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Full-Scale Engineered Barriers Experiment for a Deep Geological Repository for High-Level Waste in Crystalline Host Rock – Phase II

FEBEX II

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EXECUTIVE SUMMARY

General

FEBEX (“Full-Scale Engineering Barrier Experiment in Crystalline Host Rock”) is an international research project led by ENRESA, with financial support from the European Commission. FEBEX consists of an “in situ” full-scale test performed under natural conditions; a “mock-up” test, at almost full scale; and a series of laboratory tests, as well as modelling work (Figure 1).

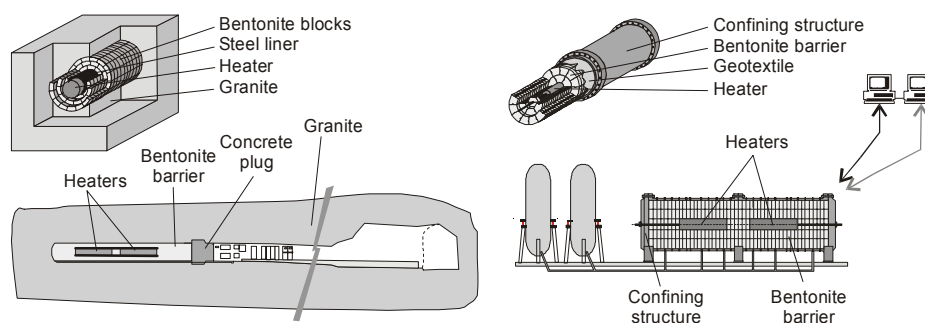


Figure 1: FEBEX “in situ” test (left) and “mock-up” test (right)

The aim of the project is to study the behaviour of the near field components for a high level radioactive waste repository in crystalline rock. The following three objectives were established:

- First:** Demonstration of the feasibility of handling and constructing an engineered barriers system.
- Second:** Study of the thermo-hydro-mechanical (THM) processes in the near field.
- Third:** Study of the thermo-hydro-geochemical (THG) processes in the near field.

The experiment is based on the Spanish reference concept for the disposal of radioactive wastes in crystalline rock (AGP Granito), in which the canisters enclosing the conditioned wastes are placed horizontally in drifts and surrounded by a clay barrier constructed of highly-compacted bentonite blocks.

The project was initially scheduled for a period of seven years (1994 to 2001). During the period 1996 to 1999 the project (phase 1) was co-funded by the European Commission as part of the 4th Euratom framework programme (1994-98) and a final report was produced, EUR 19147, 2000 [1]. However, in view of the conclusions drawn from integral analysis more than two years after the initiation of heating, the decision was taken to extend the experiment by two or three more years and to dismantle only heater No.1 of the “in situ” test, allowing the experiment to continue. The extension of the experiment is known as FEBEX II and began in September 2000.

The partial dismantling has already been carried out in the “in situ” test after five years of heating, heater No 1 has been removed and the other left in place for a continued hydration and heating phase. The materials recovered (bentonite, metals, instruments ...) have been analysed to investigate the different types of processes undergone. THM and THG model capabilities have been further developed and partially validated.

The second heater of the “in situ” test, as well as the "mock-up" test, will continue within the frame of the EU Integrated Project NF-PRO (contract FI6W-CT-2003-02389) for a period, which will depend on the behaviour of the heating and instrumentation systems. This will also provide the possibility of carrying out a retrievability exercise in the future.

“In situ” test

The operation of FEBEX II has been divided into an initial phase (from September 2000 to July 2002), this being a continuation of FEBEX I, and a second starting on the latter date, determined by completion of the dismantling of heater No. 1 and sealing of the remaining part of the test.

The following activities were carried out during the first operational phase: supervision, control and management of heating data, gas sampling and analysis, measurement of permeability to water in the clay barrier and hydraulic testing in the rock.

The work on dismantling of heater No. 1 included the following: design of the dismantling process, dismantling and sampling operation, construction of the new closure plug and additional instrumentation of the test area not dismantled.

The work performed during the second operational phase has been similar to that carried out during the first: supervision and management of heating data, gas and bentonite pore water sampling and analysis, and hydraulic testing in the rock.

The dismantling included a large number of “in situ” determinations of the humidity and dry density of the bentonite; furthermore, various laboratory characterisation tests were performed on the numerous samples extracted, with a view to analysing possible changes in the thermo-hydro-mechanical and geochemical properties of the bentonite that might have occurred during the experiment.

A multidisciplinary team studied the potential EDZ and its evolution following a 5-year heating period through “in situ” and laboratory tests.

Samples of various metallic parts (heater, steel liner, etc.) were also taken during dismantling, and the coupons of different materials that had been embedded in the clay barrier during installation were recovered, with a view to studying the corrosion caused by the effect of heating and hydration.

The measuring instruments (for temperature, humidity, pressure, etc.) were retrieved during dismantling and sent to different laboratories for analysis, the aim being to gain insight into their state following several years of operation and determine the reliability of the data obtained during the initial phase of operation.

“Mock-up” test

The objective mapped out for the “mock-up” in FEBEX II was simply a continuation of the operational phase initiated in FEBEX I in February 1997, as a result of which the activities scheduled have been supervision, control and management of the data arising from the process of heating and hydration.

However, during the first analyses performed for FEBEX II, an unexpected deviation was observed between certain of the “mock-up” monitoring data and the results of modelling, as from 700 or 800 days of the start of heating. This made it necessary to revise the hydration system in order to find out whether the cause of this deviation was incorrect operation of the experiment. The revision demonstrated that the experimental facility operated correctly.

Towards the end of November 2000, the erroneous performance of a heater power control function caused a major increase in power for a period of three days, during which the temperature increased to 240 °C in contact with the bentonite. The defect was corrected and the experiment continued normally, without any irreversible anomalies having been observed in the properties of the bentonite.

Laboratory tests

Laboratory tests have been carried out to determine parameters and thermo-hydro-mechanical, thermo-hydro-geochemical and gas generation behaviour.

A series of thermo-hydro-mechanical tests were carried out in continuation of the programme initiated in FEBEX I: oedometric tests with controlled suction, infiltration tests and the determination of retention curves at constant volume for different densities. In addition, a programme of new tests was also performed: temperature effects on the retention curves under conditions of confinement and without confinement, on swelling pressure, on hydraulic conductivity and on consolidation and swelling deformations; new porosimetry methods; swelling deformation of the clay saturated with different types of water (distilled, granitic and saline with various salts and concentrations) and various dry densities. Tests not initially foreseen in the FEBEX II programme were also performed, with a view to attempting to understand the aforementioned deviations between the “mock-up” data and modelling results: tests on permeability, infiltration with and without a thermal gradient, analysis of the repercussion on the results of the high hydraulic gradients applied in the tests to determine hydraulic conductivity and oedometric tests with controlled suction and temperature.

Basically, the thermo-hydro-geochemical test programme has been a continuation of the work initiated in FEBEX I: study of the pore water in the bentonite barrier, geochemical processes taking place at the bentonite/aqueous solution interface and processes of sorption and transport of radionuclides in the bentonite.

The FEBEX II laboratory tests on gas generation are also a continuation in keeping with the results obtained during FEBEX I.

Modelling

Three types of modelling have been performed during FEBEX II: THM and THG modelling of the clay barrier and THM modelling of the rock.

The THM modelling activities centred basically on critical analysis of the evolution of the two large-scale tests. As regards the “mock-up”, the analyses carried out were as follows: updating of the calculation and comparison with the monitoring data (almost 7 years of data); specific analysis of the difference between the monitored and computed data; and analysis of the overheating episode. For the “in situ” test, the activities included updating of the contrast between the experimental data and the modelling predictions and simulation of processes of cooling (due to the disconnection of heater No. 1), excavation and dismantling. Major efforts were made also in the experimental validation of the constitutive laws adopted in the modelling of the thermal, hydraulic and mechanical problem.

THG modelling included the following: improvement to the THG codes; improvement to the conceptual models; laboratory test modelling for checking of the models; “mock-up” modelling for contrasting the thermal and hydrodynamic predictions with the monitoring data and analysis of the deviations, and modelling of the “in situ” test and comparison of the predictions with the geochemical data obtained from the dismantling tests.

In order to study the potential damage to the rock due to the effects of excavation of the FEBEX gallery and the experiment, the stress states were calculated by means of various models for comparison with the strength of the Grimsel granite.

Results and conclusions

The most relevant results and conclusions are as follows, described schematically:

- 1) During the dismantling of heater No 1 it was observed that the installation gaps in the bentonite barrier had been completely closed and that hydration had progressed very homogeneously from the periphery inwards.
- 2) 80% of the instruments in the “in situ” test and 90% of those corresponding to the “mock-up” continue to be operational after more than 5 years since they were installed. The laboratory

analysis of those retrieved during partial dismantling of the “in situ” test indicates that the instruments still operate correctly without any loss of accuracy.

- 3) No varying trend is noticed in the THM and THG properties of the bentonite as a result of the effects of heating and hydration over more than 5 years.
- 4) There has been no modification in the original hydraulic properties of the rock as a result of either the excavation or the experiment.
- 5) Both the laboratory and “in situ” tests indicate that, to all practical intents and purposes, there is no EDZ in the FEBEX gallery.
- 6) The database on the THM properties of the FEBEX bentonite has been completed during FEBEX II and includes the effects of temperature and water type on these properties. For example, permeability has been seen to increase and retention capacity to decrease with increasing temperature and swelling capacity has been seen to decrease with increasing water salinity. In addition, a study has been made of the microstructure and its evolution as a basis for validation of the HM constitutive law.
- 7) Major progress has been made in chemical determination of the pore water and as regards the properties of sorption and transport of radionuclides.
- 8) The gas generation analyses confirm that CO₂ is by far the most abundant gas.
- 9) The THM modelling reflects the processes taking place fairly well. A detailed investigation has been made of various possible causes for the deviation between the “mock-up” monitoring data and those corresponding to modelling, including the modification of the HM constitutive model. The double porosity model is the one that best fits with the data. However, the difference in the relative humidity trend persists, particularly in the zone of highest humidity, for which reason there would appear to be a need for the research to continue, unless it is demonstrated that this difference is irrelevant from point of view of safety.
- 10) Development of the THG model has continued and, in addition to contrasting its predictions with laboratory tests, it has been possible to do this also with the results of laboratory tests performed on samples obtained during dismantling. This comparison indicates that the predictions reflect the trend of most of the chemical species, the concentration of which is greatest close to the heater and decreases with radial distance towards the periphery.
- 11) The THM modelling of the rock shows that the stresses are far lower than the resistance of the rock, for which reason it has not been damaged by either the excavation or the experiment.

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1 OBJECTIVES

Basically, the objectives of FEBEX II are a continuation of those established for FEBEX I: demonstration of the feasibility of handling and constructing a system of engineered barriers (EBS) and study of the thermo-hydro-mechanical (THM) and thermo-hydro-geochemical (THG) processes in the near field.

The objective of the demonstration, which was to be complemented with the dismantling of the “in situ” test – with observation of the state of the clay barrier and of the measuring instruments – is accomplished in FEBEX II with partial dismantling of the area of heater No. 1.

The fundamental objective of FEBEX II, however, sprang from analysis of FEBEX I, after two years of heating, when the measuring instruments and heating system were seen to have functioned well in the two large-scale tests. This analysis led to the conclusion that the THM and THG numerical models promised high expectations, inasmuch as sufficient confidence in their capacity to predict behaviour in the near field might be forthcoming. In order to achieve such confidence, it was necessary to continue theoretical development of the models and to carry out new laboratory tests to obtain parameters and validate the constitutive laws. It was considered particularly important to extend the period of experimentation in order to achieve more advanced states of hydration. For this reason the experiment with FEBEX II is not considered to be complete; rather the strategy is to extend it as much as possible over time, depending on the performance of the experimental system.

Two further studies were also added: one on a potential EDZ in the FEBEX gallery and its evolution throughout the experiment, and the second on modification of the original hydraulic properties of the rock in the near field.

2 “IN SITU” TEST

2.1 Continued operational phase

The FEBEX operational phase continued from September 2000 (start-up of the FEBEXII project) until the start of the second operational phase in July 2002, just after the performance of the partial dismantling operation (Figure 2). It comprised heating and supervision and data management of the “in situ test”, gas sampling and water permeability measurements, and the hydraulic tests in rock.

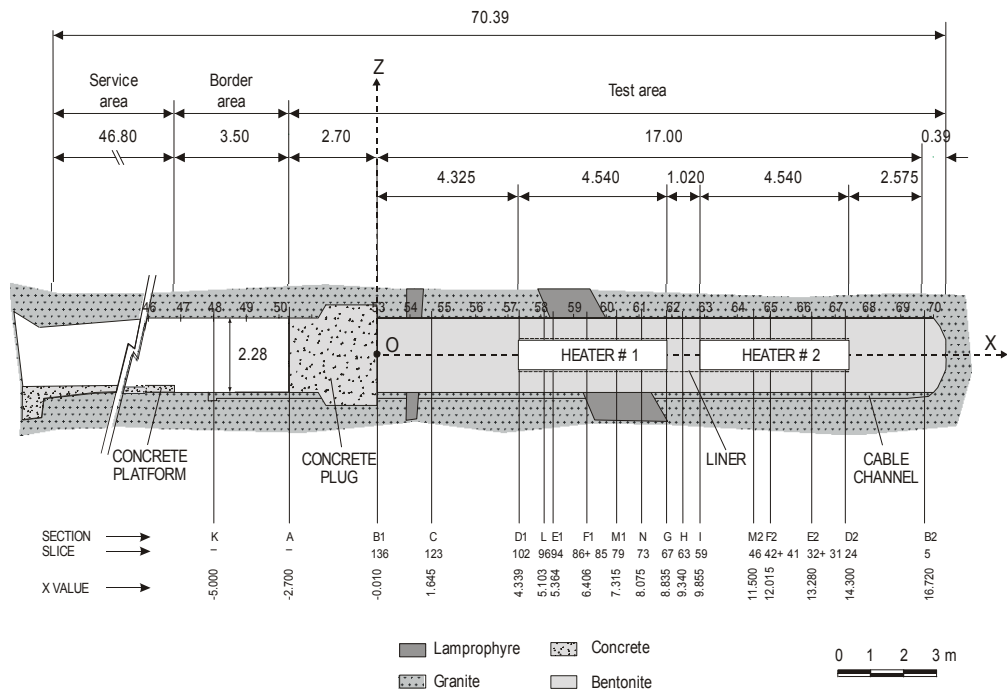


Figure 2: "In situ" test, initial configuration

2.1.1 Supervision & data management

Quarterly data reports were produced describing in detail the evolution of the experiment. The main observations during this continued operational phase were a constant, gradual increase of the applied power in both heaters, as well as a gradual increase of temperature in the buffer and rock. Humidity and total pressure also showed an increasing trend in the buffer. The percentage of operative sensors was over 80 % throughout the entire operational phase.

Heater No. 1 was turned off on 28th February 2002, following 5 years of continuous operation. Heater No 2 was kept working under normal operating conditions during the decommissioning activity and thereafter; the data from all sensors were gathered without interruption.

As planned, the supervision and data management system was improved by installing a more powerful computer at the Remote Monitoring Centre (RMC) in Madrid in late 2000. The computers used for the "in situ" tests monitoring system at GTS were replaced with new ones. At the same time, the web site for the FEBEX "in situ" test was developed within the RMC. It included mimics, graphics and numerical data on the "in situ" test, as well as the data reports and other relevant documents. All this information was made accessible to all the project participants by means of security codes.

2.1.2 Gas sampling & analysis

In situ measurements of gas generation and release in the buffer material around heater No. 1 were carried out during the continuation of the first operational phase. This investigation indicated that the draining pipes located at the gallery wall were already flooded with formation water from the surrounding host rock, the water pressure ranging from 0.2 MPa to 0.4 MPa. The draining pipes located near the heater liner were filled with gas at atmospheric pressure, with concentrations of the order of 8 vol% for carbon dioxide, 0.7 vol% for hydrogen and 0.04 vol% for the hydrocarbons. As the backfill and the gallery plug were not gas-tight, this gas generation did not generate an increase in pressure.

Water permeability measurements of the flooded buffer were performed as pressure recovery tests in the flooded draining pipes. The initial conventional evaluation indicated integral values in the range of 10^{-17} m², with a high skin factor representing a flow obstruction near the pipes. This was interpreted as being

an influence of the unsaturated buffer farther away from the pipes, while the completely saturated bentonite near the pipes had a much lower permeability. The gas permeability of the dry buffer was above 10^{-13} m^2 .

2.1.3 Hydraulic tests in rock

The field testing campaign was carried out from February to May 2001. The programmed tests comprised long term tests (several days), short duration tests (several hours) and pulse type tests. A total number of 62 pressures and 56 temperatures from 19 instrumented boreholes were recorded. A report (deliverable D3) was issued describing the tests carried out and the results obtained (see section 2.3.3).

2.2 **Decommissioning activity**

2.2.1 Activity design

The detailed design and planning of the partial dismantling activity was carried out in close cooperation with all the partners involved. During the planned dismantling activity, samples of different materials (rock, bentonite, concrete, etc) were to be taken for analysis. A document known as the “Sampling Book” (deliverable D4) was drawn up to describe how to perform the designed sampling activity in accordance with the requirements submitted by all the involved partners. This document included a sample identification and control procedure, in order to simplify matters and provide a uniform sample labelling procedure throughout the entire project.

The planning of the excavation involved numerous drillings for sampling. Ideally, undisturbed cores of both saturated bentonite from the outer backfill rings and de-saturated dry bentonite from the inner rings adjacent to the liner should be collected, with core length varying from 5-10 cm to ideally 60 cm. For this purpose, different options in terms of drilling techniques and core bits were developed and tested in wet and dry bentonite, the aim being to come up with a proven successful drilling method prior to the initiation of sampling.

The procedure for demolition of the plug was concluded and the tools for extraction of the heater (modified heater car and new winch) and removal of the buffer (new wagon and other dumping accessories) were designed and constructed within schedule by September 2000.

Also several tasks relating to design of the new plug, made with shotcrete, were performed prior to the start of the activity: a preliminary feasibility study was drawn up and an initial batch of in situ tests at the FEBEX drift was carried out in 2000 to check different shotcreting techniques. A second batch of in situ tests was carried out in 2001 to further tune the emplacement technique and to check the adherence of the concrete foreseen for use to the rock walls. As a result of the works carried out for the new plug design, a document detailing the design of the new plug was produced. The specifications of the plug were also compiled in another document.

In order to achieve the water and gas tightness of the new plug, four “cable connection boxes”, to be filled with resin, were designed and constructed. These would be installed at the rock surface in the area corresponding to the final section of the plug, before it was shotcreted, and the cables coming from the instrumentation in the remaining part of the test would be channelled through them.

The start-up of the decommissioning activity was originally planned for mid May 2001, but it was delayed one year in order to further check some divergences, detected during the period previous to that date, between the THM models and the behaviour of the buffer.

In order to improve the amount of information to be collected during the second operational phase, in July 2002 the decision was taken to install new instrumentation in the buffer. These additional instruments were to be installed before construction of the plug was completed, in instrumented pipes housed in boreholes drilled into the bentonite buffer. Accordingly, the required pipes housing the new instruments

were designed and constructed. It was decided to construct the new plug in two steps, first a 1 metre-long temporary section of plug through which the boreholes for the new instrumentation would be drilled, and then the remaining plug section.

2.2.2 Dismantling & sampling

Once their construction had been completed, the modified heater car and new winch for heater extraction and the new wagon and other dumping accessories for buffer removal were successfully transported, installed and tested at GTS late 2000.

Although the dismantling operation was delayed until 2002, some preliminary tasks were carried out in 2001 in order to avoid time constraints during the dismantling activity itself. These operations consisted of relocating part of the in-drift installations in a new monitoring area, prepared (power supply, lights etc.) at the entrance of the GTS for that purpose. The removal and re-arrangement of all in-drift electrical equipment was carried out from February to May 2001. The achieved objective was to move the computers, the power regulation units and other “big boxes” outside (to the new monitoring area), leaving in place only the sensor interfaces and the connection boxes, these being re-distributed along the drift walls in order to leave sufficient room for the dismantling activity.

The shutdown of heater No. 1, carried out on 28th February 2002, initiated the countdown for the dismantling process. The cooling process during the first two months may be observed in Figure 3.

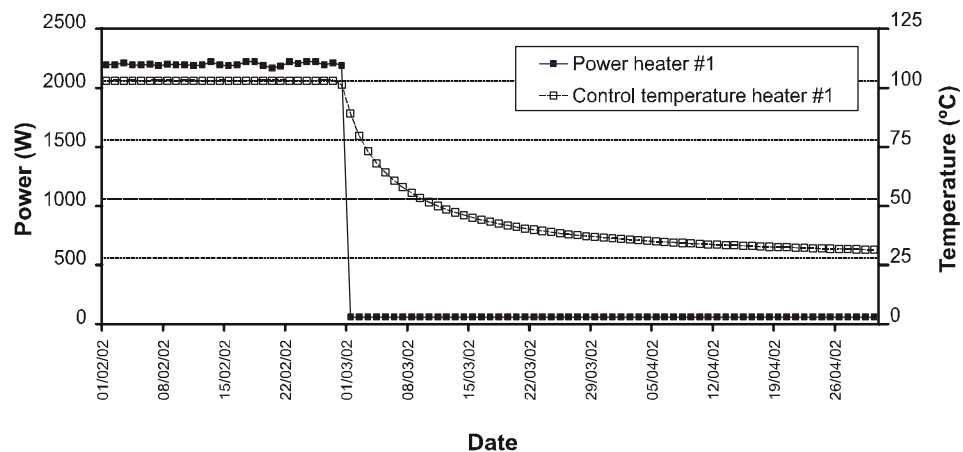


Figure 3: Cooling down of heater No 1

The dismantling works started, as planned, on April 2nd 2002, with rock sampling in the service area. Demolition of the concrete plug started on April 8th and was completed on May 28th. The method used for the demolition was breakage with a hydraulic splitter, which allowed for fast and controlled operation without jeopardising the cables passing through the plug.

The buffer was then removed and sampled, in accordance with the sampling plan, up to the front end of heater No. 1. The heater was extracted on June 19th (Figure 4). The extraction was performed quickly, smoothly and in a controlled manner. The heater was sent to Spain and sampled for corrosion analysis. The dismantling of the bentonite continued to completion on July 17th, and the whole sampling activity finished on July 23rd 2002. The sampling plan was fully accomplished, with a few minor changes introduced in agreement with the organisations involved.



Figure 4: Heater extraction

Before construction of the new plug, a dummy steel cylinder measuring 1 m in length was inserted in the void left by heater No. 1 in the centre of the buffer, and two new total pressure cells and three relative humidity sensors were installed at the bentonite front. A temporary section of the new shotcrete plug, measuring 1 m in length, was finished on July 25th, and new instrumentation for tracking of its position was installed during August.

In order to determine the properties of the temporary section of the plug obtained, the shear strength of the shotcrete/rock interface corresponding to this stage of the plug was tested “in situ”. Additionally, a total of 8 boreholes were drilled in the shotcrete plug after 28 days of hardening. Samples from the extracted cores were analysed to determine the mechanical properties of the shotcrete. Additional samples were tested to obtain hydraulic conductivity. The operations carried out up to that time are described in deliverable D7

From 1st to 7th of April 2003, three new gas injection and collection pipes were installed in the buffer for gas sampling and permeability measurements. The pipes were inserted in boreholes drilled in the buffer parallel to the drift axis, reaching up to 0.7 m beyond the rear part of the heater. Each gas pipe consisted of a 3 metre-long, stainless steel sintered filter measuring 40 mm in diameter that was longitudinally centred with the heater, and another short filter of the same type at the end of the pipe, all joined with tubes of the same diameter, and connected to the valve panel with pressure gauges and flowmeters in the open gallery. The panel was installed in September 2003 for gas extraction and injection. The entire system was tested and the pressure gauges were calibrated. Pressure data were recorded by a Data Acquisition System (DAS) installed in the main gallery.

Subsequently, six plastic pipes, each with three filters for water sampling and three humidity and temperature sensors, were installed in drilled boreholes measuring 63 mm in diameter, inserted parallel to the drift axis up to instrumented section F2 (Figure 5). The sensors and filters were located at depths corresponding to the former instrumented sections G, I and F2.

Also, two plastic pipes were installed in two boreholes parallel to the drift axis, measuring 63 mm in diameter, with two pairs of total pressure cells located at former instrumented sections I and F2, and thermocouples in sections I, F2, G, and in a new section S. The cells, placed in the radial and tangential directions, were in contact with the bentonite buffer in order to measure the total pressure at those points. The installation of these instrumentation pipes was completed by the end of May 2003. At this point, the experiment was ready for the construction of the second section of the plug.

Four “cable connection boxes” filled with resin were installed at the rock surface in the area corresponding to the second section of the plug, before shotcreting. This was done in order to pass a total

of 388 cables, corresponding to the instruments installed in the remaining test zone, through the plug without jeopardising the water tightness of the system. Following this, two total pressure cells were installed at the surface of the existing temporary plug, and a layer of a sprayable polymer product was applied on top, in order to improve the water and gas tightness of the test.

Finally, the second stage of the plug, measuring approximately 2 m in length, was built over the period 23rd-27th June 2003. It was decided to eliminate both the steel and polypropylene fibres from the shotcrete formulation, in order to make it closer to what would actually be used in a real repository. The construction process was much more efficient than during the construction of the first stage, with very little rebound material and a very good uniformity of the shotcrete (Figure 5).

The final layout of the test may be seen in Figure 6, and the appearance of the plug is shown in Figure 7. As in the case of the first stage plug, four linear displacement transducers were installed in contact with the final shotcrete surface in order to detect potential movements of the plug. Concrete sample boxes of each layer of the plug were taken, and cores were extracted from them after 28 days of hardening for analysis of mechanical properties and hydraulic conductivity, as was the case for the temporary plug.



Figure 5: Construction of second section of the plug

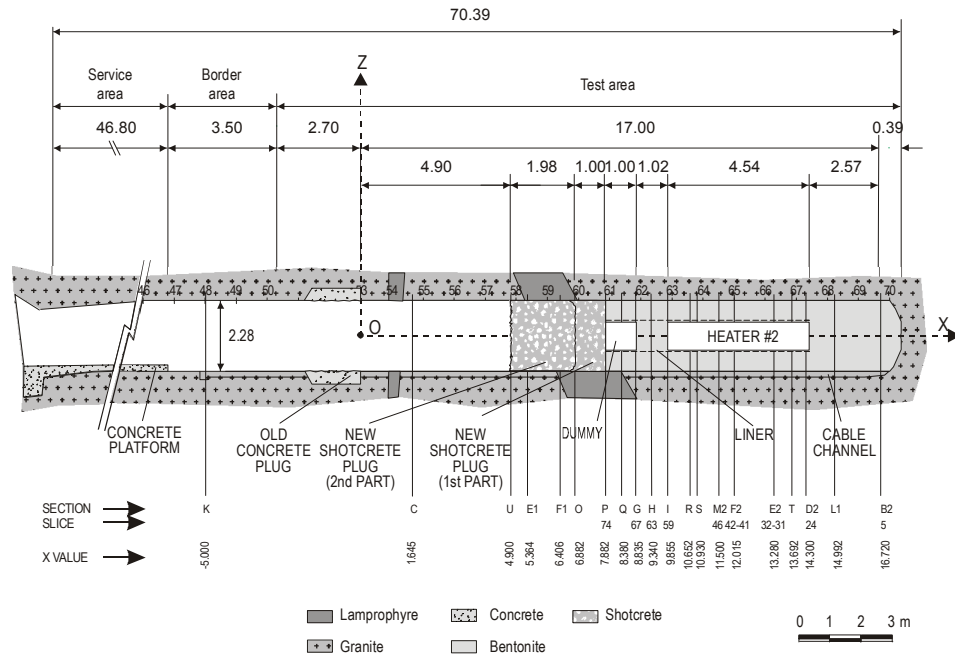


Figure 6: “In situ” test configuration following dismantling of heater No. 1

A quality assurance program was applied throughout the entire activity, from the tasks previous to the start of dismantling up to the end of construction of the plug.

Several technical reports and procedures were drawn up during this operation. They are referred to in a full report on the dismantling of heater No. 1, covering all the operations carried out, which was issued at the end of these activities (deliverable D7).

2.3 Second operational phase

The second operational phase started in July 2002, following the partial dismantling operation. It comprised the same activities as in the first operational phase: heating and supervision and data management of the “in situ” experiment, gas sampling and hydraulic testing in rock.



Figure 7: Final appearance of the plug with sensors for displacement tracking

2.3.1 Supervision and data management

Monitoring and data management have continued and quarterly data reports have been drawn up containing the data acquired during the second operational phase (deliverables D1-g and D8-a to D8-d).

Heater No. 2 has been functioning at constant temperature, and data acquisition from all the instruments continues, including the new instruments installed in the bentonite buffer and in the new plug. The readings from these sensors are coherent with those obtained from the previous ones, showing a gradual increase of humidity and total pressure in the buffer.

The Time Domain Reflectometry (TDR) system was modified and the configuration was re-installed in order to improve data access and the calculation of water content.

2.3.2 Gas sampling and analysis

Gas samples were taken for analysis between October 2003 and May 2004 (three times). The results for the gas extracted from the three filter pipes are similar. The concentration of the CO₂ and H₂ gases is decreasing drastically. The reason for this is unknown. A report was produced on these analysis (deliverable D9).

2.3.3 Hydraulic tests in rock

A large number of hydraulic tests have been performed within the framework of the FEBEX experiment. The tests span a broad range of durations and testing methods: pulse testing, which yields local values of hydraulic conductivity, recovery and short duration pumping tests, which provide information on intermediate scales, and cross-hole pumping tests, which provide information on large-scale behaviour and connectivity. The objective of these tests was to assess whether tunnel excavations and heating lead to a change in hydraulic properties. For this reason, they were performed at different stages during the project: prior to excavation of the tunnel (1995), following tunnel excavation (1996), during heating (2001) and after dismantling (2003).

The main conclusion of the comparison is that no significant trend can be detected. A few intervals display some variations between campaigns, but these variations may be attributed to incidents during testing or to uncertainties in interpretation.

2.4 Post-mortem analysis

2.4.1 Bentonite analysis

Several determinations were carried out on the bentonite samples taken during the dismantling operation. The aim was to characterise the actual state of the bentonite and to determine the possible changes that might have occurred in its thermo-hydro-mechanical and geochemical properties during the experiment, due to the combined effect of temperature, water content, joints and solutes. The conclusions drawn can be found in deliverable D11, and are summarised below:

- The distribution of water content and dry density in vertical sections presents an axial symmetry (Figure 8 and Figure 9). The average values of water content and dry density in different vertical sections along the studied zone are similar, around the heater or at a distance from it. Despite the fact that the geological characteristics of the gallery, especially with respect to water conductivity, were not homogeneous around the first heater, due to the presence of a lamprophyre dyke, there are no differences in average water content between the different sections around the heater. The average degree of saturation computed in all the retrieved bentonite is approximately 85 percent.

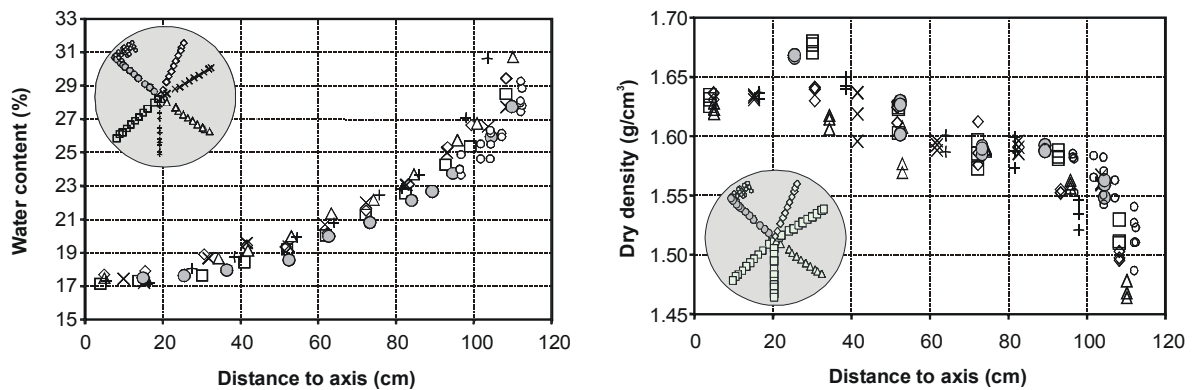


Figure 8: Water content and dry density along six radial lines in section S15 (no heater)

- The samples at the barrier have undergone an overall increase in volume, this implying a decrease in dry density from that of the compacted blocks, 1.70 g/cm^3 , to an average density of the barrier of 1.58 g/cm^3 . This is explained by the filling of all the construction gaps.
- The agreement between the measurements of gravimetric water content (by oven drying) and the measurements of relative humidity recorded by the instrumentation installed in the bentonite blocks at Grimsel is good, this corroborating the correct performance of the “in situ” sensors.

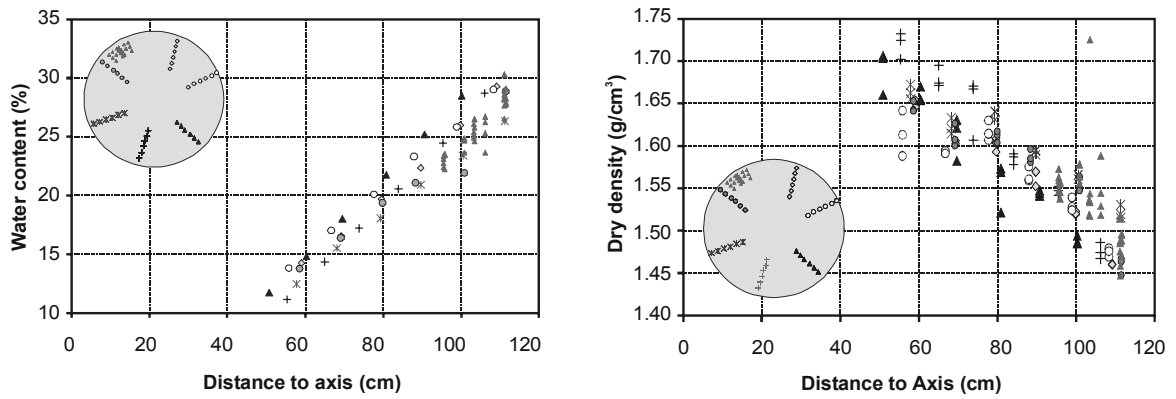


Figure 9: Water content and dry density along six radial lines in section S22 (around heater)

The mineralogical and geochemical characterisation of the Grimsel samples suggests that no major modifications occurred in the bentonite during the experiment. Temperature appears to be the main potential factor inducing mineralogical and geochemical changes:

- Cationic exchange capacity has increased with respect to the initial value, due mainly to the overall increase in exchangeable potassium and calcium. An increase in exchangeable sodium has been observed towards the granite. In the case of calcium, there is an increase in content at the heater contact and at the bentonite-granite interface.
- Hydration of the bentonite at the external blocks in contact with the granite produces the dissolution and dilution of the more soluble trace minerals in the bentonite (sulphates, carbonates and chlorides), which are transported towards the inner part of the barrier. As a result, saline fronts are generated due to the different mobility of the dissolved ions: the tendency of Na, Ca and Mg concentrations is similar to that of chloride, while sulphate mobilisation is significantly retarded with respect to chloride. Salt movement is faster in the heater sections than in the zone without temperature effects.
- The chemical and mineralogical composition of the bentonite from the section in contact with the concrete plug is rather similar to that of the raw bentonite.

The results concerning changes in THM properties may be summarised as follows:

- The water retention capacity of the samples from Grimsel has not appreciably changed after five years of being submitted to repository conditions.
- The hydraulic conductivity of the samples from Grimsel is clearly related to dry density and the latter in turn is related to the position of the block in the barrier.
- The swelling capacity of the FEBEX bentonite has not changed irreversibly after five years of being subjected to repository conditions.
- Pre-consolidation pressures below 10 MPa have been measured for all the Grimsel samples, these being lower in the samples from the external ring of the barrier. This means an important decrease with respect to the initial pre-consolidation pressure (around 40 MPa), this being accounted for by the microstructural changes associated with the volume increase experienced during hydration.
- The uniaxial strength of the bentonite is higher in the direction of compaction of the blocks than in the perpendicular, and tends to be lower for the samples that were subjected to higher temperature.

- Thermal conductivity increases with the water content of the clay and is consequently higher in the case of the blocks in the external ring. However, the blocks in the internal and intermediate rings present lower conductivities than expected in view of the theoretical values. This might suggest a certain decrease in thermal conductivity related to heating.
- The experiments performed in remoulded samples with joints parallel and perpendicular to the percolation flow show that, upon saturation, the medium becomes homogeneous and the joints seal completely, the hydro-mechanical properties of the material depending only on its dry density. However, in the case of unsaturated samples, the hydrodynamic properties of the clay are modified by the existence of joints parallel to the infiltration flow.

Finally, it may be said that the slight modifications observed in the chemical and mineralogical composition of the bentonite cannot be clearly correlated with any important variation in macroscopic thermo-hydro-mechanical properties, except possibly as regards an increase in the plasticity of the samples from the outer ring, which might be linked to the increase in exchangeable sodium that takes place near the gallery wall.

2.4.2 Granite (EDZ) analysis

Any excavation gives rise to a damaged zone around the opening (EDZ). As regards radioactive waste storage, the important point is to know whether this damaged zone may alter the rock properties relevant to long-term safety; in particular permeability, since the EDZ around the underground opening in granite may provide enhanced pathways for radionuclide migration,

A multidisciplinary team studied the potential damaged zone around the test drift and its evolution over a 5-year period of heating. The research program included laboratory and in-situ investigation, and results were compiled in deliverable D12.

Laboratory investigation

- Microfracturing and porosity: The ^{14}C -polymethylmethacrylate (^{14}C -PMMA) technique was applied for quantitative and qualitative study of the spatial distribution of porosity in the EDZ of the drift, in addition to complementary microscopy and scanning electron microscopy (SEM) studies.

No clear zones of increased porosity were observed in the tunnel wall of the test area when analysing the granite samples taken during dismantling using the PMMA method. The samples from the service area did not differ from the samples from the test zone. A clear increase in porosity to depths of 10-15 mm from the test area tunnel wall was detected in lamprophyre samples.

According to the SEM/EDX analyses, the excavation disturbed zone in the granite matrix extended to depths of 1 - 3 mm from the surface of the wall.

- Gas permeability test: The permeability measurement is a good indicator for assessing the existence and evolution of the EDZ. Gas permeability tests were carried out on two core samples measuring 1 m in length, again from the service area and from the heated zone.

Permeability ranges between $8.4 \cdot 10^{-19} \text{ m}^2$ (lowest measurable by the experimental setup) and $3.5 \cdot 10^{-18} \text{ m}^2$, this pointing to the absence of marked damage. Although there was an increase in permeability over the first 20 cm of the sample from the heated zone, this cannot be linked to the existence of a damaged zone. Indeed, no discrepancies higher than one order of magnitude were observed along this sample, the maximum permeability measured remaining below that provided by the natural heterogeneity of the virgin rock.

- Acoustic investigations: Measurements were performed of the propagation times of ultrasonic waves through a cylindrical granite block extracted from the wall of the test area, the objective being to determine the existence of an EDZ according to the velocity distributions obtained. The block measured 38.8 cm in diameter and 40 cm in height.

The main results showed a preferential direction, with higher velocities in the study of horizontal trajectories, and in a second interpretation with an evolving figure with velocity vectors (Figure 10). Some other local heterogeneities were encountered. However, no special decrease in velocity towards the gallery wall was appreciated; this meaning that there is no evidence of EDZ in the first 40 cm of granite in the FEBEX gallery.

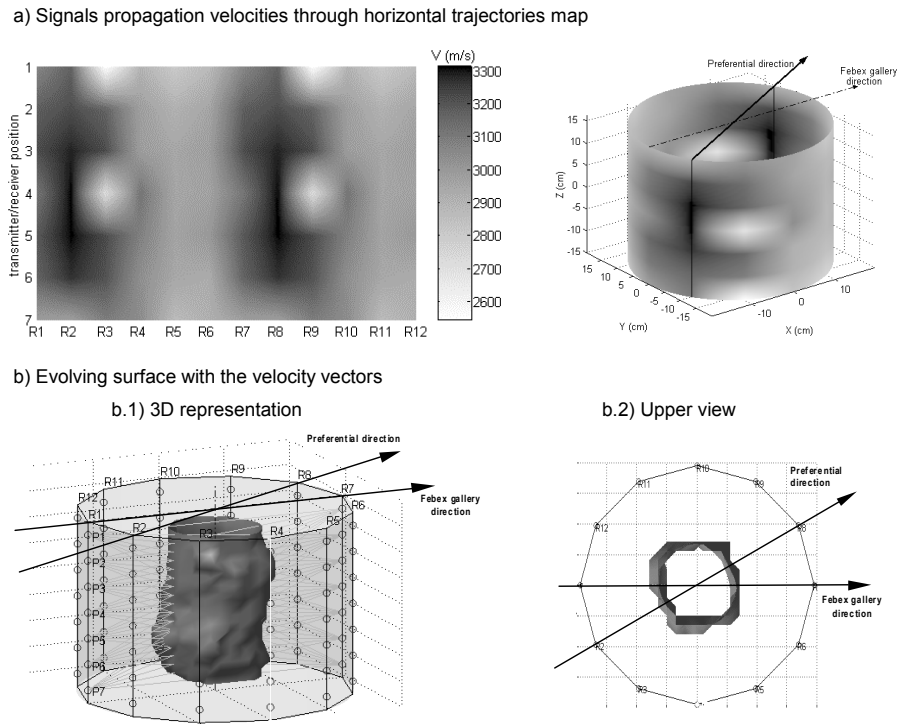


Figure 10: Results for tomographic measurements

Other acoustic investigations performed on two additional 1 metre-long core samples, taken both from the service area and from the test zone, have shown no significant changes in P-wave velocity. These results indicate that the thermo-mechanical loading experienced by the rock mass during the FEBEX experiment does not affect the elastic behaviour of the Grimsel granite.

In situ investigation:

The hydraulic connectivity of the artificially induced and natural fractures is the property that essentially determines the effects of the EDZ on groundwater flow. In order to characterise the hydraulic connectivity of the fracture networks in the tunnel near-field and to determine the permeability distribution along artificial/natural fractures intersecting the tunnel, a surface packer system with gas injection was developed and used in seventeen selected locations throughout the FEBEX drift, both in the heated and non heated zones.

Only two locations with higher permeability were detected: one is a natural fracture in the lamprophyre dyke and the other is the interface between lamprophyre and granite. The permeability of the granite matrix in the EDZ of the tunnel drilled by TBM is comparable to that of the undisturbed rock mass ($<5 \cdot 10^{-19} \text{ m}^2$). The transmissibility of the fractures may amount to $1 \cdot 10^{-15} \text{ m}^3$.

The thermal and mechanical conditions induced by the experiment during heating and hydration have no significant influence on hydraulic parameters (permeability and porosity), but may affect the residual water saturation of the granite in the EDZ and again, in the long-term, re-saturation.

2.4.3 Corrosion analysis

During the dismantling, samples from different corrodible metallic parts of the experiment were collected and sent for analysis. The analysed parts included heater No. 1, a section of liner, a number of corrosion coupons (placed for that purpose within the buffer during the installation of the experiment) and some sensors from the instrumented section, which were found to be severely corroded during dismantling. Deliverable D13 was produced on those analyses. The following results were obtained:

- Heater No. 1: This showed slight uniform generalised corrosion over its entire surface, with oxide layers of less than 20 microns in thickness in all the cases examined. No localised corrosion phenomena were observed.
- Liner: The morphology of the corrosion detected on the liner was generalised and non-uniform, with maximum values of penetration of the corrosion of approximately 130 microns on the external surface and 200 microns on the internal surface. No localised corrosion phenomena were observed.
- Corrosion coupons: No generalised and/or local corrosion was observed on the stainless steel and titanium specimens. The carbon steel coupons showed very slight generalised corrosion, with average corrosion rate values of 0.10 $\mu\text{m}/\text{year}$; no localised corrosion phenomena were detected. The copper coupons showed average corrosion rates of 0.71 $\mu\text{m}/\text{year}$ for the Cu-ETP, and 0.74 $\mu\text{m}/\text{year}$ for the Cu10Ni alloy. The corrosion suffered by the Cu30Ni alloy was negligible.
- Sensors: The high humidity, together with the presence of sulphate-reducing bacteria (SRB) in the bentonite housing the sensors are the reasons underlying the significant corrosion observed in these components. The sulphur rich corrosion products, as well as the morphology of the corrosion, indicate localised corrosion phenomena most probably induced by sulphate-reducing bacteria. Cracking typical of stress corrosion induced by the presence of chlorides and/or products resulting from the metabolic activity of the SRB was also observed. In the case of the carbon steel components, the corrosion observed was of the generalised type, with the practical destruction of the component being observed on occasions.

As a general conclusion, the corrosion processes have not progressed significantly in the drier zones of the barrier, whereas their effects are more noticeable in the more humid zones where the conditions of moisture and temperature have favoured the action of sulphate-reducing bacteria. Hence, microbiological activity shall be taken into account when addressing possible corrosion processes in future installations.

2.4.4 Instruments analysis

The instruments retrieved during dismantling were sent to different laboratories for analysis in order to obtain first hand information on their actual status after several years of “in situ” operation, as well as on the reliability of the data obtained during the first operational phase of the experiment. Deliverable D14 was produced on those analyses. The following results were obtained:

- Temperature sensors (thermocouples): The data obtained seemed to be accurate when compared with measures from temperature sensors incorporated in other instruments and with the expected evolution provided by the models. The temperature trend has been quite uniform during the operational phase, this being the parameter with the highest symmetry throughout the experiment. According to calibration data, the behaviour of the temperature sensors was excellent, except for those few which were damaged by corrosion. The accuracy of the still operative dismantled thermocouples has not varied since the time of installation (below $\pm 1^\circ\text{C}$).

- Humidity (capacitive type, psychrometers and TDRs): In general, the readings provided by each sensor type match quite well with the others and also with the predictions provided by the models. The evolution of humidity was more three-dimensional than that of the temperature.
 - The capacitive type sensors have far exceeded the initially expected operative lifetime. The readings provided by these sensors were accurate and, given their wide range, the data obtained from them is very useful for modellers when the hydration process starts from low water contents and is sufficiently slow, as in this case.
 - Psychrometers proved to be very fragile for the bentonite buffer environment with regard to mechanical resistance and contamination with salts from the bentonite, although their readings, especially in the outer buffer ring, matched the capacitive readings. On the other hand, the psychrometers in the granite provided reasonable readings (very low suction) and seemed to be less affected by salt contamination.
 - TDRs in the bentonite buffer also proved to be fairly fragile for such an environment. Furthermore, two distorting effects were identified which have affected the calculated water content and made it necessary to re-interpret the data from the start of the experiment, for TDRs in both bentonite and in granite.
- Total pressure cells on the rock surface: In general, the behaviour of these cells has been as good as initially expected for all the sensors based on the vibrating wire technique. The only difficulty arose as a result of the weakness of the embedded thermistors used for temperature compensation of the vibrating wire signal, some of which failed. In these cases, nearby temperature readings were used instead.

Also, in situ re-calibrations were carried out on the pressure cells installed at the gallery wall in the dismantled zone, which served to apply an offset correction to the data obtained from these cells from the start of the experiment. The application of this correction improved the coincidence of pressure evolution for the cells at the same sections.

- Other vibrating wire type sensors:
 - Pore pressure sensors in bentonite: Only a few of these showed problems. These sensors generally provided very low readings, showing positive values only at the most humid parts, located at the outer part of the buffer. However, as a general conclusion, it may be inferred that the registered pore pressure values were tightly dependent on the temperature in the buffer.
 - Total pressure cells in bentonite: Half of the retrieved cells were out of order during operation, in some cases due to damage to the cables during installation. It may be stated that in general their performance was similar to that of the cells installed at the rock surface.
 - Heater displacement sensors: Unfortunately the two recovered sensors were severely damaged by corrosion, as a result of which it was not possible to obtain results from calibration; furthermore, the confidence in their readings was low and they did not match the measures taken during the dismantling.
 - Bentonite block displacement sensors: All these sensors were operative throughout the entire operation. These displacement transducers, installed “floating” in specific bentonite blocks in the intermediate ring of the buffer, gave very small length variations (in the range of 1-2 mm), with an initial small but fast expansion, followed by slow contraction that changed steadily to an expansion movement.

- Other sensors:
 - Hydraulic pressure in rock boreholes: Internal packer pressures and borehole interval pressures were measured by means of conventional pressure transducers installed outside the sealed area, at the end of nylon type plastic tubes. These sensors are working under standard conditions and can be checked or replaced if necessary, as occurred in certain cases.
 - The so-called experimental sensors: Potentiometer type bentonite displacement sensors, clinometers and gas flow pipes. 100 % of the LVDT type clinometers and potentiometers for displacements within the bentonite barrier failed due to complete flooding of some of these instruments, up to the associated electronics. In fact, the gas pipes are strictly speaking not sensors but devices to sample gas and water. However, only those protected by an external metallic tube survived intact the swelling of the bentonite.
 - Gas draining pipes: The three pipes mounted close to the gallery wall were broken into small pieces as a result of bentonite expansion and the resulting heterogeneous stress. Nevertheless the porosity of the ceramic material still exists and additionally a residual volume was present between these broken materials, as a result of which water sampling and pore pressure measurements via the PFA pipes was possible.

The three pipes installed in the boreholes in the bentonite backfill close to the heater were not broken and could be extracted without problems. The permeability to water and gas did not show any significant change in comparison with new pipes.

This investigation indicated that ceramic pipes might be used in areas with isotropic stresses. In areas with anisotropic stresses, such as the wall of backfilled galleries, these pipes will break; nevertheless, the broken pipes have enough porosity for the performance of permeability measurements and the extraction of gas and water samples.

In general, the results obtained show that the instruments performed well, with good mechanical resistance, especially in the non-experimental sensors (Figure 11), and low levels of drift with regard to the readings acquired prior to installation.

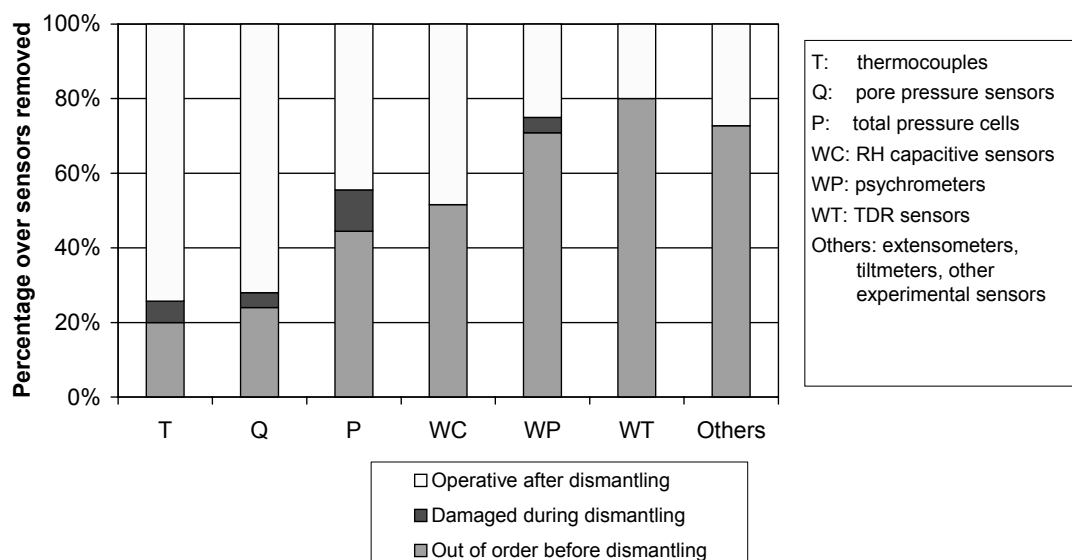


Figure 11: Status of sensors removed during the dismantling

3 “MOCK-UP” TEST

The installation phase of the “mock-up” was carried out between October ‘96 and January ‘97. The operational stage – simultaneous hydration and heating– started on February 4th 1997, “day 0” on the time scale.

Three days before the beginning of the operational stage, a volume of 634 litres of water injected at high flow (3.5 l/min) completely flooded the voids, allowing for the closure of the gaps between blocks through swelling of the bentonite. The water injection pressure has been between 0.5 and 0.6 MPa since that date and a pressure-controller has been installed to establish the nominal value, 0.53 MPa. The water volume injected is calculated from the masses of the water tanks, corrected by the nitrogen injection pressure. The calculated rate of water injection follows an asymptotic curve, as expected, with lower rates as time goes by. The total volume of water injected was 1024.3 litres as of 08/07/2004.

The operational power to the heaters has been supplied in three phases: 250 W/heater during the first 6 days of operation (to 65 °C measured at the heater-bentonite interface), 500 W/heater during the next 4 days (to 95 °C measured) and automatically controlled from there on (to achieve the target temperature of 100 °C at this interface). The temperature steady state in the clay barrier is achieved in a short time (15 days) and generates temperature gradients with maximum values close to the heater surface. Over the last two years, and because of problems with the isolation of the electric resistances, the heaters have been operated at a constant power (700W/heater) with the temperature close to the 100°C target.

As a result of a malfunction towards the end of November 2000 (day 1391), the control program supplied the total heating power (around 2700 W/heater) for more than 36 hours, until the temperature at the sensors in the heaters reached the resistance safety value (300°C). This overheating was automatically stopped, but not before the temperature within the bentonite had achieved values of around 240 °C. This dried the bentonite around the heaters and generated a thermal pulse.

The THM parameters measured within the bentonite are temperature, total pressure, fluid pressure and relative humidity at equilibrium (RHE); while the controlled boundary conditions are both thermal (power supply and heater temperature, outside structure temperature, and room temperature) and hydraulic (injection pressure and volume).

Temperature

After the initial transient state, the test was conducted in a quasi-stationary temperature state until the overheating event that generated thermal waves; subsequently, the quasi-stationary state was completely recovered in less than 18 days (Figure 12). The thermal gradient within the bentonite around the heater is 0.03 °C/m.

The temperature data show good homogeneity throughout the test. The initial variations observed between sensors located at selected radial distances in the same section (0.20, 0.39, 0.58, and 0.77 m, respectively) are less than 2 °C.

The properties that control the behaviour of the clay under a thermal load are thermal conductivity, specific heat and the thermal expansion coefficient. In addition to these factors, the final temperatures in the barrier are strongly related to the degree of saturation of the bentonite.

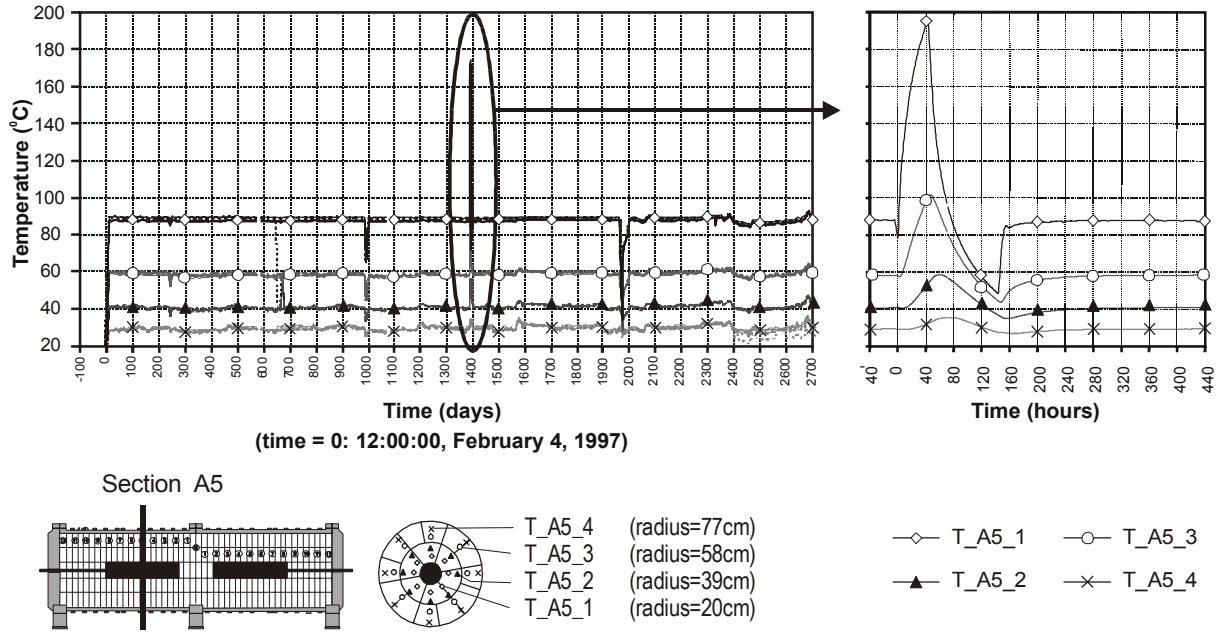


Figure 12: Temperatures in section A5: complete test and overheating enlargement

Relative humidity (RH)

The RH sensors allow for monitoring of the hydration drying-wetting process. Figure 13 shows the evolution of relative humidity (RH) at various distances from the heater in a “hot” section.

Depending on the location of the RH measurement (distance to the hydration surface and thermal gradient imposed on the sensor) different behaviours may be observed. The values measured clearly show the effects of evaporation (drying) and condensation (wetting) in different zones of the barrier. The values measured at 10 cm from the hydration surface of the structure suggest that the bentonite in this external zone is fully saturated.

In sensors located close to the heater the following phases may be distinguished: (i) a sharp increase in RH value, which appears to be related to the vapour phase generated by the initial heating; (ii), continuous heat transfer from the heaters produces drying of the clay, this causing decreasing RH; (iii) after some time, hydration reaches the dried zone and overcomes the drying process, increasing the RH values.

This transient indicates the redistribution of water, a process with slower dynamics than thermal transfer. So, 360 days are required to reach the minimum value of RHE, and 1080 days to recover the initial values in the ring closer to the heater; however, achieves a relative minimum in 270 days but without retrieving the original value, this indicating the adsorption of water through the vapour phase.

During overheating, sharp peak values of RH were once again observed in the inner rings. This supports the idea that a new drying of bentonite occurred, generating sufficient vapour to flow through the location of the sensor. This vapour outflow from the heaters seems to be radial and redistributes water within the bentonite.

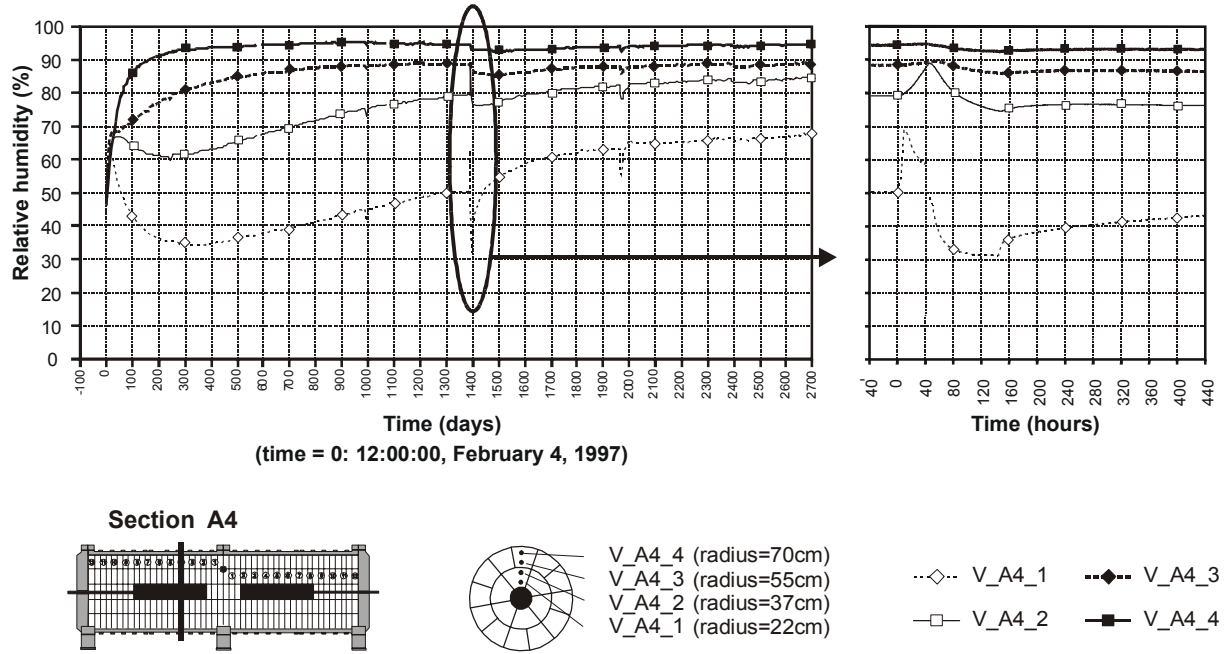


Figure 13: RH in section A4: complete test and overheating enlargement

The sensors placed in zones without heaters (“cold” sections) show higher RH values, reaching almost full saturation according to the retention curves.

The RH evolution curves in all sections show tendencies similar to those described above. The only differences are related to the relative radial and longitudinal positions with respect to the heaters (hot and cold zones).

The synchronous evolution of the different RH sensors indicates that their behaviour is a real process in the RHE (relative humidity of equilibrium) of the material. It is not an artefact. This evolution is shown as a decrease of magnitude in the more saturated zones of the external ring in the barrier. From above, the water inflow is radial and homogeneous, modified only by the implicit THM behaviour of the barrier.

Total pressure

Under hydration, bentonite develops a mechanical pressure by swelling, recorded by the total pressure sensors located at selected radial distances (35.0 cm and 66.5 cm), oriented in the three main directions.

Axial pressures range from 4.5 to 9.0 MPa, radial pressures from 5.0 to 8.0 MPa and tangential pressures from 5.0 to 10.0 MPa. The pressures are in accordance with the swelling pressure values of bentonite measured in the laboratory: 10 and 6 MPa for dry densities of 1700 and 1600 Kg/m³, respectively.

The higher-pressure values are located within the outer ring due to the evolution of the saturation front. In fact, the average-pressure values in this zone and their slow increase might indicate full saturation of the buffer (Figure 14).

On the other hand, the smaller pressure values in the inner rings might indicate two different processes: the redistribution of stresses coming from the outer rings or the extension of saturation into this zone. Small variations in the pressure evolution appear to be linked to external temperature variations.

Overheating produced small pressure value peaks and redistributed total stresses and water content within the bentonite through the heating-cooling cycle generated. Recovery of the values existing previous to overheating does not occur so quickly as in the temperature or RHE sensors, but is more pronounced in

the sensors placed in the outer ring (Figure 14). In general, approximately one year is required for values to be recovered in the saturated part of the outer ring, both cold and hot zones, 220 days in the non-saturated part of the hot zone, and 180 days in the non-saturated part of the cold zones. Sensors measuring axial and tangential stresses seem to be more affected.

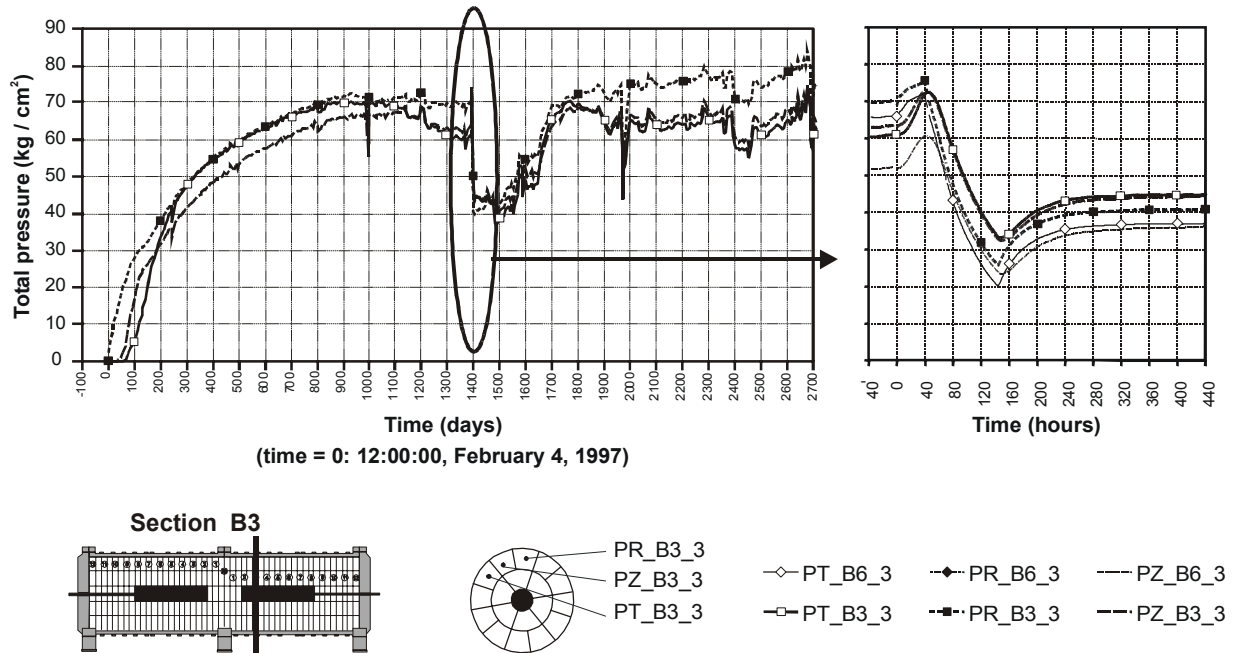


Figure 14: Total pressures in section B3: complete test and overheating enlargement

The more saturated materials undergo a lower pressure peak than the less saturated ones, but the absolute decrease respect to the previous values is higher. It seems that pressure loss is more intense for the higher degrees of saturation, and longer for the hotter materials. This might indicate a competition between two transfer processes, thermal and hydraulic, and their location in the experiment (the thermal in the outer saturated zone and the hydraulic, in the vapour phase, in the inner non-saturated zone).

Some local extremely high-pressure values (up to 10.5 MPa) may be explained by considering the locally combined effects: XYZ coordinates, dry density of the block (higher than 1800 Kg/m³ in the core blocks), sensor installation (place carved in the block), local swelling pressure (depending on hydration and temperature) and/or development and concentration of local stresses due to readjustment between blocks.

Fluid pressure

The measured values cannot be assigned to water or gas pressure without uncertainty, mainly in the inner ring. Only some variations seem to be related to the arrival of water, in all cases for sensors located in the outer rings. There are fluctuations apparently related to temperature variations.

Almost 700 days are required for some increase to be observed in fluid pressure within the outer rings, both in the hot and in the cold zones. This time increases to 900 days in the inner rings of the cold sections, showing a dependence on the fluid temperature (through water viscosity).

During overheating, sharp peak values of fluid pressure, generated in the inner rings, support the idea introduced above in relation to the drying of bentonite. Values are recovered in the outer rings after overheating; but values in the inner ring continue to vary slowly or remain almost negligible (Figure 15).

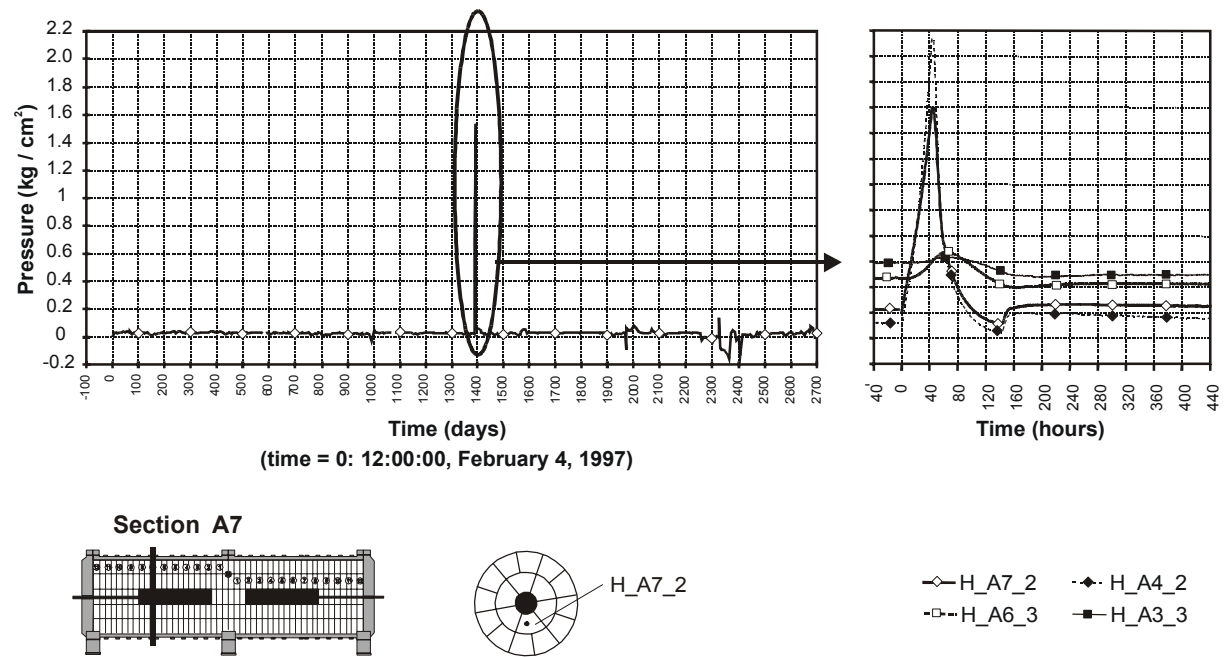


Figure 15: Fluid pressure in section A7: complete test and overheating enlargement

Operational behaviour of the experiment components

The “mock-up” test exceeds its design operation time of 3 years, functioning correctly. The reliability of the instruments is fairly good; while the reliability and performance of the heaters are sufficient (the low-voltage constant-power operation must extend their life expectancy and prevent them from any further damage). The data acquisition and control systems are working satisfactorily.

More than 90% of the sensors remain operative (Figure 16), but it is not possible to guarantee their future behaviour.

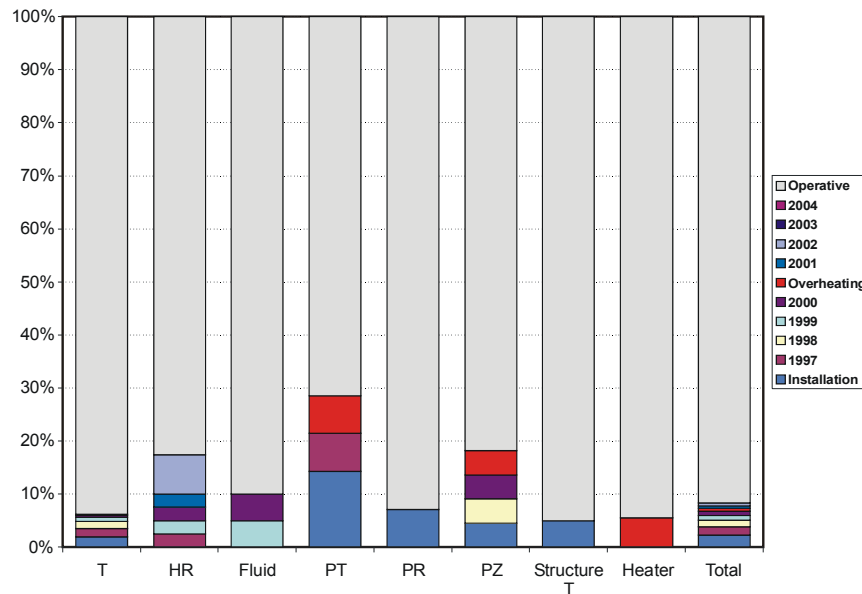


Figure 16: Evolution of sensor breakdown (operative sensors in grey)

4 LABORATORY TESTS

4.1 THM laboratory tests

4.1.1 Continuation of the tests initiated during FEBEX I

The mechanical behaviour of compacted bentonite was investigated during FEBEX I through the performance of a test programme carried out in suction-controlled oedometers. A deeper insight into the behaviour of compacted bentonite, and of the basic mechanisms controlling it, has been achieved during FEBEX II using an elasto-plastic framework that incorporates the interplay between micro-structural and macro-structural fabric levels in a simplified manner. Most of the main features of behaviour are correctly reproduced by the model: yield phenomena, dependency of swelling strains on applied stresses, stress path dependency of strains, and compound stress paths in swelling pressure tests.

In order to study the thermo-hydro-mechanical processes during water infiltration, the results of infiltration tests performed during FEBEX I and II were back-analysed as a boundary value problem using the CODE_BRIGHT code. The numerical model is capable of reproducing the global tendencies observed in the small-scale tests: both the results related to the evolution of the main variables of the test and those related to the post-mortem study. The combination of this kind of tests and coupled THMC numerical analysis can help to achieve a better understanding of the behaviour of the FEBEX bentonite under repository conditions.

In the retention curves at constant volume (Figure 17) it has been observed that the repercussion of initial dry density on the value of water content reached is more obvious as suction decreases. The hysteretic behaviour of the clay has also been made clear, the water contents reached during drying being higher than those obtained during the previous wetting (in confined samples), and the water contents in the wetting paths lower than those reached for the same suction in the previous drying (in unconfined samples). The degrees of saturation obtained in the wetting paths at constant volume, for suctions lower than around 10 MPa, are higher than 100 percent because they were calculated considering the density of the water as 1.00 g/cm³, which was shown to be untrue for high plasticity materials.

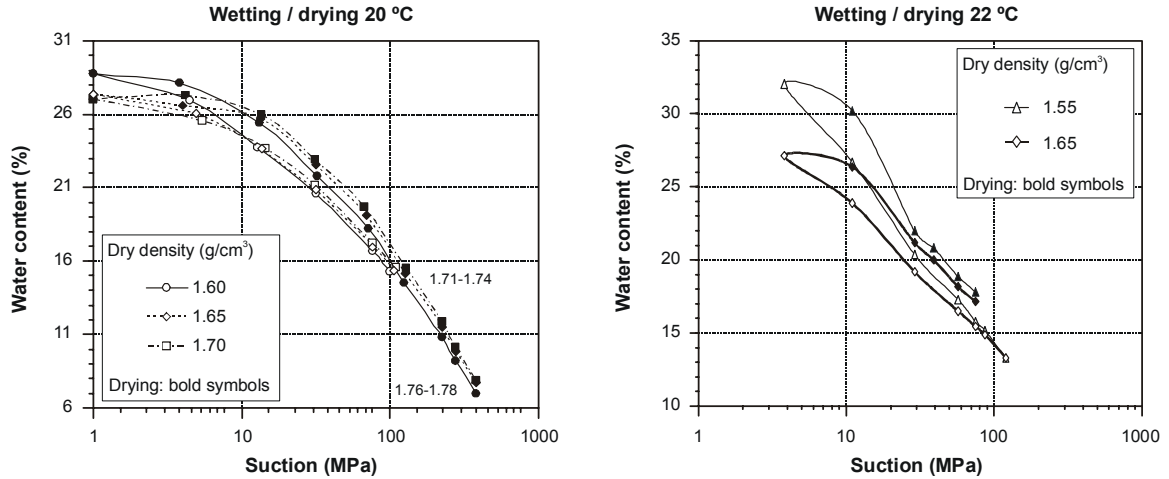


Figure 17: Retention curves at constant volume in wetting/drying paths (left: at 20°C, final dry densities indicated in g/cm³; right: at 22°C)

4.1.2 New THM tests

Temperature effects on water retention curves in confined and unconfined conditions have been determined and swelling pressure, hydraulic conductivity and swelling and consolidation strains as a function of temperature were successfully measured. Different experimental techniques and items of equipment were developed to study thermally-induced changes under partially saturated states, covering a wide range of suctions.

Both in confined and unconfined conditions, the retention capacity at higher temperature seems to be slightly lower: At a constant degree of saturation, the higher the temperature of the sample the lower its suction (Figure 18a). The way in which temperature increases the water saturated permeability of FEBEX bentonite was measured, although this measured increase is slightly lower than what would be expected on the basis of the thermal changes in water kinematic viscosity (Figure 18b). Thermo-chemical effects altering clay fabric (flocculation or dispersion), porosity redistribution (creating preferential pathways or blocking macro-pores) and pore fluid chemistry (affecting viscosity) might be relevant issues regarding the effect of temperature on permeability.

Bentonite swelling strains are a function of temperature: At high temperatures the swelling capacity of clay decreases (Figure 19a). In the same way, a clear decrease of swelling pressure as a function of temperature (down to 2.5 MPa at 80 °C) was observed (Figure 19b). Oedometric tests have shown that saturation seems to induce a decrease in the apparent pre-consolidation pressure, regardless of the temperature of the tests. Samples with hygroscopic water content (suctions around 100 MPa) are very stiff for vertical pressures of up to 8 MPa. This phenomenon does not appear to depend on temperature, which indicates that the effect of temperature on the elastic behaviour of bentonite is small. On the other hand, temperature increases the compressibility of bentonite, both saturated and unsaturated, which would imply that a certain reduction in the size of the elastic domain takes place with temperature. Nevertheless, the deformation of bentonite is more dependent on the stress and suction path than on temperature. In tests with suction reduction, structure changes due to hydration are more relevant in the subsequent mechanical behaviour of bentonite, than the effects of temperature.

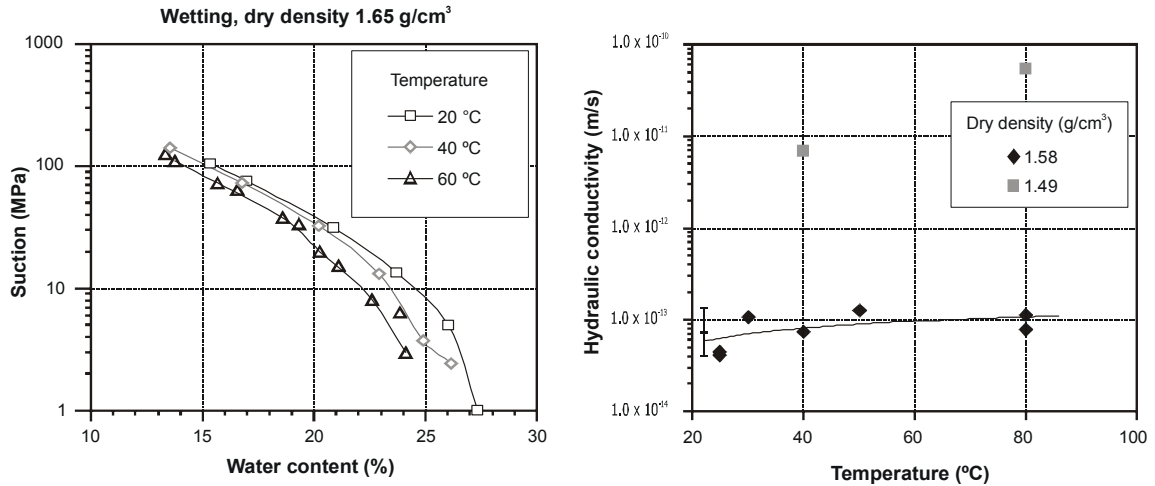


Figure 18: Effect of temperature. Left: on retention curves at constant volume. Right: on hydraulic conductivity

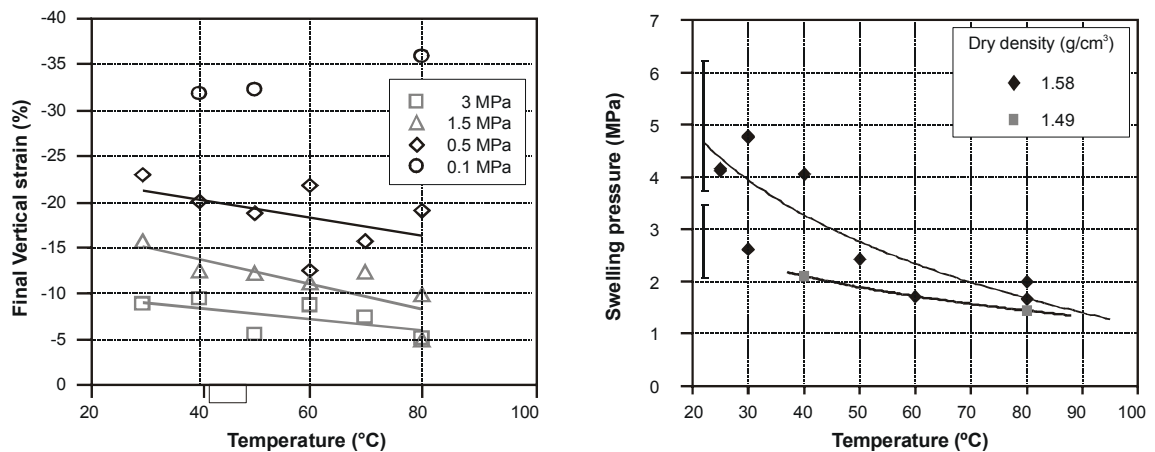


Figure 19: Left: final strain of samples compacted to dry density 1.60 g/cm³ saturated with deionised water under different vertical pressures and temperatures. Right: swelling pressure as a function of temperature

In summary, the FEBEX bentonite remains suitable as a sealing material in HLW repositories (from the hydro-mechanical point of view) for temperatures of up to 80 °C, as it maintains its high water retention capacity, low permeability and self-healing ability. No data are as yet available for higher temperatures, although extrapolation of the results points to the preservation of properties at least up to 100 °C.

Mercury intrusion porosimetry and environmental scanning electron microscopy (ESEM) provided promising results for the characterisation of the bentonite microstructure. In the as-compacted state, the dominant intergranular pore mode conceals the inter-aggregate porosity, which cannot be distinguished. Loading paths reduce larger pores (*i.e.* inter-granular pores, Figure 20a). Suction reduction influenced the inter-aggregate pore size mode: On progressive wetting, the hidden and latent inter-aggregate pore size mode systematically emerged (Figure 20b), due probably to the progressive splitting of the original structure of the pseudo-morphs. The emerging inter-aggregate porosity was detected only when liquid water was transferred. On the other hand, the ESEM observations indicate that the changes induced by hydration under isochoric conditions tend to favour the existence of structures similar to those observed in compacted slurry samples, which present a more uniform structure than the one observed in unsaturated

samples. The use of digital imaging techniques made it possible to verify that at micro-scale level, where chemical phenomena prevail, strains are almost reversible, as considered in the two-level elasto-plastic models.

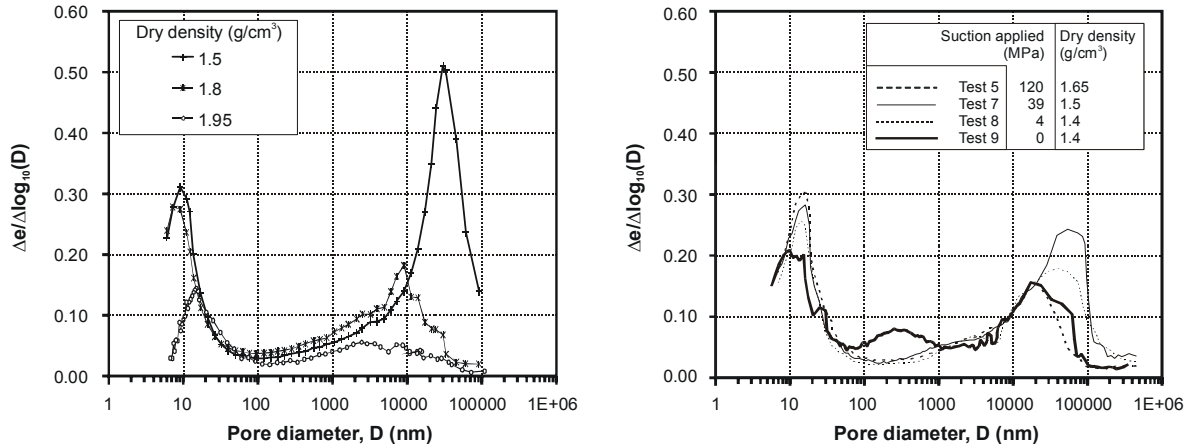


Figure 20: Left: porosimetry of samples compacted to different dry densities with water content of approximately 13-14%. Right: evolution of porosimetry on wetting at constant volume for an initial dry density of 1.65 g/cm³

The swelling strains of clay upon saturation with different kinds of water (deionised, granitic and saline with different salts and concentrations) were measured as a function of initial dry density and vertical load. The effects of salinity on bentonite stiffness and permeability were also investigated. Fits between final swelling strain and vertical pressure as a function of initial dry density were found for each kind of water. A higher swelling capacity was observed in samples saturated with deionised water, although this difference becomes less evident for higher vertical loads (Figure 21a). The swelling strains measured when the samples were soaked with different saline concentrations are similar to the strains measured in suction controlled oedometer tests in which a final suction equal to the osmotic suction of the saline solutions is applied. The hydraulic conductivity of bentonite increases with saline concentration when saline water is used as the permeating agent, especially in the case of low clay densities (Figure 21b).

4.1.3 New tests proposed to understand the behaviour observed in the “mock-up”

New tests were proposed in order to understand the unexpected reduction in water uptake rate observed in the “mock-up” test in relation to modelling results. Specifically, permeability tests, infiltration tests with and without thermal gradients, a study of the repercussion of the high hydraulic gradients applied for the determination of hydraulic conductivity on the values obtained and two new suction and temperature controlled oedometer tests were undertaken. The main conclusions from these new activities are as follows:

- The permeability of compacted bentonite appeared to remain constant for 700 days.
- The infiltration tests have shown that the permeability to water vapour of dry bentonite is very high. On the other hand, the initial saturation of compacted bentonite takes place more quickly under a thermal gradient than at laboratory temperature. The increase of hydraulic conductivity with temperature would account for this. Subsequently, the water intake is higher for the sample tested at room temperature, since the hot zones of the sample tested under a thermal gradient remain desiccated for a long period (Figure 22).

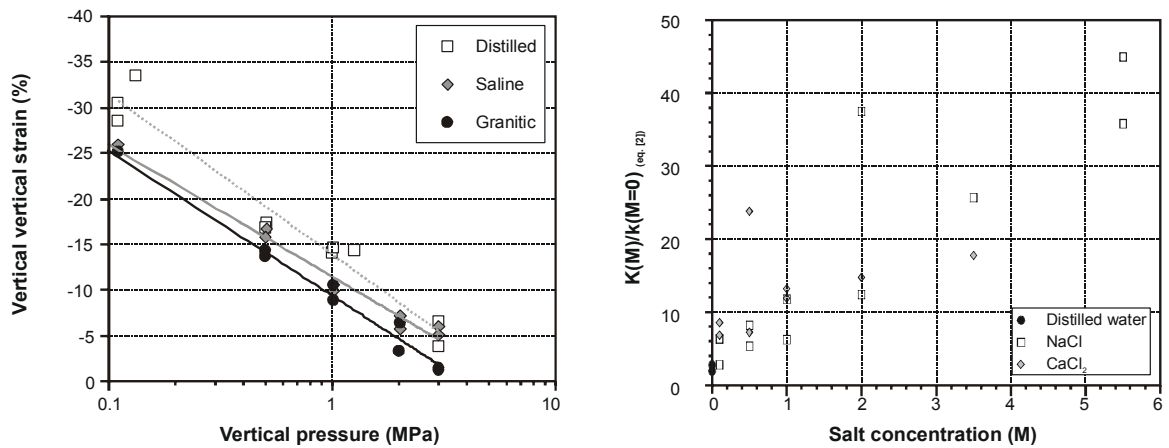


Figure 21: Left: final strain of samples of dry density 1.60 g/cm^3 saturated under different vertical pressures with different waters. Right: rate between permeability estimated from oedometric tests on samples saturated with different solutions, and permeability at the same void ratio measured directly using distilled water

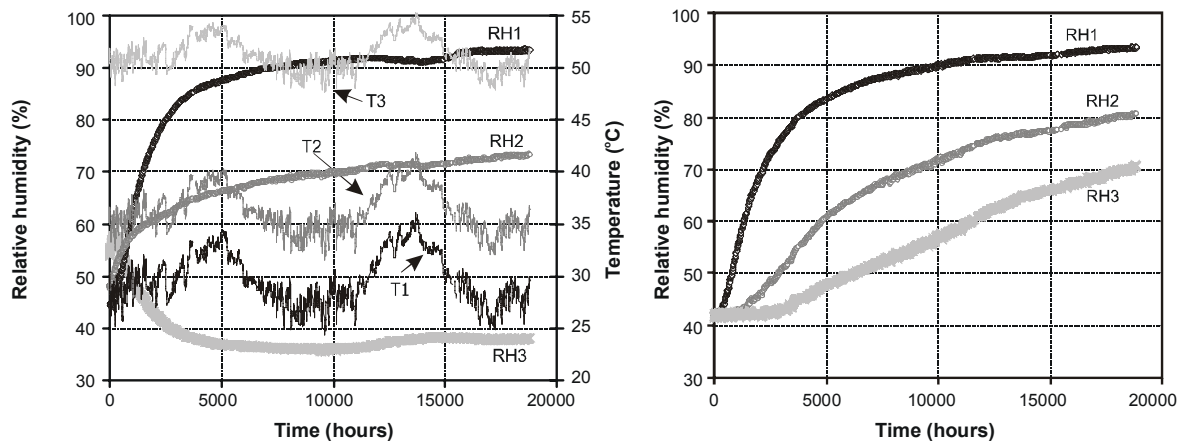


Figure 22: Evolution of relative humidity in infiltration tests performed under thermal gradient (left) and at isothermal conditions (right) (sensor 1 placed 30 cm from the bottom, sensor 2 at 20 cm and sensor 3 at 10 cm)

- Analysis of the bentonite permeability tests performed during FEBEX I made it possible to prove the independence existing between the hydraulic gradient applied and the hydraulic conductivity obtained. However, it seems that gradients higher than 0, of around 5000, and even higher in the case of the highest densities, are necessary to have a measurable flow which would point out the existence of a threshold gradient. The measurement of hydraulic conductivity under low hydraulic gradients was also undertaken. The preliminary results indicate that there is no dependence of hydraulic conductivity on the value of the hydraulic gradient.

In summary, most of the thermo-hydro-mechanical features of compacted bentonite have been experimentally studied. In general, the behaviour of the clay may be explained taking into account its double structure. The interactions between the two structural levels are responsible for the main features of the mechanical aspects of this behaviour. On the other hand, temperature-induced transfers between

intra-aggregate adsorbed water –of a density higher than that of free water– and inter-aggregate free water might explain most of the temperature-related features observed.

4.2 THG laboratory tests

4.2.1 Studies of pore water in the clay barrier

The pore water chemistry of highly compacted bentonite cannot normally be obtained by direct measurement. Rather, indirect methods based on geochemical modelling must be applied. A methodology was developed for determining the FEBEX bentonite pore water composition. In order to calculate the pore water composition of the FEBEX bentonite in its initial condition and in the compacted and saturated states, detailed physico-chemical characterisation studies were performed. These included (i) aqueous extracts at different solid to liquid ratios to determine chloride and sulphate inventories, (ii) determination of the cation exchange capacity and cation occupancies and (iii) determination of selectivity coefficients for the major cation exchange reactions. An important issue in calculating the pore water chemistry in high clay content media is to distinguish between the different types of water and their distribution in the clay/water system (double layer water, interlayer water and free pore water).

Nitrogen and water vapour adsorption-desorption isotherms, together with c-lattice spacing determinations, were used to identify the different states and location of the water. Six domains were distinguished, which are related to the different states and location of the water. Moreover, these domains also corresponded to the d001 spacing obtained from XRD measured at each water activity. The maximum amount of internal water in the FEBEX bentonite is ~30-36%. Water is mainly adsorbed in the interlayer space, but 3-6% of water is external water adsorbed on the external surface of the stacks, edges and OH groups.

Uptake of water occurs in three discrete stages as the montmorillonite structure expands. The distribution of water in the interlayer of the FEBEX bentonite powder may be classified in: a) monolayer hydrated state, which corresponds to a water content of 10.2%; b) two-monolayer hydrated state, which may be defined by two sub-states: i) formation of the second solvation shell, which corresponds to a water content of 18.3% and, ii) the filling of the free siloxane cavities and possible adsorption of water at external surfaces, which corresponds to a water content of 21.4%; and c) three-monolayer hydrated state, which corresponds to a water content of 31.9%. The FEBEX smectite stacks under laboratory conditions (RH = 50-60%) have two monolayers of water (d001 = 15.2 Å). In wetting experiments, the FEBEX montmorillonite expands in the c-dimension to acquire a maximum of three monolayers of water (d001 = 19.0 Å). However, in compacted bentonite, the amount of water depends on dry density.

Thus, it was found that most of the water in the powder bentonite with its hygroscopic water content (as received bentonite) resides in the interlayer space. Measurements indicated that ~5% may be regarded as being external water, implying a chloride concentration of 0.42 M, since the chloride inventory in the FEBEX bentonite is ~22 mmol/kg. The pH of the system is fixed by equilibrium with the atmosphere ($P_{\text{CO}_2} = 10^{-3.5}$ bar) and saturation with the carbonate phases present. Considering these premises, the pore water in equilibrium with the as received FEBEX bentonite was calculated to be Na-Ca-Mg chloride type with a high ionic strength, 0.66 M, and pH ~7.4.

A key issue in the geochemical modelling of the bentonite as a function of its dry density was the Cl⁻ accessible porosity, which was obtained from through-diffusion experiments. The bentonite pore water after re-saturation under constant volume conditions ($\rho_d = 1.65 \text{ g/cm}^3$) was calculated to be Na-Ca-Mg chloride type with a high ionic strength, 0.9 M, and pH ~7.4. Pore water chemistries at other initial dry densities may be readily calculated if the corresponding Cl⁻ accessible porosity values are available.

With a view to acquiring more detailed knowledge of the hydration behaviour of the bentonite, the natural FEBEX clay hydration was compared to that of the homoionic Ca or Na-clay and bi-ionic Ca/Na smectite with different Ca/Na ratios. The effect of the exchange complex on the bentonite hydration properties was

studied. Bentonite with variable amounts of exchangeable Na/Ca were prepared and studied under different relative humidity atmospheres.

The pure Ca-bentonite samples adsorb more water than the sodium samples, although close to saturation all the samples tend to behave similarly, regardless of sodium-calcium content. The Ca ion in the bentonite is surrounded by a larger number of water molecules than Na. Thus, the swelling of the Ca-bentonite starts at low relative humidity, forming a double layer of water molecules: First surrounding the cations and then occupying the free spaces among the groups of water molecules coordinated to the cations. The tri-layer complex forms only at very high relative humidity. The Na ion has a smaller number of coordinated water molecules than Ca, and forms one monolayer of water molecules, so the adsorbed water will fill the interlayer, will condense in capillary form in the micropores and may be adsorbed on the external surface. The Na sample can swell freely until a gel is formed. Several equation models were used to interpret the adsorption isotherms.

As a result of interaction with the granitic waters, as in the case of the Grimsel experiment, the bentonite may become more Ca enriched and eliminate its free water (intra- or inter-aggregates), which will enter the interlayer and form a bilayer. The trilayer can be formed only close to saturation, when the intra or inter-aggregate spaces may start to refill.

The water adsorbed by bentonite, equilibrated at different relative humidities, was extracted for isotopic analysis in order to deduce the mechanism of bentonite hydration and distinguish between the different types of water. The technique of vacuum extraction of water was implemented for this project, taking into account also the gravimetric and DTA-TG methods. The isotopic analysis of interstitial waters extracted from the bentonite indicated $\delta^{18}\text{O} = -0.83\text{‰}$ and $\delta^2\text{H} = -31\text{‰}$. These values might approximate to the average isotopic value of interstitial waters of bentonite in the Serrata de Níjar area in the Cabo de Gata region. For the Ca-exchanged bentonite, the water extracted at saturation is similar in value to that of the original sample. Samples equilibrated at other relative humidities show more negative δ values. This fact might be due to the different diffusion rates of light isotopes versus heavy ones. Lighter isotopes are more reactive than heavy isotopes. For samples at low relative humidity, the water vapour in the interlayer of the bentonite will come from the lightest atoms of oxygen and hydrogen. The relative proportion between the isotopes of ^{18}O and ^2H in the bentonite water, depending on the different relative humidity, may therefore affect ion diffusion and solute transport in the interstitial solutions.

The experiences regarding the squeezing extraction methods to obtain pore water from MX-80 bentonite have shown that most of the components of interest, such as Na^+ , K^+ , Ca^{2+} , Mg^{2+} , Si^{4+} , Cl^- , SO_4^{2-} , HCO_3^- and pH, may be determined without significant difficulties from squeezed pore water samples. However, S^{2-} , Fe^{2+} and Fe_{tot} appeared to be difficult to determine. Additionally, it was found that the density of bentonite affects the concentration of the pore water. Typical for successive extractions of pore water fractions is a decrease in the concentration as a function of increasing density. This is due to the exclusion caused by the overlapping electrical double layers. Reporting the density interval during squeezing is, therefore, most important for the interpretation and comparison of the results. The modelling of the data obtained by squeezing MX-80 bentonite samples at different densities saturated with external solutions of different ionic strengths suggested that the squeezed water comes both from the large pores and from the interlamellar pores, the relative amounts depending on the density of the sample.

The rheological properties of FEBEX bentonite suspensions saturated with different Na/Ca ratios were studied. The suspensions behave as a plastic fluid at low shear rates and as a pseudo-plastic fluid at higher shear rates. In all cases, the increase in solid concentration induces an increase in the viscosity of the suspension. This behaviour is strongly affected by the composition of the exchange complex. A high content of exchangeable Na raises the suspension viscosity. For instance, in order to prepare a suspension of similar viscosity (15 mPa·s), only 10 % of pure Na-bentonite is needed while 55 % of solid is needed for the Ca bentonite. The low viscosity of Ca samples produces an increase in suspension fluency and its contribution to mass transport. As regards nuclear waste repositories, the bentonite at the granite interface takes up Ca from the percolating solutions and becomes progressively enriched in Ca. According to the results obtained, under conditions of high input of groundwater to the interface, the increase in

interlayered Ca may contribute to suspension of the smectite in the percolating solutions that might fill and seal fractures.

4.2.2 Geochemical processes at the bentonite/solution interface

The dissolution of bentonite phases under barrier conditions is a process that should be included in any predictive model, since this reaction may be accelerated in zones with favourable conditions (concrete barriers or plugs, acidic fronts, or accumulation of organic matter or micro-organisms). The hydraulic properties of the barrier do not provide the flux required for producing and maintaining a massive dissolution initially, but this process might initiate locally and then spread and increase through fractures and discontinuities. Thus, dissolution studies were carried out. Smectite, plagioclase and volcanic glass were separated and studied in flow-through reactors. Temperature, pH, flow rate, solid/solution ratio and input solution were controlled.

The results indicate that the change in dissolution rates within the pH range from 7 to 8.5 is small at constant temperature. However, important variations are observed outside this interval. The most important effect of temperature is observed in the glass, and it is very small in plagioclase. In conclusion: a) The bentonite dissolution rate increases by four when temperature rises from 25 to 50°C; b) the contribution of plagioclase dissolution to the overall rate seems to be negligible. It allows us to assess that the process is governed by smectite and tuff; c) at 25°C, the smectite makes a 70% contribution to the overall rate; d) at 50°C, tuff dissolution increases by nine, representing two thirds of the total, whereas the smectite dissolution rate only doubles. This is a very important fact, because the conditions within the barrier are quite similar to those of smectite formation in natural environments and the dissolution product of the accessories may produce additional smectite.

4.2.3 Processes of radionuclide sorption and transport in the bentonite

Accessible porosities for HTO (for all clay densities) and $^{36}\text{Cl}^-$ (for clay densities up to 1.2 g/cm³) were obtained directly through saturation experiments. In these experiments the water-saturated bentonite samples were introduced in a reservoir with the tracer until equilibrium concentration was reached. The measurement of tracer activity in the clay pore water allowed for direct measurement of the accessible porosity. Alternative estimates of accessible porosity were accomplished in through-diffusion experiments with constant concentration and through concentration profile experiments, which provided redundant, albeit less precise, methods for estimation. Similar values of accessible porosities were obtained with the three methods.

The results showed that in the FEBEX bentonite the accessible porosity for HTO agrees very well with total porosity, this implying that all the pores in compacted bentonite are available for the diffusion of neutral species. Different results were obtained in the case of Cl^- , for which the accessible porosity is significantly smaller than total porosity, even at the lower densities (at 1.65 g/cm³, the porosity accessible to Cl^- is ~3%). Results for chloride clearly show that the FEBEX bentonite displays a significant anionic exclusion.

For HTO, the independently measured values of apparent diffusion coefficient (D_a), effective diffusion coefficient (D_e) and accessible porosity (ϕ) satisfy the relation between effective and apparent diffusion coefficients for conservative tracers. The consistency of the transport parameters measured using different methods confirms that these methods are appropriate and that the values obtained are correct. The experimental values may be adjusted using exponential functions of the type $D_{a,e} = A \cdot e^{-B\rho_d}$, where A and B are constants and ρ_d is the bentonite dry density. Thus, accessible porosity and apparent and effective diffusion coefficients in the FEBEX bentonite may be easily estimated at any dry density by interpolation.

Diffusion experiments performed using non-conservative tracers (U, Eu and Nd) allowed the diffusion database needed for the modelling of transport processes of the “in situ” and “mock-up” tracer tests to be

completed. The K_d of various radionuclides was directly determined in the compacted clay, for comparison of the values with those determined by batch experiments or indirectly by diffusion tests.

Batch sorption experiments of Cs(I), Sr(II) and U(VI) have been carried out on homo-ionic (Na and/or Ca) SWy-1 montmorillonite to obtain a mechanistic understanding of sorption in bentonite. The sorption of caesium in both the FEBEX and the SWy-1 homoionised clays showed non-linear behaviour. Since caesium may be present in solution only as the species Cs^+ , the non-linear sorption indicates the existence of at least two different sorption sites. The first sorption site is of "high" affinity and low capacity, whereas the second type of sorption site is of "low" affinity and high capacity ($\sim$ the CEC of the clay). In the light of the kinetic experiments carried out in the FEBEX montmorillonite, the adsorption of caesium seems to involve a rapid exchange reaction (hours) and a slower component (days), which seems to be an anomalous behaviour pattern for ion-exchange reactions. This slow process is in evidence only when very low tracer concentrations are used ($<10^{-9}$ M), due to the very low density of the high affinity sites ($\sim 3 \times 10^{-8}$ eq/g) compared to the bentonite cation exchange capacity. In relation to the concept of high affinity and low affinity sites, the sorption process may be described in two steps: adsorption on the planar sites (rapid process) and diffusion to less available but highly selective sites (slow process). The existence of "low" and "high" affinity sites for caesium sorption in clays is usually explained by considering that caesium may be exchanged with hydrated cations in basal/interlayer sites (low affinity sites) and may sorb, in a highly selective manner, in frayed edge sites (FES, high affinity sites). FES sites are not present in expanding clays like smectite but develop in weathered micas and illite.

The SWy-1 montmorillonite contains $\sim 1\%$ illite, consequently a caesium sorption model was developed for SWy-1. This model is based on the proposition that the uptake of Cs in argillaceous rocks is dominated by the illite clay mineral component due to its FES sites. It successfully modelled the sorption results both in the Na and in the Ca-clay system. The first assumption of the model is that, in addition to the montmorillonite component, Cs sorption in SWy-1 is governed by cation exchange reactions affecting the illite mineral component. For the purposes of calculating Cs sorption in SWy-1, the cation exchange capacity of the illite was assumed to be equal to 0.20 eq/kg. The uptake of Cs on illite is envisaged as taking place on three site types, each having different capacities and affinities, known as frayed edge (FES), type II and planar sites. These site capacities were scaled to the illite content in the SWy-1 system and fixed. Thirdly, selectivity coefficients for Cs-Na were taken directly from previous studies.

On the other hand, illite was never detected as a "pure" phase by XRD in the FEBEX clay, the mineralogical studies showing that the smectite phase is actually made up by illite-smectite mixed layer containing 10-15 % of illite layers. The existence of smectite-illite mixed layer may possibly lead to the existence of FES-like sorption sites in FEBEX bentonite; however, the illite in the illite-smectite mixed layer may not behave exactly in the same manner as a pure illite phase. This may be the main reason why modelling of the Cs sorption data in accordance with the aforementioned model (considering a 10% content of illite in the FEBEX bentonite) was not successful. Therefore, the sorption of caesium on the FEBEX bentonite was interpreted using a 2-site model (2 "generic" sites), considering ion-exchange in both the "high" affinity and "low" affinity cases. This model satisfactorily reproduced the experimental data.

Sorption edges (0.01 and 0.1 M Na-SWy-1) and isotherms (0.1 M Na-SWy-1, pH 7.2 and 0.005 M Ca-SWy-1, pH 7.6) have been determined for strontium. At $\text{pH} < \sim 9$, the data may be interpreted by means of a simple cation exchange mechanism. The sorption edges and isotherm in Na-SWy-1 and the sorption isotherm in Ca-SWy-1 were modelled with $\frac{S_r}{N_a} K_c = 4.5$ and $\frac{S_r}{C_a} K_c = 1.0$ respectively. With pH values above 9, a clear increase in sorption occurred for the 0.1 M Na-SWy-1 edge data, which is due to a surface complexation mechanism.

Sorption experiments for uranium, in both the FEBEX and the SWy-1 homoionised clays, were carried out. The edge data indicated that there is a clear influence of pH, which is indicative of a surface complexation mechanism. An effect of the Na background electrolyte concentration was observed at low pH, which is characteristic of cation exchange. The sorption edge and isotherm data were interpreted in

terms of both uptake mechanisms, and were successfully modelled using the 2-site protolysis non-electrostatic cation exchange/surface complexation model.

4.3 Gas generation tests

The gas generation tests performed during FEBEX I indicated that carbon dioxide is the only gas component of importance released from the backfill material in the temperature range between 20 and 100 °C under aerobic or anaerobic conditions and for exposure times of up to 100 days. Screening tests with much longer exposure times at 100 °C indicated that the amount of released gases was increasing. Therefore, the FEBEX I investigation programme was continued within FEBEX II.

Glass ampoules with a volume of 500 ml were filled with 10 or 100 grams of bentonite ground from the compacted blocks. Since the type of gas (air or nitrogen) in the residual volume of the ampoules had not influenced the gas generation in phase I, only laboratory air was used to fill the residual volume. In addition, 10 or 100 ml of Grimsel groundwater were added to one half of the ampoules. After filling, the ampoules were sealed to make them gastight and placed in an oven at 100 °C for 1, 10, 100, 300, 1000 and 2000 days. A total 55 ampoules were prepared for the entire investigation programme.

This investigation again indicated that carbon dioxide is the only gas generated and released from the bentonite at a temperature of 100 °C. The results for the natural dry and wet stages (additional 10 ml water per 10 g bentonite) as a function of exposure time are shown in Figure 23. In the wet stage, up to 1.8 m³ per 1000 kg of bentonite of carbon dioxide were released, and equilibrium appears to be reached under the existing physico-chemical conditions. In the natural dry stage of the bentonite, up to 0.4 m³ per 1000 kg of bentonite of carbon dioxide were released, and equilibrium appears not to be reached. The reason for this difference might be that in the dry stage, carbon dioxide is partly adsorbed to the internal surfaces of the clay. In the wet stage water is adsorbed and carbon dioxide is desorbed and released into the residual volume. When the amount of bentonite in the ampoule is increased from 10 to 100 g, the specific amount of carbon dioxide released decreases, this meaning that with a higher concentration of carbon dioxide in the residual volume of the ampoule, back reaction will take place. It is most likely that carbon dioxide is generated by oxidation of the organic components in the clay in the presence of oxygen adsorbed to the clay.

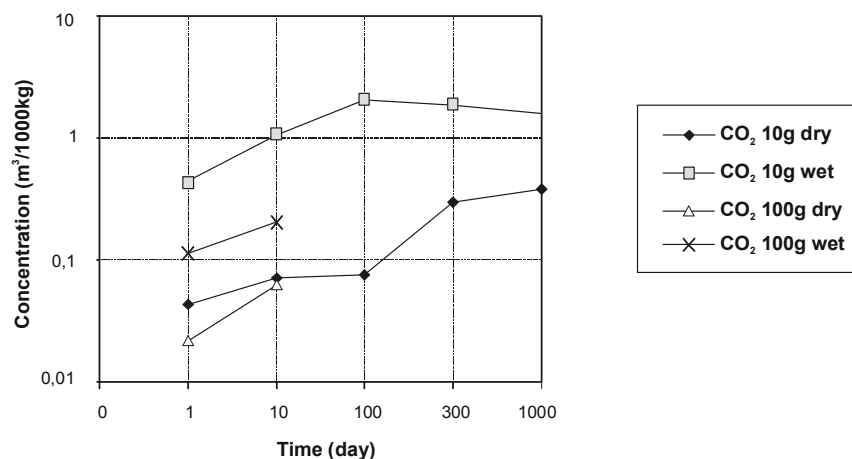


Figure 23: Release of carbon dioxide from the bentonite in the natural dry and wet stages as a function of exposure time at 100°C

5 MODELLING

5.1 THM modelling

The main activities in the area of THM modelling have focused on critical analysis of the evolution of the large-scale experiments. As regards the “mock-up” test, three main kinds of analyses may be distinguished:

- Performance of concurrent analyses and comparison with experimental results.
- Analyses to assist in the interpretation of “mock-up” test evolution, more especially the examination of certain differences between the test results and numerical predictions.
- Analysis of the short-term effects of the overheating episode in the “mock-up” test.

As regards the “in situ” test, the activities have focused on the following:

- Updating of the comparison between experimental results and model predictions in the engineered barrier and host rock.
- Simulation of the cooling, excavation and dismantling processes.

Additionally, important efforts have been made in the experimental validation of the constitutive laws adopted in the modelling of the thermal, hydraulic and mechanical problem. Different laboratory tests (oedometric, swelling pressure, permeability and large cell tests, among others) have been used to define the constitutive laws and to obtain their parameters.

5.1.1 “Mock-up” test modelling

- Performance of concurrent analyses and comparison with experimental results.

The last records considered in the comparisons were obtained on 18th September 2003, corresponding to day 2417 as from starting of the heaters (i.e. approximately 6.62 years). The model used in this simulation is that denoted as OBC (Operational Base Case).

The model yields good results in relation to the thermal problem. This is reflected, for example, in the comparison with the power emitted by the heaters, Figure 24. As regards the hydraulic problem, until day 900 (approximately) of the test, the model provides a successful reproduction of hydraulic parameters concerning water entry in the test (Figure 25) and the distribution of relative humidities, as indicated by Figure 26 and Figure 27 (time variation). From day 900 onwards, certain differences are observed between the hydraulic behaviour of the test and the model predictions. In terms of water entry, the model results progressively move away from the experimental data. As regards the evolution of relative humidity, it may be noted that in the heater regions (sections A4 and B4, Figure 26) there is a significant reduction in the rate of relative humidity increase. On the other hand, when a ‘cold cross-section’ (section away from the heater) is examined, the differences in the progress of hydration are less perceptible (Sections A10 and B10, Figure 27). Note that some minor differences between the model and test results may also be detected in these sections as from day 2000 (approximately). In Figure 25 and Figure 26 may be observed the influence of an unplanned overheating episode (which took place close to day 1391) on the evolution of barrier hydration. The tendency observed before the overheating appears now to have been recovered, with a clear slowing down of the rate of water intake compared to the model predictions. As regards the mechanical problem, the results are good, with the stresses responding to the modifications of hydration pattern due to the strong hydro-mechanical coupling of the problem. The predictions are particularly good for

data before overheating. This event had a noticeable effect on the mechanical problem in the ‘hot cross sections’ (section involving heaters).

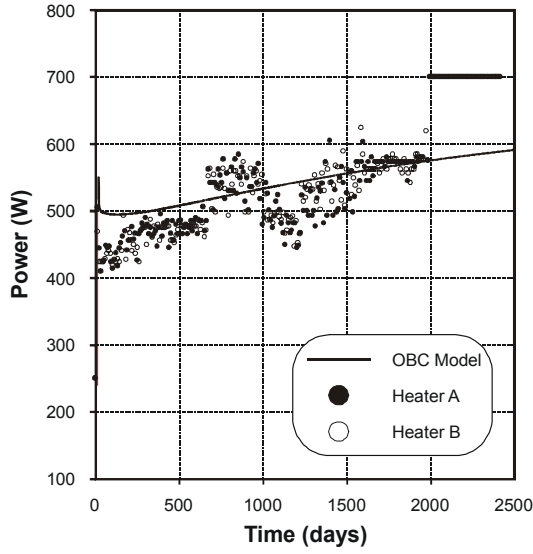


Figure 24: Evolution of heater power in the ‘mock-up’ test. Observed and computed values. (OBC model)

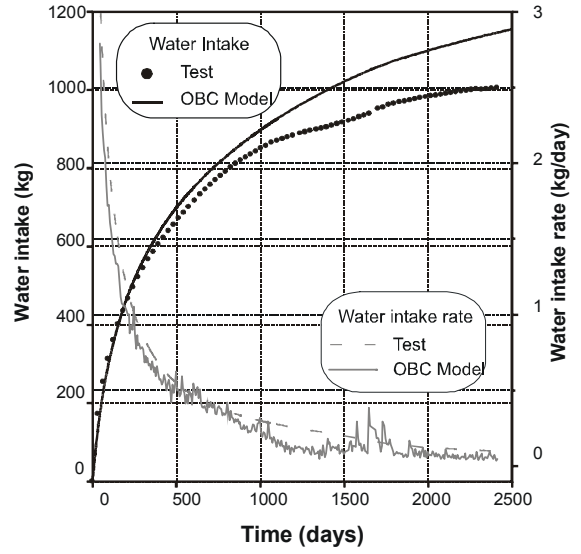


Figure 25: Evolution of water entry in the ‘mock-up’ test. Observed and computed values (OBC model)

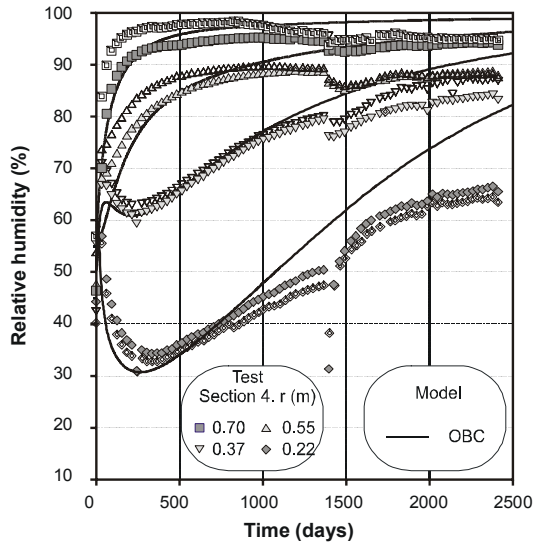


Figure 26: Evolution of relative humidity in the ‘mock-up’ test. Sections A4-B4 (‘hot cross-section’). Observed versus computed values (OBC model)

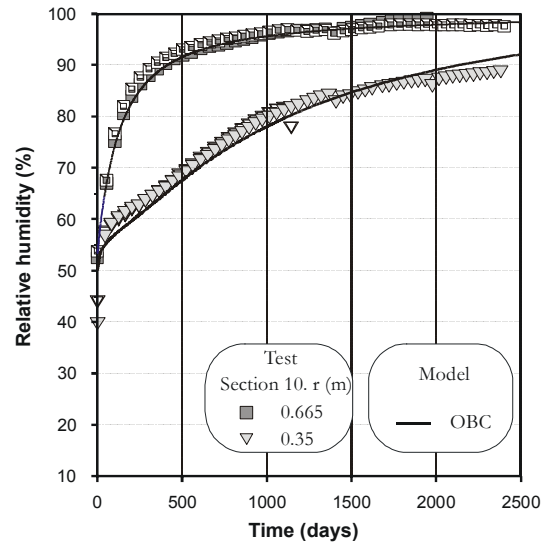


Figure 27: Evolution of relative humidity in the ‘mock-up’ test. Sections A10-B10 (‘cold cross-section’). Observed versus computed values (OBC model)

- Analyses to assist in the interpretation of “mock-up” test evolution.

The analysis of the differences between “mock-up” data and model results has received preferential attention during this period. The understanding and explanation of the apparent decay in the rate of hydration of the barrier are viewed as being an important aspect related to the performance of reliable long-term predictions. Once it had been verified that there were no problems in the water supply system, and also that changes in the parameters of the THM constitutive laws could not explain the unexpected behaviour of the barrier, research focused on the identification of other processes that might be responsible for the apparent slowing down of barrier hydration. A series of preliminary analyses have been performed using ‘non-standard flow models’. Three principal lines of research have been explored: 1) Existence of a threshold gradient, 2) thermo-coupling effects and 3) microfabric evolution. The inclusion of chemical effects, and their THM couplings, in the study of barrier evolution is envisaged for future work. In view of the results obtained, it may be said that each phenomenon might explain, to some extent, the unforeseen response of the experiment. The changes in the microfabric are considered to constitute the most promising phenomenon for explanation of the behaviour of the barrier because there is some experimental evidence to support its existence. Therefore, a more detailed analysis of the effects of the clay fabric changes has been carried out using a double structure framework. The use of such type of model seems to be suitable for the case of the FEBEX bentonite, in which the two pore levels actually exist. The modelling results may be considered very satisfactory, since the main tendencies of the observed behaviour have been correctly reproduced. For instance, in Figure 28 and Figure 29 the results of the double structure model (‘Dou’) are presented together with experimental data; the ‘OBC’ predictions are also shown (dashed line). It may be observed that the evolution of water intake is very accurately reproduced by the ‘Dou’ model. The model clearly captures, in qualitative terms, the evolution of relative humidity, especially in the internal zones. Good results are also obtained for the thermal and mechanical problem. In contrast to the ‘OBC’ model, the ‘Dou’ model predicts slow hydration of the barrier. This is qualitatively in agreement with the tendency observed in the barrier.

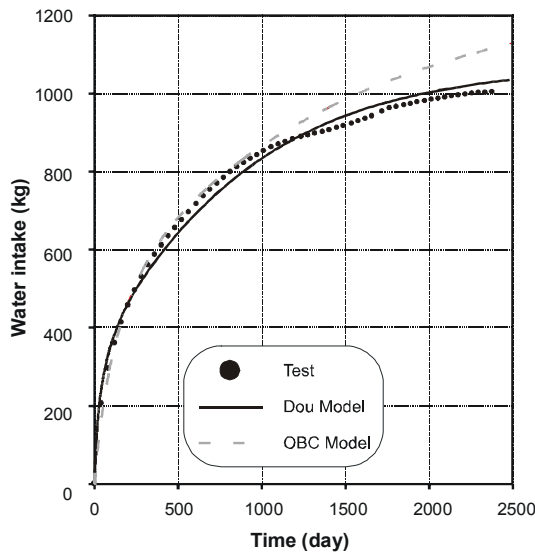


Figure 28: Water intake. Observed versus computed values of ‘Dou’ and ‘OBC’ models

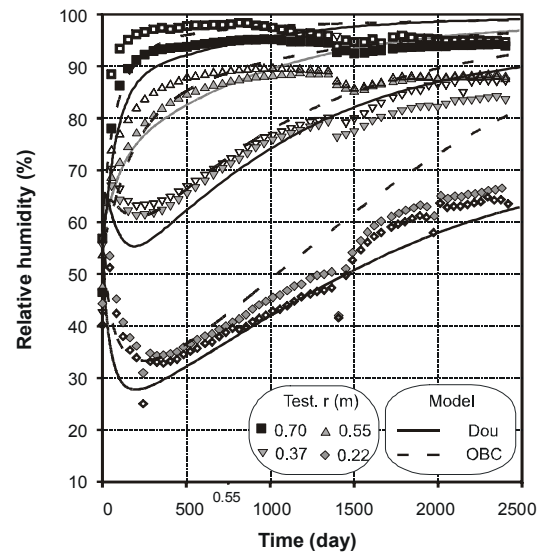


Figure 29: Relative humidity. Sections A4-B4. Observed versus computed values of ‘Dou’ and ‘OBC’ models

- Analysis of the short-term effects of the overheating episode in the “mock-up” test.

Numerical analysis has been performed to explain and reproduce the irreversible behaviour observed in the FEBEX bentonite during the accidental overheating that took place on day 1391 of the experiment. It has been shown that the model is able to reproduce the major features of the observed mechanical behaviour in response to a complex history involving temperature and suction changes.

5.1.2 “In-situ” test modelling

- Updating of the comparison between experimental results and model predictions in the engineered barrier and host rock.

The results of the ‘in situ’ test have been updated until May 5, 2004, 2650 days (~7.3 years) after the start of heating.

Clay barrier: The model successfully captures the general thermal behaviour of the test. This suggests that the physical assumptions of the model are correct and that the differences may be due simply to discrepancies in the adopted parameters. For instance, Figure 30 presents the evolution of the power emitted by heater No. 2. It may be observed that the model correctly reproduces the tendency to increase power when heater No. 1 is switched off. As regards the hydraulic (i.e. Figure 31) and mechanical problems, it may be concluded that the response of the model is satisfactory overall, with the various phenomena adequately reproduced.

Host rock: The comparison between the numerical simulation and the observed THM behaviour in the host rock demonstrates that the performance of the model is once again satisfactory. It may be observed that the model captures very well the effect that the cooling of heater No. 1 and the barrier excavation have on rock mass behaviour (i.e. Figure 32 and Figure 33).

- Simulation of the cooling, excavation and dismantling processes.

A complete numerical analysis of the dismantling process of the ‘in-situ’ test has been performed, including the modelling of the cooling and excavation stages. The model results presented in Figure 30 to Figure 33 include the simulation of the dismantling process.

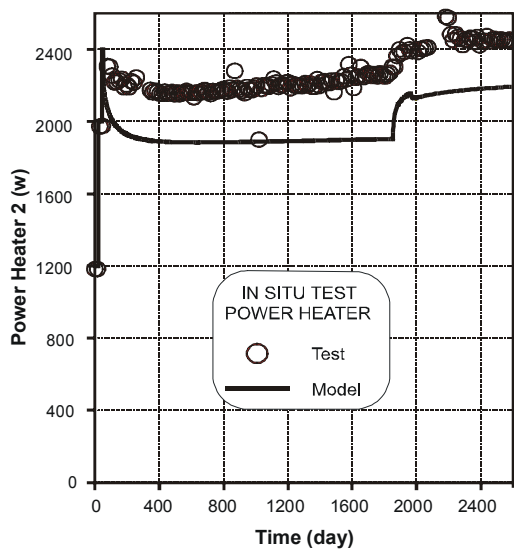


Figure 30: Heater 2 power. Observed and computed values, “in situ” test

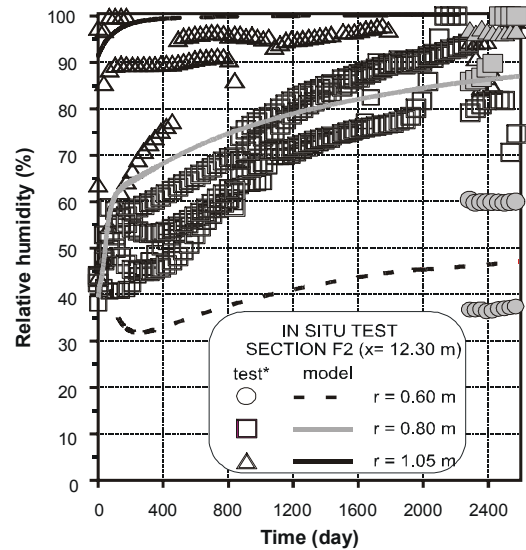


Figure 31: Relative humidity in section F2 of the “in situ” test. Observed and computed values. (*bold symbols correspond to sensors installed after dismantling)

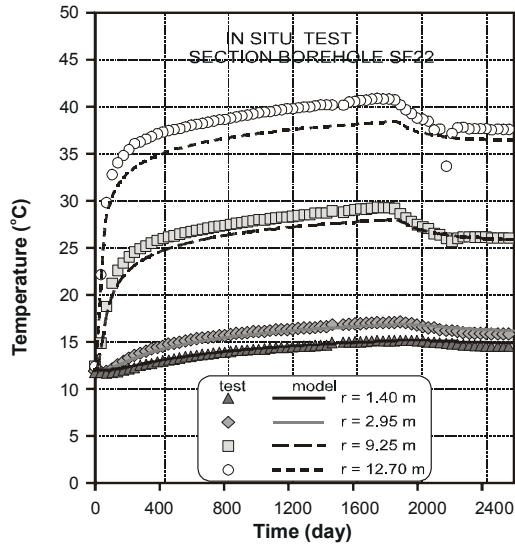


Figure 32: Temperatures in borehole SF21. Observed and computed values, “in situ” test

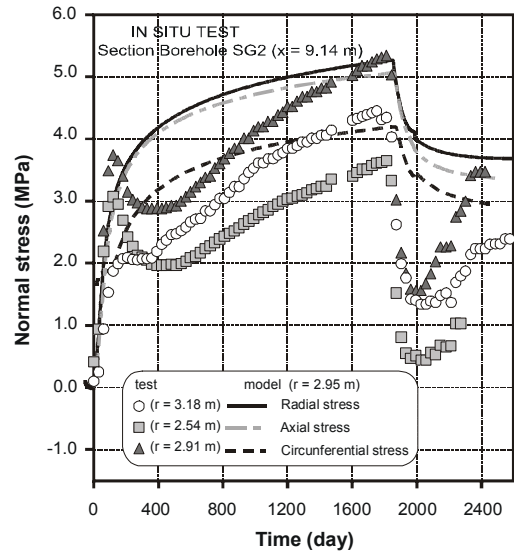


Figure 33: Normal stresses in borehole SG2. Observed and computed values, “in situ” test

5.2 THG modelling

5.2.1 Improvements in THG codes

The following features have been implemented in FADES-CORE:

- Accounting for more appropriate speciation models under high salinity conditions by implementing Pitzer equations for the computation of solute activities.
- Computation and checking for charge balance, using methods which preserve charge balance even when diffusion coefficients are different for each chemical species.
- Including double porosity models.
- Accounting for changes in porosity caused by dissolution/precipitation phenomena.
- Implementing a constitutive law for permeability as a function of ionic strength derived from the Diffuse Double Layer Theory.
- Accounting for chemical kinetic processes.
- Implementing the option of automatic estimation of flow, heat, solute transport and geochemical parameters in order to allow for more efficient and comprehensive use of the available data.
- Incorporating algorithms which improve the numerical efficiency in solving coupled solute transport and geochemical reactions, especially for kinetically-controlled processes.

5.2.2 Improvements in THG conceptual models

- Accounting for the dependence of hydraulic conductivity with ionic strength *and cation exchange composition*.
- Redox processes.

- Evaluation of the relevance of gaseous species.
- Anion exclusion effects for selected anions.
- Identification of the main geochemical processes triggered by corrosion products.
- Dependence of permeability on pore water chemistry.

The data reported and published have been adjusted to theoretical expressions which relates the permeability to the ionic strength of pore water.

5.2.3 THG modelling of laboratory tests

Improvements in THG models have been checked and tested by using data from laboratory tests. Aqueous extract tests have been modelled in order to improve the estimation of bentonite pore water chemistry under ambient conditions ($w = 14\%$). A long-term permeability test has been interpreted numerically using single and double porosity models and three conceptual geochemical models. The results from modelling indicate the following:

- Anion exclusion is a relevant process for chloride transport – models without exclusion fail to reproduce the breakthrough curve of chloride. Chloride can access 35% of the mobile-part pores and 58% of the immobile pores.
- The measured data fall within the bands of computed breakthrough curves with three possible conceptual geochemical models using a single porosity model.
- Major discrepancies between model results and measured data are found for bicarbonate, which might be related to changes in the pressure of $\text{CO}_{2(g)}$, these not being considered in the model.
- Chloride and sodium data tend to support the double porosity model.

5.2.4 THG modelling of the “mock-up” test

The THG model of the “mock up” test has been updated and improved throughout FEBEX II. The following tasks have been performed:

- Calibration of the thermo-hydrodynamic model using thermal and hydrodynamic data.
- Modelling of unexpected trends in hydration. The effect of permeability increasing with ionic strength has been evaluated. Simulations have also been produced for “cold areas”, i.e. areas of the buffer far from the heaters.
- Modelling of the “overheating episode”.
- Updating of predictions of thermo-hydro-geochemical evolution and tracer migration through the barrier.

The relevance of cross diffusion has been addressed for the purpose of preserving charge balance in THG models. Numerical analyses of the THG model for the “mock-up” test and cell CT23 indicate that the model results change significantly due to cross diffusion. Cross diffusion coefficients are especially relevant for chloride and sodium. Accounting for permeability changes caused by changes in ionic strength in the THG model of the “mock-up” test leads to an improvement in the adjustment of measured cumulative water inflow and relative humidity. However, there are still discrepancies between the

modelling results and measurements, which might be explained in terms of double porosity behaviour and swelling phenomena.

5.2.5 THG modelling of the “in situ” test

Data from the dismantling of the “in situ” test were used to test and validate THG models of the EBS. Firstly, the THG model of the “in situ” test was updated and improved in keeping with the conclusions drawn from the THG model of the “mock-up” test. A recalibration of the TH model has been performed. Pre-dismantling THG predictions were prepared, which were used for comparison with the measured geochemical data. Numerical predictions of deuterium migration were performed and compared to the measured data.

Analysis of the available deuterium data does not allow clear conclusions to be drawn, due to the lack of accuracy of such data and uncertainties regarding the breakage of glass ampoules. Although the precision of the deuterium data for aqueous extract samples is 0.8 ‰, this analytical error translates into large errors for bentonite pore water values. The reinterpreted deuterium data show a high degree of scatter and a lack of any clear trend. Model predictions of deuterium transport with and without ampoule breaking fall within the values of the data available. The deuterium added in glass ampoules probably diffused to such an extent through the bentonite that no signs of the initial pulse remain after 5 ½ years of diffusion.

Numerical predictions of the hydro-geochemical evolution of the “in situ” test have been compared to the geochemical data measured and collected after the dismantling of heater No. 1. Most chemical data have been obtained with aqueous extract methods, which require the use of geochemical models for their interpretation in order to account for the geochemical processes undergone by the bentonite samples during aqueous extraction. The comparison of predicted and measured values using the available data indicates that:

- THG predictions capture the trends of most chemical species.
- Most chemical species show their largest concentrations near the heater and decrease with radial distance.
- The data in one of the sections analysed fall within the band of computed values.
- Aqueous extract sulphate data show trends different from those of the squeezing data. The model predictions are more coherent with squeezing data than with aqueous extract data.

5.3 THM modelling of the rock mass

As part of the study on the possibility of a potential EDZ being generated in the rock surrounding the gallery, various numerical analyses were performed on the “in situ” test: a one-dimension of THM simulation, several two-dimensional TM analyses and a three-dimensional TM calculation.

The stresses calculated using these models were compared to the available data on the resistance of the Grimsel granite. The results show that the maximum stresses – generated both by excavation and by the experiment – are much lower than the minimum strength of the rock. In other words, the numerical analyses of the stress states also indicate that the rock has not been damaged close to the gallery wall. This is yet a further indication of the non-existence of an EDZ in the FEBEX gallery.

6 ASSESSMENT OF RESULTS AND CONCLUSIONS

6.1 “In situ” test

The activities performed with regard to the “in situ” test have met the objectives defined in the work plan:

- The FEBEX demonstration objective has been completed, on the one hand, through direct observation and analysis of the state of the bentonite barrier - which closely agree with the forecasts regarding the closure of all the voids and the homogenisation of the barrier with hydration - and, on the other hand, by checking the status of the measuring instruments.
- Apart from contributing to verification of the forecast behaviour of the barrier, the data provided by the post-mortem laboratory tests on the bentonite have served to check the reliability of the monitoring data and, consequently, increase confidence in the comparison with the results of modelling. They have also served to check the predictions of the geochemical model.
- The non-existence of an EDZ in the FEBEX gallery is of value only in relation to the Grimsel granite massif and, perhaps, that of the FEBEX gallery. However, the study methods used may be generally applied to any massif. The same may be said of the non-variation of the hydraulic properties of the rock massif near field.
- The shotcrete technology tested for the closure plug of the non-dismantled part of the test may be of use in a real repository.

6.2 “Mock-up” test

The only objective established for the “mock-up” was the supervision, control and management of the monitoring data, in order to continue checking of the model predictions. This has been accomplished according to planning.

6.3 Laboratory tests

The main objectives proposed for the THM and THG investigations during FEBEX II have been fulfilled.

With respect to the THM studies, the information on the aspects affecting the retention capacity of the bentonite has greatly increased, as has knowledge of the effects of temperature and salinity on several hydro-mechanical properties. The water infiltration mechanisms are also better understood, which has allowed for improvement of the models. Several techniques for characterisation of the bentonite microstructure have been tested. As a result, a deeper insight into the behaviour of compacted bentonite, and the basic mechanisms controlling it, has been achieved by taking into account the interplay between the microstructural and macrostructural levels. However, further complementary studies may be necessary to provide more information on the mechanisms influencing pore size distribution changes in high active clays. More research effort must be dedicated to the study of certain specific aspects, such as the existence of a threshold hydraulic gradient, water flow under low hydraulic gradients, the effect of osmotic and temperature gradients on this flow and, more generally, current knowledge of the physico-chemical aspects of clay microstructure should be related to the macroscopic behaviour of compacted bentonite.

Regarding THG activities, considerable progress has been made in the acquisition and modelling of bentonite pore water chemistry. Different types of water have been distinguished and characterised. The effect of pore water composition on anionic exclusion is an interesting issue to be studied in the future. The influence of the exchangeable cations of bentonite on water adsorption capacity has been analysed. Furthermore, the factors affecting the dissolution of bentonite have been identified. The sorption experiments have allowed for the determination of quasi-thermodynamic parameters for Cs and U. Exponential relations have been found between the diffusion coefficients of HTO and chloride and the

dry density of the FEBEX bentonite, this allowing these parameters to be easily determined at any dry density. Further studies should be devoted to analysis of the influence of water salinity on the anion exclusion processes that take place in bentonite and, consequently, on the diffusion coefficients.

The results obtained during FEBEX I on gas generation in bentonite have been confirmed.

6.4 Modelling

FEBEX II came about on the basis of the two following ideas: 1) good performance of the heating system and of the instruments in both large-scale tests, which authorised continuation of the test, and 2) the good expectations existing regarding the prediction capacity of the THM and THG models. At the same time, the need for certain theoretical improvements and, mainly, improvement in determining certain parameters and constitutive laws, also pointed to the need for FEBEX II.

Noteworthy improvements have been achieved as regards acquisition of the parameters and constitutive laws, as pointed out in evaluation of the laboratory tests. Progress has been made also in development of the theoretical models.

The THM modelling reflects the processes fairly well both overall and quantitatively, especially in the short term. The THG modelling captures the concentration tendencies of almost all the chemical species. In addition, in the attempts to resolve the causes of the differences between the “mock-up” thermo-hydro-dynamic data and the model predictions, more detailed insight has been gained into the behaviour of the clay barrier and it has even been possible to improve the adjustment of certain aspects. However, there are still gaps in knowledge of the processes, as is demonstrated by the clearly different tendencies shown by relative humidity between the monitoring data and the results of modelling, especially in the more hydrated zone of the barrier. Consequently, there is a need for research to continue on this divergence, which might have consequences for other hydration-dependent variables, unless this was demonstrated to be irrelevant from the point of view of repository safety assessment.

7 REFERENCES

7.1 FEBEX Project internal deliverables

D1a to g; AITEMIN; Sensors data report (1st op. phase), #20 to #26

D2; GRS; Gas sampling and analysis report (1st op. Ph.), including results on gas generation tests

D3; AITEMIN; Hydro-geological tests report (1st op. Phase)

D4; AITEMIN; Dismantling plan v.2

D7; AITEMIN; Dismantling of the heater 1 at the FEBEX "in situ" test (v1)

D8a to d; AITEMIN; Sensors data report (2nd op. phase) #27

D9b; GRS; Gas sampling and analysis report (2nd operational phase), including results on gas generation tests #2

D10; AITEMIN; Hydro-geological tests report (2nd op. phase)

D11; CIEMAT; Bentonite analyses report

D12; G3S; EDZ report

D13; AITEMIN; Corrosion analysis report

D14; AITEMIN; Instruments analysis report

D15a and D15c to l; CIEMAT; Sensors data report #14 to #24

D15b; CIEMAT; Sensors data report overheating episode

D16; CIEMAT; Hydration water analysis report

D17/3; CIEMAT; Results on THM laboratory tests #3

D18/3; CIEMAT; Results on THG laboratory tests #3

D19/3; UPC; Final report on THM modelling results (incorporates D21, Final THM analysis of the “In situ” test; and D22, Integrated THM-G analysis of the laboratory and “In situ” test)

D24a, UDC; Update of the thermo-hydro- geochemical model of the mock-up test.

D25; UDC; THG Final THG modelling report

D26; UPM; THM analysis of the rock mass #1 ((In preparation))?

7.2 Other references

ENRESA. FEBEX project. Full-scale engineered barriers experiment for a deep geological repository for high level radioactive waste in crystalline host rock. Final Report. Madrid Publicación Técnica 1/2000.

ENRESA. FEBEX internal report, ref.70-ST-H-0-4 v1.0. Full-Scale Engineered Barrier Experiment in Crystalline Host Rock- Phase II. Test Plan.

EUR 19147 EN, 2000. Project report, Full-scale engineered barriers experiment for a deep geological repository for high-active waste in crystalline host rock (FEBEX project). European Commission, Nuclear Science and Technology.

APPENDIX

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