, the Callovo-Oxfordian layer has been selected for the repository feasibility study (Figure 6.1). It is surrounded by two geological formations (underlying Dogger and overlying carbonated Oxfordian) containing water-bearing sedimentary horizons with low permeabilities and slow runoff (approximately one kilometer per hundred thousand years for the Darcy water velocity). The structural framework is stable, with natural stresses oriented in a stable manner for the past 20 million years. The site is located apart from large regional faults such as the Marne fault towards the southwest (Figure 6.1).

The depth of the Callovo-Oxfordian roof varies from 420 m at the underground research laboratory (URL) to over 600 m along the dip direction. The thickness of the layer varies from 130 m at the laboratory to 160 m towards the north.

Figure 6.1: 3D geological block diagram of the Meuse / Haute-Marne site

The 3D seismic data obtained on the URL site show no fault with a vertical throw exceeding 2 meters within the layer. Directional boreholes confirm the absence of secondary (subseismic) faults. Moreover, only a few microfissures, stable and not affecting the water flow, have been observed in over 4 km of core samples. Some of them are sealed with sulphates (celestine) which indicates a precociously tight formation during the compaction of the deposits.

The characteristics of the Callovo-Oxfordian layer have been acquired shortly after its deposition. The layer has subsequently remained undisturbed, as indicated by Sr and δ13C isotopic markers, geological thermometers (maximum palaeotemperature of approximately 40 °C) and the near absence of minerals formed at a later date (beyond 10 million years).

6.1.2 Mineralogy and porewater chemistry of the Callovo-Oxfordian argillites

The Callovo-Oxfordian formation consists of clay mineral representing up to 60 % of its mass, as well as silts (fine quartzes) and carbonates. It is from a mineralogical viewpoint laterally homogeneous.

Vertically, the proportions of the main mineralogical phases vary and are structured into three sedimentary sequences. The upper sequence is characterized by a higher carbonate content. The Callovo-Oxfordian argillite resembles tectosilicates (essentially quartz) and carbonates (essentially

__________________________________________________________

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calcite) embedded in a fine matrix formed out of swelling and non-swelling phyllosilicates (clay minerals) that contain a small quantity of organic matter and sulphides (0.5 to 1% each). The morphology of the minerals is representative of two distinct origins:

- detrital minerals settled by marine sedimentation (quartz, carbonated bioclasts, clay minerals)
- calcite precipitated on site in the sea or remobilized after deposition

The clay minerals constituting the matrix consist of illite, interstratified illite/smectite, chlorite and kaolinite. They are assembled in the form of aggregates a few microns in size. The lower part of the Callovo-Oxfordian is marked predominantly by R1 interstratified illite/smectite (ordered I/S with 20 to 40% of swelling smectic layers). An abrupt transition was systematically identified in all boreholes towards the upper part of the argillites with a predominance of R0 interstratified illite/smectite (disordered I/S, with 50 to 70% of swelling smectic layers).

Different water salinities have been observed in the Callovo-Oxfordian and surrounding formations, 3 to 4 g/l in the argillite porewater (see Table 6.1), around 4 g/l in the Dogger and 0.9 g/l in the calcareous Oxfordian. High salinity of the interstitial water in the Callovo-Oxfordian indicates an absence of hydraulic exchanges with water-bearing formations. It confirms the low permeability of the argillites and the very slow displacement of ions in solution.

**Table 6.1: Most probable water composition (and plausible alternative) of Callovo-Oxfordian argillites at the Bure URL**

<table>
<thead>
<tr>
<th>Parameters</th>
<th>reference</th>
<th>alternative</th>
</tr>
</thead>
<tbody>
<tr>
<td>Eh (mV)</td>
<td>-156</td>
<td>-180</td>
</tr>
<tr>
<td>pH</td>
<td>7.0</td>
<td>7.3</td>
</tr>
<tr>
<td>ionic force (mol/l)</td>
<td>0.12</td>
<td>0.09</td>
</tr>
<tr>
<td>Alkalinity (meq/l)</td>
<td>2.5.10⁻⁵</td>
<td>1.4.10⁻⁵</td>
</tr>
<tr>
<td>Cl (mol/l)</td>
<td>3.0.10⁻²</td>
<td>1.5.10⁻²</td>
</tr>
<tr>
<td>S(VI) (mol/l)</td>
<td>3.4.10⁻²</td>
<td>3.1.10⁻²</td>
</tr>
<tr>
<td>Na (mol/l)</td>
<td>3.2.10⁻²</td>
<td>2.6.10⁻²</td>
</tr>
<tr>
<td>K (mol/l)</td>
<td>7.1.10⁻³</td>
<td>6.2.10⁻³</td>
</tr>
<tr>
<td>Ca (mol/l)</td>
<td>1.5.10⁻⁵</td>
<td>1.1.10⁻⁵</td>
</tr>
<tr>
<td>Mg (mol/l)</td>
<td>1.4.10⁻⁵</td>
<td>1.1.10⁻⁵</td>
</tr>
<tr>
<td>Fe (mol/l)</td>
<td>3.3.10⁻⁴</td>
<td>7.1.10⁻⁴</td>
</tr>
<tr>
<td>Si(aq) (mol/l)</td>
<td>9.4.10⁻⁵</td>
<td>9.4.10⁻⁵</td>
</tr>
</tbody>
</table>

### 6.1.3 Mechanical properties

The argillites have mechanical properties favouring the feasibility of underground engineered structures at the depth of the Callovo-Oxfordian layer in the transposition zone in which the URL is situated (simple compression resistance > 21 MPa).

### 6.1.4 Hydraulic properties

The total porosity of the argillites is around 15 to 18%. The pores have an average size of 50 nm. That implies that half the porosity is occupied by bound water.

Owing to these textural properties, permeability of the argillites is low and ranges from 5.10⁻¹⁴ to 5.10⁻¹³ m/s. The diffusion coefficient values are also low, particularly for anions. The effective diffusion (De) coefficient values have been assessed at:

De = 5.10⁻¹² m²/s for an accessible porosity value of 5% in the case of anions

De = 2.5.10⁻¹⁰ m²/s for an accessible porosity value of 18% in the case of cations.
The argillaceous mineralogical composition of the argillites gives the Callovo-Oxfordian formation high retention capabilities for cations.

6.1.5 Thermal properties

6.1.5.1 Thermal conductivity

Thermal conductivities of argillites have been either calculated on the basis of the thermal-diffusivity measurements taken on cores from boreholes EST104 and HTM102 through the “flash” method (Homand, 1998) or measured directly through the “divided-bar” method (GdR ForPro, 2002).

Results show a correlation between the thermal conductivity, the porosity and the mineralogical composition. For this reason, there are significant differences in the thermal conductivity of the Callovo-Oxfordian argillites within the formation (Su, 2002a; Figure 6.2).

![Figure 6.2: Vertical evolution of thermal conductivity as measured on samples from boreholes EST104 and HTM102 (François, 1998)](image)

All upper horizons contain more quartz carbonate and have less significant porosity, the latter implying a higher thermal conductivity. The average thermal conductivities parallel and perpendicular to the stratification amount 2.2 and 1.6 W/m/K respectively.

The central horizon corresponds to the maximum-clayey zone and is characterised by the lowest conductivity value. Parallel and perpendicular conductivities to the stratification amount 1.9 W/m/K and 1.3 W/m/K respectively.

All lower horizons include a thin carbonated episode of several metres in thickness which induces a lower average porosity and, consequently, a higher thermal conductivity.

6.1.5.2 Specific heat

The specific-heat of argillites was measured on samples from borehole EST104 (François, 1998). The specific heat of saturated argillites varies only slightly with depth. At 20°C, it reaches an average of 1,096 J/kg/K. The highest values are found in the carbonated beds (i.e., 515-527 m for borehole EST104). At 100°C, the results are more dispersed (standard deviation/average reaches 10 to 15%) resulting from the variability on clay and carbonate concentrations between the different...
6.2 THM characterisation in laboratory

6.2.1 Impact of temperature on the short term mechanical behaviour

The impact of the temperature on the short term mechanical behaviour was studied through uniaxial-compression tests (3 at ambient temperature and eight tests at higher temperatures) and triaxial-compression tests (9 at ambient temperature and 35 at higher temperatures) with temperatures as high as 100 °C.

Test results do not indicate any impact of the temperature on the strain modulus within the spectrum of tested temperatures (T < 100 °C) (Figure 6.3) (Bauer, 1997).

The rise in temperature can lead to a reduction of argillite strength. UCS is 30 % less when temperature reaches 80-100 °C, but no net reduction is visible under triaxial compression.

Beyond the rupture the argillites behave more ductile during triaxial tests when the temperature reaches 80-100 °C.

The influence of a thermal cycle was analysed by 15 triaxial tests carried out at ambient temperature on pre-dried samples at 100 °C. Results show that:

- moduli of dried samples tend to be slightly higher than those measured on non-dried samples when the water content of argillite is above 6.2 %. No net tendency was noticeable on other samples
- no influence of temperature on rupture and damage characteristics

In conclusion, until now no study has ever detected any significant impact of temperatures up to 100 °C.
°C on the mechanical characteristics of deformability, strength or damage. Either that impact, if it exists, is low enough to be obliterated by the dispersion of results, or the number of available tests is not sufficient to reach a sound conclusion.

6.2.2 Impact of temperature on the long term mechanical behaviour

Since 1994, Antéa and G3S-LMS have conducted several creep-test campaigns under specific temperature conditions (Antea 1999; Gasc 2002; Gasc & Malinsky 2002; Chanchole 2004). Those campaigns include uniaxial, triaxial, mono-stage and multi-stage tests.

The key result is that the creep rate increases with temperature (Figure 6.5 and Figure 6.6). It is practically multiplied by a factor of 1.5 when the temperature increases by 30°C (from 20 °C to 50 °C) and by a factor of about 3, on average, when the temperature increases by 60 °C (from 20 to 80 °C) (Figure 6.6b, Gasc 2002).

Multi-stage tests at a constant temperature of 80 °C show that the creep rate varies between $3.5 \times 10^{-11}$ and $3.5 \times 10^{-10}$ s$^{-1}$ depending on the value of the deviator and on the timescale. However, as shown in Figure 6.6a, even under these temperature conditions the creep rate is progressively cancelled over time for deviator values less than or equal to 10 MPa, but remains at a value of about $10^{-10}$ s$^{-1}$ for a 15 MPa deviatoric stress.

Independent of the temperature all the creep tests can be interpreted by a Lemaître model. The impact of the temperature on the creep rate is taken into account by the mean of the Arrhenius law, which is frequently used for viscoplastic rocks.

![Figure 6.5: Impact of temperature on creep tests with a 12-MPa deviator, (borehole EST104, geomechanical units C and E (Gasc, 1999)](image-url)
Figure 6.6: Impact of temperature on creep a) axial deformation over time for three deviators at
ambient temperature and at 80°C; b) synthesis of strain rates versus deviatoric stress at two
temperatures (black triangles : ambient, red squares: 80°C), (borehole EST205, geomechanical unit
C)

6.2.3 TM and THM coupling parameters in argillites

In porous-media mechanics the key parameters characterising TM and THM couplings are:

- the drained linear thermal dilatation coefficient \( \alpha_0 \)
- the differential thermal dilatation coefficient \( \alpha_m \)
- hydro-mechanical coupling parameters: Biot coefficient (b) and Biot modulus (M).

The pseudo-undrained thermal-dilatation coefficients were measured by an automatic dilatometer
(Homand, 1998) and with a heating-bath system (Antéa, 2001). The measurements indicate that:

- The thermal-dilatation coefficient under pseudo-undrained conditions ranges between:
  - 0.8 and 1.2 \( \times 10^{-5} \) K\(^{-1}\) in a direction parallel to the stratification
  - 1.2 and 1.9 \( \times 10^{-5} \) K\(^{-1}\) in a direction perpendicular to the stratification

- The thermal dilatation of the rock is linear up to 90°C. Above that temperature significant
  non-linear behaviour appears and may induce shrink of the material 100 and 130°C

- Desaturation seems to increase the thermal-dilatation coefficient, but exceptions exist.

Reference values under pseudo-undrained conditions:

Average linear thermal-dilatation coefficient:
isotropy hypothesis: $\alpha_{\text{average}} = 1.28 \cdot 10^{-5}$ K$^{-1}$; anisotropy hypothesis: $\alpha_\parallel = 1.0 \cdot 10^{-5}$ K$^{-1}$; $\alpha_\perp = 1.55 \cdot 10^{-5}$ K$^{-1}$.

The differential thermal-dilatation coefficient, $\alpha_m$, also called “the isochoric drained thermal fluid mass contribution coefficient” was deduced from a theoretical model:

$$\alpha_m = (b-\Phi) \alpha_0 + \Phi \alpha_\text{fl} = 1.95 \cdot 10^{-5}$$ K$^{-1}$

where Biot coefficient $b = 0.6$, the porosity $\Phi = 15\%$, the linear thermal-dilation coefficient of water $\alpha_\text{fl} = 1.0 \cdot 10^{-4}$ K$^{-1}$ and the drained thermal-dilation coefficient $\alpha_0 = 1 \cdot 10^{-5}$ K$^{-1}$ (hypothesis).

Obviously, uncertainties on $b$, $\Phi$ and $\alpha_0$ may lead to uncertainty on $\alpha_m$.

6.3 In-situ THM characterisation

6.3.1 Thermal disturbance during the REP experiment

The REP experiment is a vertical mine-by test equipped with hydromechanical sensors (Armand 2006). Pore pressure measurements are associated with a temperature recording in the same chamber of the instrumented borehole. During the lining of this zone (concrete pouring), the concrete curing created a temperature increase at the shaft rock wall face and the thermal effect has been observed in the rock mass on the temperature, the pore pressure and deformation sensors.

The temperature profile around REP is given in Figure 6.7. It can be shown that the temperature diffusion around the shaft is nearly isotropic and not affected by stress anisotropy. The thermal conductivity is isotropic in the bedding plane (close to horizontal).

Figure 6.8 gives the overpressure created by the temperature increase during the curing phase of the lining (and the reverse effect during the cooling phase). The coefficient of the pore pressure variation with temperature ranges from 0.225 MPa/°C to 0.29 MPa/°C.

![Figure 6.7: Maximum temperature variation observed versus distance from the shaft wall](image)
6.3.2 TER experiment (heating experiment)

The main objective of the heating experiment (TER) is to determine the thermal properties of argillites in its natural state. The second objective of the heating test is to provide the first knowledge on in-situ THM processes in saturated argillites. The scientific program includes also sample testing to compare the results at different scales. The thermal effect on the damaged zone is studied in this experiment by measuring the permeability before and after the thermal loading.

The TER experiment is located at the main level of URL (490m deep) at the corner of two galleries (Figure 6.9) (similar to the HE-D design). The heated area is located approximately 6 m far from the wall of the GEX drift in order to avoid the damaged or desaturated zone around this GEX drift. The pore pressure is measured around the heating borehole between 0.5 m and 1.5 m. Both the pore pressure and the temperature can be monitored in each chamber. The chambers also offer the possibility to connect a hydraulic system to carry out some pulse tests in it (permeability characterization).

Three boreholes are dedicated to monitor the temperature around the heater in 3 directions (normal, parallel, and at 45° of the bedding plane). They are 0.6 m to 1.8 m far from the heater (Figure 6.9). The test lasted more than 205 days.

Figure 6.8: Pressure and temperature variation at a distance between 2.1 and 4.1 from the shaft wall

Evolution over time of overpressures throughout the heating and cooling phases is given in Figure 6.10, that of deformation is in Figure 6.11.

The two pore pressure peaks recorded on sensor TER1401 suggest a partly-drained response of the...
argillite. Even after a 200-day cooling period, the pore pressures did not resume their initial state before the heating phase. The other sensors show a continual increase of pore pressures with temperature, thus indicating that, due to their position, thermo-consolidation is not sufficient to absorb the pressure increase by thermal expansion.

Figure 6.10: Evolution over time of pore overpressures generated during the heating phase

Figure 6.11: Evolution over time of the measurements recorded manually on extensometer TER1301, compared to automatic measurements in borehole TER1302

6.4 Related chemical aspects

Callovo-Oxfordian argillites contain interstratified illite/smectite clay minerals: R1-type at the base of the formation and R0 type in the upper half. The smectitic portion is likely to be modified due to the rise in temperature. Two complementary approaches, experimentation and modelling, were used to identify and quantify possible mineralogical transformations.

Experiments conducted on pure poles of smectite confirm the data mentioned in the literature for temperatures in the order of 300 °C. However, analyses supplementing X-ray diffraction (chemical, microprobe, etc.) show that part of the closed flakes resulting from those experiments corresponds only to dehydration and not to an irreversible chemical transformation of those flakes. As soon as
temperatures are below 120 °C, smectites remain stable. Only interlayer sites are affected by cation exchanges and it is possible to detect a change in the location of the charge within smectites in relation with the temperature.

All detected transformations depend highly on the physico-chemical parameters concerned. Besides temperature, it is necessary to take into account the initial chemical composition of the smectite, the chemical composition of the fluid and the liquid/solid ratio.

Similarly, it seems that the presence of organic matter may play a role in the kinetics of the transformations of clay materials (Michel, 2006). In fact, a physical phenomenon of preferential adsorption of the organic matter on the clay surfaces appears during the pyrolysis experiments in a confined environment under increasing temperatures (200 to 365 °C). X-ray diffraction suggests that the presence of organic matter would tend to slow down the mineralogical transformation of clays.

Callovo-Oxfordian clays remain very stable at temperatures close to 200 °C, provided that the particles are larger than 40 µm in diameter and that the liquid/solid ratio decreases, even though it remains higher than those in the natural environment.

It may therefore be possible to conclude that the mineralogical transformations of Callovo-Oxfordian interstratified clay minerals due to a radwaste repository will be minor because the argillite water content is lower than 10 % and the temperature will always be below 100 °C in the argillite, what is much below the 200 °C of the experiment.

It is impossible for increasing the argillite temperature from 25 to 80 °C to result in a phenomenon of illitisation without any additional source of potassium. Over the temperature spectrum under investigation, the only constitutive potassium-bearing phase of the argillite is oversaturated and is consequently unable to constitute the required source of potassium for the illitisation process to occur.

6.5 THM modelling

Accompanying the conception and the result analysis of THM in-situ experiments, different kinds of modelling have been carried out on the Callovo-Oxfordian argillites.

6.5.1 Numerical modelling of the REP experiment

Two thermo-mechanical models (a 2D strain plane and a 2D axisymmetric model) have been performed in order to study the TM responses of the host rock during the pouring of liner. The modelling considers thermo-elasticity without taking into account THM coupling. The corresponding parameters are:

- Young modulus: \( E = 9000 \) MPa (from in-situ dilatometer tests)
- Poisson coefficient: \( \nu = 0.3 \)
- linear thermal expansion (assumed isotropic): \( \alpha = 1.28 \times 10^{-5} \) K\(^{-1}\)
- thermal conductivity: \( \lambda_{//} = 2.2 \) W/m/K (in the horizontal plane) and \( \lambda_{\perp} = 1.6 \) W/m/K
- heat capacity: \( C_p = 935 \) J/kg/K

To simplify the model, the boundary condition imposed on the rock wall is the temperature history measured inside the lining (Figure 6.12) without taking into account the concrete.

The temperature evolution at different distances obtained by the two models are depicted on Figure 6.13. It can be observed that the results are very similar (the differences are less than 0.1 °C).

The temperature evolution at different distances from the shaft wall is well predicted by the modelling, but amplitudes of the temperature peak are overestimated due to the used simplified
boundary condition. There is a temperature gradient across the lining. Because of this, the temperature at the rock wall face is smaller than in the concrete.

These models highlight the fact that the pouring of the rings of concrete between 459 and 465 m depth in the shaft does not significantly affect the temperature profile at 467 m (Armand, 2006). This confirms that the horizontal thermal conductivity of argillite is rather predominant.

This elastic model is unable to reproduce the strains observed in the shaft. The displacements observed with extensometers indicate the time-related behaviour of the rock mass around the shaft. A full coupled THM numerical modelling considering the variation of the permeability at the vicinity of the shaft wall reveals to be of interest.

![Temperature history measured inside the concrete lining of the shaft](image1.png)

**Figure 6.12:** Temperature history measured inside the concrete lining of the shaft

![Comparison of temperature evolution calculated by both models (depth -467 m)](image2.png)

**Figure 6.13:** Comparison of temperature evolution calculated by both models (depth -467 m)

### 6.5.2 Numerical modelling of the TER experiment

#### 6.5.2.1 Thermal analysis

The experiment was conducted by two numerical models. The first one was entrusted to CEA, the
Direct thermal modelling by CEA

The thermal analysis is conducted by using the heat equation (Fourier’s law) in transient regime. A 3-D model was considered in order to simulate the overall test with a side extension in the order of 20 m. Eleven materials are covered in the calculations. All materials contained in the heating probe are assumed isotropic. For the argillites, the selected parameters are:

- specific heat of the saturated rock: \( C_p = 1,000 \text{ J·kg}^{-1}·\text{K}^{-1} \)
- anisotropic thermal conductivity: three cases around the parameters measured on samples
  - case 1, \( \lambda_{//} = 2.2 \text{ W·m}^{-1}·\text{K}^{-1}; \lambda_{\perp} = 1.48 \text{ W·m}^{-1}·\text{K}^{-1} \)
  - case 2, \( \lambda_{//} = 1.9 \text{ W·m}^{-1}·\text{K}^{-1}; \lambda_{\perp} = 1.3 \text{ W·m}^{-1}·\text{K}^{-1} \) (reference parameters)
  - case 3, \( \lambda_{//} = 2.0 \text{ W·m}^{-1}·\text{K}^{-1}; \lambda_{\perp} = 1.25 \text{ W·m}^{-1}·\text{K}^{-1} \)

The overall results show that the 3-D thermal model reproduces satisfactorily the test and that the thermal-diffusion process is well understood. However, the comparison between the different cases indicated that it is difficult to detect the best set of parameters from the three cases studied.

Determination of thermal parameters by inverse modelling by UPC

The purpose of inverse modelling is to estimate the specific heat \( C_p \) of the rock, as well as the thermal-conductivity parameter \( \lambda \), which is, based on the basis of the temperature field measured in-situ, considered to be isotropic.

The resolved equation is the one for energy-conservation. A single phase is considered as an equivalent porous medium. Thermal conductivity and specific heat are considered to be constant. Their value is the result of inverse modelling.

The principle of the back analysis is to minimise the error between measurements and calculation results, by repeating the calculations for different pairs of thermal-conductivity and specific-heat values. The error is calculated as follows:

\[
\varepsilon = \frac{1}{n_{MP}} \sum_{i=1}^{n_{MP}} \left( \sum_{j=1}^{n_{t}} \left( T_{\text{real}}(j) - T_{\text{sim}}(j) \right)^2 \cdot \frac{\Delta t(j)}{t_{\text{heat}}} \right)
\]

where:
- \( T_{\text{real}}(j) \) represents the temperature measurements achieved in-situ
- \( T_{\text{sim}}(j) \), the calculation results during the corresponding time, \( j \)
- \( \Delta t(j) \), the time interval between two temperature measurements
- \( t_{\text{heat}} \), the time during which measurements are analysed (47 days)
- \( n_t \), the number of time intervals involved
- \( n_{MP} \), the number of comparison points, i.e., the number of temperature sensors.

Two kinds of modelling are performed: an axisymmetric modelling in which the medium is assumed isotropic and a 3D modelling in which the medium is anisotropic.

In the first case, the heating element is not explicitly discretised. Heating is simulated by an applied flux on the borehole wall. A total of 110 variations of axisymmetric calculations were performed for thermal-conductivity values ranging from 1.2 to 2 W·m\(^{-1}\)·K\(^{-1}\) and for specific-heat values ranging from 800 to 1,200 J·kg\(^{-1}\)·K\(^{-1}\). The error, calculated over all temperature sensors, is shown in Figure 6.14. The minimum error is obtained with \( \lambda = 1.75 \text{ W·m}^{-1}·\text{K}^{-1} \) and \( C_p = 1,005 \text{ J·kg}^{-1}·\text{K}^{-1} \). The
quasi-verticality of iso-error lines shows a high dependency of the thermal field to the thermal conductivity and a low dependency to the specific heat.

Figure 6.15 provides a comparison between measurements and simulations related to the direction. The axisymmetric modelling underestimates the temperature in the direction parallel to the bedding and overestimates it in the vertical direction. The anisotropy of thermal conductivity is put in evidence.

![Figure 6.14: Axisymmetric thermal calculations: error map generated on the basis of axisymmetric thermal calculations by varying thermal conductivity and specific heat](image)

**Figure 6.14:** Axisymmetric thermal calculations: error map generated on the basis of axisymmetric thermal calculations by varying thermal conductivity and specific heat

![Figure 6.15: Axisymmetric thermal calculations: Comparison between measured and calculated temperatures in directions parallel and perpendicular to the bedding](image)

**Figure 6.15:** Axisymmetric thermal calculations: Comparison between measured and calculated temperatures in directions parallel and perpendicular to the bedding

The purpose of 3-D thermal analysis is to estimate both thermal-conductivity parameters of argillites, \( \lambda_\perp \) and \( \lambda_\parallel \), (\( \lambda_\perp \) the vertical thermal conductivity, \( \lambda_\parallel \), the horizontal one). The estimated value of the specific heat by the axisymmetrical analysis (\( C_p = 1,005 \text{ J·kg}^{-1}·\text{K}^{-1} \)) is used for those calculations.

A total of 315 calculations were performed. The resulting error map is shown in Figure 6.16. The minimum error corresponds to the values of 2 W·m\(^{-1}·\text{K}^{-1}\) and 1.3 W·m\(^{-1}·\text{K}^{-1}\) for \( \lambda_\parallel \) and \( \lambda_\perp \), respectively. Those values are close to the values measured on samples (1.9 and 1.3 W/m/K parallel and perpendicular to the bedding, respectively).
6.5.2.2 Thermo-hydro-mechanical coupling analysis

The inverse THM-coupling analysis was performed by UPC using the Code_Bright to understand the evolution of the pore pressures and the deformation during heating and cooling.

The method used estimates the permeability and thermal expansion of the porous medium by performing an inverse analysis of the pore pressure and deformation fields. It should be noted that those parameters have a direct impact on the pore pressures and deformations of a porous medium during the heating process.

Resolved equations and parameters taken into consideration for the argillite

A linear elastic law was considered for the argillite. The modelling used the reference parameters except the value of the thermal conductivity \( \lambda_{\text{mean}} = 1.75 \, \text{W/m/K} \) which was taken from the above mentioned inverse isotropic model. The purpose is to minimise the error between the measured pressure and deformation fields and those resulting from the THM calculations. Different calculations are performed by considering a pair of intrinsic permeability and thermal expansion values for each of them. The error is calculated by replacing the temperature \( T \) in Equation 6.1 by the pore pressure \( p_w \) for the hydraulic field and by the deformation standard \( \varepsilon \) for the kinematic field. The values used for the intrinsic permeability range from \( 10^{-21} \) to \( 10^{-18} \, \text{m}^2 \). The linear thermal expansion varies from \( 10^{-8} \) to \( 10^{-4} \, ^\circ\text{C}^{-1} \). The values for the thermal expansion of the solid grain and the skeleton are considered to be equal, assuming that the heating process does not induce any structural alteration.

The temperature field has already been described above and is not affected by the interstitial-pressure and deformation fields.

An axisymmetric model was used and the heating element is not explicitly discretised. Heating is simulated by applying the heat flux as in the experiment (277 and 925 W during phases 1 and 2, respectively).

A total of 1,320 calculations were performed. The error representation for each of those calculations for the pore pressure and the deformation fields is shown in Figure 6.17(a) and (b), respectively.
The error is dissociated from the coefficient for linear thermal expansion, when the latter is lower than 10^{-5} °C^{-1} and becomes negligible in comparison to the coefficient for the thermal expansion of water (1.13 \times 10^{-4} °C^{-1}). Consequently, the pore pressure is mainly controlled through the intrinsic permeability of the argillite. In that case, the deformation mechanism of the medium follows the principle of effective stress.

The error concerning the deformation field increases rapidly with the linear thermal expansion of the solid, when this latter one exceeds 10^{-4.7} °C^{-1}. This means that the deformation field appears to be controlled more and more by the thermal expansion coefficient of the solid.

As the permeability of the argillite increases, the error concerning the pore pressure becomes more stable, which seems to be logical since no pore pressure is generated once a certain permeability level has been reached. On the contrary, when the permeability decreases, both the induced pore pressures and the error increase.

The \textit{de minimis} zone of the error map for pore pressures (\(k_w = 10^{-19.5} \text{ m}^2\)) is offset compared to the error map for deformations (\(k_w = 10^{-19.75} \text{ m}^2\)). It is possible to grant a higher level of confidence to the former than to the latter, since deformations evolve within a range of very low values that are close to the measuring capacity of the instruments being used.

Comparisons between the measurements and calculations carried out with three different sets of parameters taken in the \textit{de minimis} zone of the error map for pore pressures (Table 6.2) are given in Figure 6.18 (pore pressure) and Figure 6.19 (strain).

| Table 6.2: Variations in THM-calculation parameters and associated errors |
|---|---|---|---|---|---|
| | \(k_w [\text{m}^2]\) | \(-\log (k_w)\) | \(\alpha_T [\text{K}^{-1}]\) | \(-\log (\alpha_T)\) | \(\epsilon \text{ (pressure)}\) | \(\epsilon \text{ (deformation)}\) |
| THM-I.2.A | 2.8.10^{-20} | 19.55 | 1.10^{-7} | 7 | 0.113 | 8.9.10^{-4} |
| THM-I.2.B | 3.16.10^{-20} | 19.5 | 5.10^{-6} | 5.3 | 0.131 | 8.9.10^{-4} |
| THM-I.2.C | 4.46.10^{-20} | 19.35 | 2.10^{-5} | 4.7 | 0.166 | 11.10^{-4} |

The intrinsic permeability assessed by this method (2.8 to 4.5.10^{-20} \text{ m}^2) is very close to the one measured in situ (5.10^{-21} to 5.10^{-20} \text{ m}^2). THM-I.2.A corresponds to the area where the thermal-expansion coefficient is very low in comparison to that of water, THM-I.2.B to the area where the
error is minimised on both the pore pressure and deformation map (area consistent with reference values). THM-I.2.C corresponds to a thermal expansion coefficient of 2.10^{-5} °C^{-1}, which is the upper limit of the experimental data.

Figure 6.18: Comparison between the tree results of modelling and measured pore pressures

In general, it should be noted that the three cases give very close results. The pore pressure is overestimated for chamber TER1401 and underestimated for chamber TER1404. That observation could be correlated with a small anisotropy in the permeability of the argillite, although it was not detected by hydraulic tests in boreholes. Simulations suggest that the pore pressures, at the end of the cooling period, do not resume their initial state prior to heating. The behaviour of sensor TER1405 during cooling is unexplained.

For some measurement intervals, intervals 1 to 4, intervals 5 to 8, for example, the simulation results are quite inconsistent with respect to the measurements. This is obviously due to the convergence of the drifts delineating the TER zone.

With regard to intervals 9 to 12, the slope inversion between phases 1 and 2 and the compression-extension cycle associated with the heating-cooling period is well reproduced by modelling.
However, the initial extension phase as measured \textit{in situ} for intervals 8 to 10 does not exist in the numerical simulations. It is therefore possible to assume that measurements are incorrect due to their low value.

It is important to note that the deformation mechanism of the porous medium in simulation A (THM-I.2.A) is only associated with the pore pressure development. The very good reproduction of measurements for a negligible value of the solid thermal expansion, except in interval 12, seems to indicate that the actual value of the thermal expansion coefficient is close to the inflection point of the valley of the error map of the pressure field (Figure 6.17a), i.e. the moment when the solid thermal expansion starts to have an impact.

At the opposite, the simulation C (THM-I.2.C) results for the intervals located close to the heating probe suggest that the value of the solid thermal expansion coefficient is too high: those high values would have been reproduced by measurements, the precision of which keeps improving for more significant deformations.

Simulation B (THM-I.2.B) results fit best to \textit{in-situ} data and seems to provide the best estimate in terms of error on pore pressures and deformations.
6.6 Discussion

6.6.1 Uncertainty
On THM behaviour

In generally, large uncertainty exists on the THM coupling parameters that control the temperature overpressure, especially the thermal expansion coefficients \( \alpha \), and differential thermal expansion coefficient of \( \alpha_m \). Secondly, large uncertainty remains on the thermal effect on the damage and rupture thresholds. Finally, the temperature effect on the creep rate need more investigation.

On confinement properties

Following aspects seem need to be more understood:

The influence of temperature on sorption equilibrium: argilitte and swelling clay reactivity with temperature (\( T < 120^\circ C \))

Thermodynamic data acquisition (e.g. the equilibrium constants for solids) and kinetic data (e.g. the dissolution/precipitation kinetic constants) for the clay minerals at temperatures below 120°

Relationship between temperature and effective diffusion coefficients: empirical for anions from some scarce data must be better understood. Experimental approach has to be developed for cations.

6.6.2 R & D programme 2007-2010

Following R & D programme is established for following three years:

Observations and measures of the thermal fissuring at a microscopic scale

Theoretical developments of the THM behaviour using a micro-macro approach

THM load tests on samples allowing reducing the uncertainties on the THM coupling parameters

Experimental characterization of the thermal load impact on damage and failure criteria

New long term load tests on samples under thermal and mechanical paths close to those around cells and drifts for assessing the temperature impact on argillites deformations

A summary characterization of the THM behaviour beyond the functioning domain of the disposal (between 90°C and 120°C)
7 Conclusions

The present state-of-the-art report gives a general view on the THMC behaviour of three potential radwaste repository host formations: Boom Clay, Opalinus Clay and Callovo-Oxfordian Argillite. The state of the art in the field of THM is mostly related to the laboratory characterization, in-situ investigation and modelling of selected THM related in-situ tests. The main feature of the THM behaviour for each host rock, the range of the most important THM parameters, the in-situ observations are presented. The accompanied uncertainty is highlighted and analysed. The modelling results of the selected in-situ tests are included. The capacity, the limitation of the developed/applied models are discussed. The associated future developments on the constitutive models are thus underlined.

Consequently, this state of the art allows to

- delineate the most important temperature-dependent material properties
- define the most important coupled processes and parameters
- assess the effect of discrete fractures and fracture connectivity on the effective hydraulic properties and to determine the importance of chemical impact
- derive/evaluate the most appropriate conceptual models and numerical codes as well as to notice the remaining uncertainties on the THM properties of the clays

Various laboratory experiments have been performed by GRS on both Callovo-Oxfordian argillites and Opalinus Clay, including thermal expansion, pore pressure, swelling pressure and long term deformation, strength, self-sealing as well as the THM processes, which allow a comparison on the THM characteristics of these two materials. Detailed results are given in technical annex 3.

The state of the art in geochemistry is mainly related to the experimental and modelling researches on the mineralogy transformation, reactivity of the clays as well as the geochemical disturbance in the nearfield of the disposal system. Especially the temperature related geochemistry perturbation is analysed in detail.

In summary, the state of the art shall give important information and a database to all TIMODAZ partners to continue the related research in TIMODAZ project.
8 References

8.1 References for Boom Clay


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References for Opalinus Clay


8.3 References for the Callovo-Oxfordian Clay


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9 Appendix

- Technical annex 1 : detail version of D2
- Technical annex 2 :
  - Scoping calculations by ULg
  - Scoping calculation by CIMNE
- Technical annex 3 :
  - GRS contribution, Laboratory experiments on the THM behaviour of clay rocks

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