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PEBS

Long-term Performance of Engineered Barrier Systems

PEBS

Final Scientific Report

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Executive summary

The fundamental basis of geological disposal concepts for spent nuclear fuel and high level radioactive wastes is generally a multi-barrier system. The engineered barriers play a central role in this system to ensure the containment and long-term retardation of radionuclide release. Understanding the performance of engineered barrier systems (EBS) is therefore crucial to evaluate the safety of disposal concepts of radioactive waste in geological formations.

The 7th Framework EURATOM project PEBS was initiated in 2010 to study the complex interaction of thermal, hydraulic, mechanical and chemical (THMC) processes in clay-based EBS for geological repositories. During the four year project, investigations were performed by 17 partners from Europe, China and Japan, including waste management organisations, research institutes and consultants.

The work performed within PEBS involved several laboratory and in-situ experiments, covering a broad range of time and spatial scales. The experimental results provided the database for the validation and enhancement of coupled numerical simulations. New material models were developed and applied for the extrapolation of the observed EBS behaviour to the long-term performance. A special focus was the integration of existing and newly gained knowledge on the EBS evolution in order to constrain the conceptual and parametric uncertainties in the context of long-term safety assessment.

With the described comprehensive scientific approach, the PEBS project was thus able to

- deepen the knowledge and understanding of the THM-C evolution of the EBS;
- provide a more quantitative basis for relating the evolutionary behaviour of the EBS to its safety functions as a repository system component;
- clarify further the significance of residual uncertainties for long-term performance assessment.

In addition to the scientific objectives, the dissemination of the essential results to the broad scientific community within the EC, China and Japan was an important aim of the project. The consortium used its expertise for public information purposes and to promote knowledge and technology transfer through training.

1. Introduction

1.1. Project context

The evolution of the engineered barrier system (EBS) of geological repositories for spent fuel (SF) and high level radioactive waste (HLW) has been the subject of many national and international research programmes during the last years. The emphasis of these research activities was on the elaboration of a detailed understanding of the complex coupled thermo-hydro-mechanical and –chemical (THM-C) processes, which are expected to evolve in the EBS in the early post closure period of the repository. From the perspective of radiological long-term safety, an in-depth understanding of these coupled processes is of great significance, because the evolution of the EBS during the early post-closure phase may have a non-negligible impact on the radiological safety functions at later stages of the repository's lifetime. Process interactions during the resaturation phase (heat pulse, gas generation, non-uniform water uptake from the host rock) could impair the homogeneity of the safety-relevant properties of the EBS (e.g. swelling pressure, hydraulic conductivity, diffusivity).

In previous EU-supported research programmes such as FEBEX, ESDRED and NF-PRO, remarkable advances have been made to broaden the scientific understanding of THM-C coupled processes in the near field around the waste canisters (NF-PRO 2008, ESDRED 2009). The experimental data bases were extended on the laboratory- and field-scale and numerical simulation tools were developed. As one conclusion of these previous research activities, a need was stated for integrating this in-depth process understanding into constraining the conceptual and parametric uncertainties in the context of long-term safety assessment. It was recognised that Performance Assessment (PA) related uncertainties could not be reduced significantly with the newly developed THM-C codes due to a lack of confidence in their predictive capabilities on time scales which are relevant for PA. To gain confidence in the simulations of the coupled processes in the canister near field a general need was stated for:

- Systematic and traceable validation procedures, which allow qualifying the predictive capabilities of the THM-C codes with quantitative performance indicators such as post-experimental evaluations (e.g. evaluations of blind predictions, dismantling of experiments and post-experimental analyses);
- Adaptations in the PA methodologies, which would allow the transfer of improved THM-C related process understanding into the corresponding safety function indicators for the EBS.

An integrated approach was required to set up the scientific validation procedures in a context relevant for PA purposes. Thus, validation experiments had to be conducted on the real scale (in-situ experiments, large scale mock-up experiments) to avoid scale effects. Furthermore, the assessed THM-C processes, the experimental conditions and the experimental times had to be specified by the needs of PA.

1.2. Project objectives

Based on the existing knowledge, the project PEBS aimed at bridging the gap between the improved scientific understandings of THM-C processes and the actual needs of PA to specify EBS-related safety function indicators. This included the development of systematic validation procedures for THM-C models, allowing for a quantitative evaluation of their predictive capabilities through a traceable prediction-evaluation process. The improved understanding of THM-C processes fed into an adapted assessment of the long-term safety functions of the EBS, through extrapolation of the short-term processes and analysis of their impact and propagation of uncertainties.

The detailed scientific and technical objectives of PEBS were:

- To review recent advances in the current state-of-the-art (methodology, data, knowledge and understanding) concerning the processes in the early evolution of the EBS and their treatment in performance assessment;
- To discuss how the short-term transients will/may affect the long-term performance and the safety functions of the repository;
- To evaluate the key thermo-hydro-mechanical and chemical processes and parameters occurring during early evolution of the EBS;
- To provide for a reliable good quality experimental HM, THM and THMC data base for the model validation process through laboratory and in-situ experiments;
- To evaluate the predicted evolution of the EBS using the experimental data as performance indicators and to improve the THM-C models through calibration and further code development;
- To use the improved THM-C process models for extrapolation to long-term evolution of the EBS taking into account normal and altered scenarios;
- To relate the experimental and modelling results and uncertainties to the long-term safety functions of the repository components and to the overall long-term performance of the repository;
- To give feedback and guidance for repository design and construction as well as to future research and development (R&D).

In addition to the scientific and technical objectives, the dissemination of results to various stakeholders was a major aim of the PEBS consortium. One Work Package within the project was dedicated to dissemination and training activities aiming at

- making the acquired data, knowledge and expertise accessible to the broad scientific community within the EU and abroad;
- making the acquired expertise available for public information purposes;
- promoting knowledge and technology transfer through workshops and training.

1.3. Project structure

The PEBS project was divided into seven Work Packages (WP) (Table 1). The scientific work was performed in the research and technological development (RTD) WP 1-4 and WP B. WP 5 was dedicated to dissemination activities and WP 6 to project management. Figure 1 gives an overview on the Work Packages and their subdivision in different Tasks.

Table 1: Work Packages of the PEBS project.

#	Title	WP leader
WP 1	Analysis of system evolution during early post closure period: Impact on long-term safety functions	SKB
WP 2	Experimentation on key EBS processes and parameters	enresa
WP 3	Modelling of short-term effects and extrapolation to long-term evolution	GRS
WP 4	Analysis of impact on long-term safety and guidance for repository design and construction	nagra
WP B	China-Mock-Up Test on Compacted Bentonite-Buffer	中核集团核工业北京地质研究院 CNNC Beijing Research Institute of Uranium Geology
WP 5	Dissemination	BGR
WP 6	Project Management	BGR

Figure 2 illustrates the workflow between the RTD Work Packages. In WP 1 a review of recent advances in the state-of-the-art regarding the processes in the early evolution of the repository and their treatment in performance assessment, in particular the relationship to EBS safety functions. This clarified the needs for additional laboratory and in-situ experiments, to support the assessments of normal and altered evolution scenarios. WP 2 and WP B provided a reliable experimental data bases for THM-C processes in bentonite barriers, considering different time and spatial scales. The obtained data was integrated into WP 3 and WP B for the validation, calibration and enhancement of the numerical models. The extrapolation of the numerical analyses to the long-term evolution of the EBS took into account the scenarios defined in WP 1. Finally, WP 4 related the experimental and modelling results and uncertainties to the long-term safety functions of the repository components and to the overall long-term performance of the repository, giving feedback and guidance for the EBS repository design and construction. The scientific-technical outcomes of these Work Packages were spread to scientific community within and outside the EU. The consortium used its expertise for public information purposes and promoted knowledge and technology transfer through training. WP 5 bought together all the mentioned activities concerning dissemination and training.

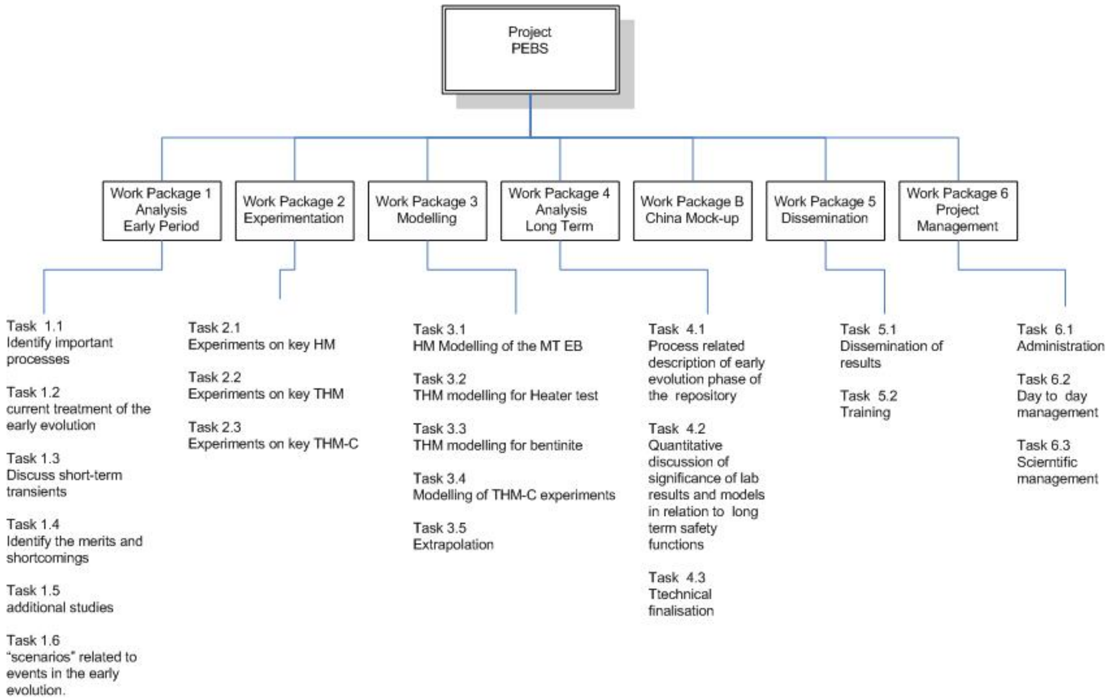

Figure 1: PEBS Work Package structure.

1.4. Project consortium

To achieve the project objectives and to guarantee the relevance of the research, the PEBS project required a strong multidisciplinary team involving the major European, Chinese and Japanese radioactive waste management organisations together with nuclear and other research institutes, universities, consultants and industrial partners. The organisations which participated in the PEBS project are listed in Table 2.

The waste management organisations as end-users ensured with their participation that the outcome of the PEBS project is of direct use for the waste disposal programmes and the interaction with different stakeholders. Their role within the project was to:

- integrate the results of the project with those from the national programmes;
- set priorities in types of waste, engineered barriers, repository designs and host rocks that were considered in project;
- manage research performed in underground research laboratories (URL);
- perform parts of the R&D.

The role of the nuclear research institutes within PEBS was to:

- bring together a multidisciplinary and complementary expertise in laboratory experiments, in-situ testing in URLs, numerical modelling, and safety assessments for the different research domains;
- ensure the dissemination of knowledge and technology within the scientific community;

- ensure the accessibility of the results for the intended end-use;
- manage and preserve the knowledge and expertise acquired within the project.

The role of the organisations including universities, consultants and industrial partners within PEBS was to complement the skills of the above mentioned partners with their specific competences and experiences in the fields of:

- design, implementation and evaluation of in-situ experiments;
- development and implementation of measuring systems and techniques, instrumentation, monitoring and field testing methods;
- design, implementation and evaluation of thermo-hydro-mechanical and geochemical laboratory experiments;
- characterisation and analysis of materials and material interfaces relevant in the EBS;
- advanced numerical analyses of coupled thermo-hydro-mechanical and -geochemical processes, occurring in the engineering barrier during the various stages of the repository;
- code development and enhancements of highly sophisticated coupled thermo-hydro-mechanical and -geochemical models;
- mining, civil and environmental engineering.

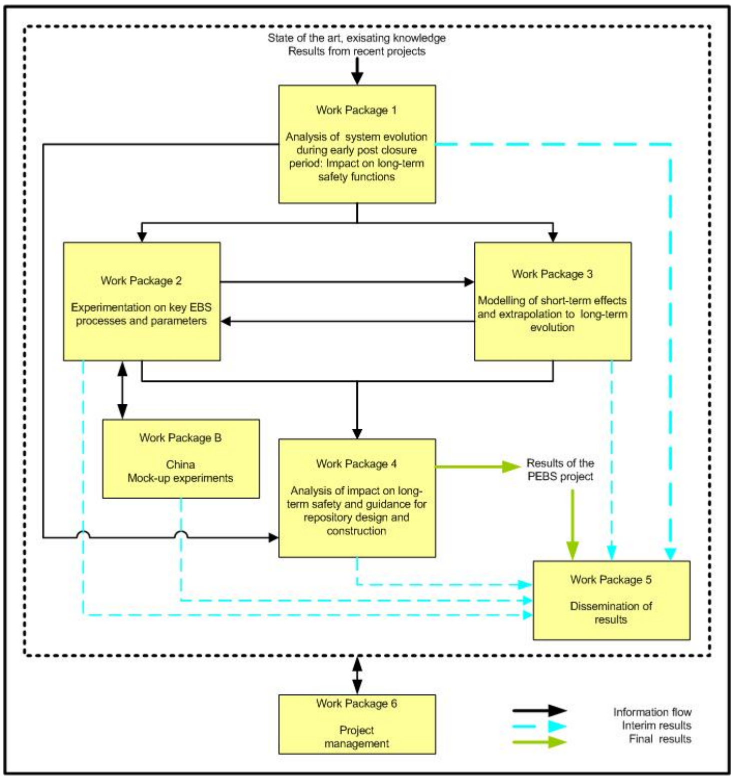

Figure 2: PEBS Work Package workflow.

Table 2: Beneficiaries in the PEBS consortium.

	Aitemin	Spain
	ANDRA	France
	BGR	Germany
	BRIUG	China
	CIEMAT	Spain
	CIMNE	Spain
	Clay Technology	Sweden
	ENRESA	Spain
	Golder	Spain
	GRS	Germany
	JAEA	Japan
	Nagra	Switzerland
	SKB	Sweden
	Solexperts	Switzerland
	TK Consult	Switzerland
	UAM	Spain
	UDC	Spain

2. WP 1 – Analysis of system evolution during early post closure period: Impact on long-term safety functions

2.1. Objectives

The objectives of WP 1 in the PEBS project were to identify the important processes, describe how they are treated currently in long-term safety/performance assessments, discuss how the short-term transients will/may affect the long-term performance and the safety functions of the repository and to consider the key uncertainties in the current treatment. According to the PEBS Description of Work, the work in WP 1 was broken down into six tasks:

1. Identify important processes during the early evolution of the EBS. This task involved a listing of the processes that are considered in description of the evolution of the EBS in safety assessments. This task also reviewed the outcome of the NF-PRO project. The listing was given as input to the expectations from the experiments done in WP 2.
2. Describe the current treatment of the early evolution of the EBS in long-term safety assessments for HLW and spent nuclear fuel. This task dealt with how the processes described in Task 1 were treated in the assessments, which type of models, assumptions and boundary conditions were used. This task was closely connected with the work in WP 3.
3. Discuss how the short-term transients will/may affect the long-term performance and the safety functions of the repository. The purpose of this task was to connect the processes to the safety functions in the repository – i.e. what impact will a process have on the overall performance of the repository. This task was continued within WP 4.
4. Identify the merits and shortcomings of the current treatment. This task made a summary about the uncertainties related to the processes as well as to the treatment of the processes. This included uncertainties in boundary conditions, data and in the conceptual models.
5. Discuss the needs for additional studies of these issues and how they can support future assessments. Based on the results of Task 4, lists of issues that can be handled by the PEBS project was generated. These lists gave guidance to the work in WP 2 and WP 3.
6. Define “scenarios” related to phenomena in the early evolution of the EBS. This task was an integration of the all the previous. The purpose was to define “cases” of EBS evolution that could be treated in WP 4. The work in WP 1 progressed during the first 12 months of the PEBS project. After that the assessment activities were handled in WP 4.

According to Task 1-6, the product of WP 1 was a list of “scenarios” or “cases” related to events in the early evolution of the EBS that should be an integration of the entire study. The list served as an input to the analysis of impact on long-term safety and guidance for repository design and construction performed in WP 4.

2.2. Beneficiaries involved

The scientific work in WP 1 was mainly performed by the national waste management organizations involved in PEBS. The countries represented were:

- France (ANDRA)
- Germany (GRS)
- Spain (ENRESA)
- Sweden (SKB)
- Switzerland (Nagra)

SKB was in charge of the scientific and technical coordination of this Work Package. BGR, as the project coordinator, was involved in this WP with management duties.

2.3. Execution of work

The key output from WP 1 was a summary of the treatment of the early evolution of the EBS in safety assessments with examples from Sweden, France, Switzerland, Spain and a brief description of how the issues are treated in Germany. This included a discussion on how the early evolution of the EBS could affect the long-term safety functions.

2.4. Main results

In the WP 1 report the repository concepts from Sweden, France, Switzerland and Spain were presented. Despite the differences in repository concepts the safety functions defined for the engineered clay barriers are similar. Most safety functions are common and the value for the criteria are very similar, despite the fact that the expected performance of a bentonite buffer is rather different between a concept in diffusion-controlled clay rock and one in fractured rock. The key processes occurring in the EBS in the early evolution of the repository that may affect the long-term performance are identical for all concepts on a fundamental level. However, the significance as well as the treatment of the processes in the safety assessment can differ between the concepts. In particular, the importance for repository safety of satisfying the buffer safety function criteria is greater in the case of fractured crystalline rock than in clay rock. The key processes identified were:

- Water uptake in clay components of the EBS,
- Mechanical evolution,

- Alteration of the hydro-mechanical properties.

The water uptake/saturation does not have any direct effect on the performance of the repository. However, in most cases, the repository is designed to operate under saturated conditions while it is constructed under unsaturated conditions. Therefore, it is important to include a description of the saturation process in the assessment of long-term performance.

During the early stage of the repository evolution, the deposited buffer blocks will take up water from the surrounding bedrock. The water will expand the mineral flakes and the buffer will start swelling. The swelling will be restricted by the rock wall and a swelling pressure will develop. The process is dependent on the properties of the buffer as well as on the local hydraulic conditions and the saturation state of the tunnel backfill. After final saturation, the hydraulic conductivity of the buffer will be very low and the swelling pressure will be high.

This process is common for all concepts with a bentonite buffer and is also relevant for bentonite seals. The timescale for the saturation process is however strongly dependent on the boundary conditions.

In terms of numerical simulations, the "standard THM model" is able to make reasonably good predictions for THM buffer evolution in the FEBEX experiment and conservatively characterize the safety relevant parameters (e.g. swelling pressure, hydraulic conductivity). There is however a discrepancy in the water saturation process of the buffer; the simulated hydration rates are generally larger than the experimental values. There is hence uncertainty in the conceptual model and several new processes have been postulated (e.g. threshold hydraulic gradient, thermo-osmosis, water adsorbed density) in order to improve the "standard model" predictions. Parameter uncertainty also exists, although it is generally deemed less important, at least in the FEBEX context.

The sealing ability is essential for the engineered clay barriers in all repository concepts. This is normally achieved by a swelling pressure and a low hydraulic conductivity. The swelling pressure may also impact the barriers in the repository. The mechanical properties of the installed EBS, that may consist of a mixture of blocks, pellets and engineering voids, will be entirely different from the situation after full saturation. It is therefore important to understand:

1. The mechanical evolution during the saturation phase,
2. The final situation after equilibrium.

Friction within the clay and between the clay and rock/canister may lead to permanent density gradients within the barrier. A good knowledge of the mechanical evolution is necessary to ensure that a given design is sufficient to meet the performance targets.

The mechanical processes in the EBS normally includes the swelling and swelling pressure from the buffer/seal as well as other stress-strain-related processes that can cause mass redistribution within the buffer, for example thermal expansion, creep and a number of interactions with the canister and the near field rock.

After the deposition, the buffer is initially inhomogeneous due to the gaps between the buffer blocks and/or pellets (depending on concept) and the rock and canister surfaces. When water from the rock fills the outer slot and enters the bentonite blocks there will be swelling of the blocks and compression of the pellets and expansion into voids.

At first the swelling will be pronounced because of the overall low bulk density of the pellet-filled slots and voids. The resistance to compression is thus small compared to that of the buffer. This means that the outer part of the blocks will swell to a lower density than the average density expected after complete homogenisation. Ultimately, the water will be drawn so deeply into the blocks that the swelling pressure compresses both the gap and the swollen outer part of the blocks. With time, saturation is achieved and the compression of the outer part and the expansion of the inner part will come to some kind of equilibrium. However, the buffer will not be a completely homogenous material due to inner friction in the bentonite and hysteresis effects; a small density gradient is expected to persist.

Besides mechanical effects, the buffer's hydraulic conductivity and diffusion properties are also altered by swelling.

Other phenomena that could lead to mass redistribution, expansion or contraction of the buffer include creep, shear movements and convergence of the deposition hole, canister movements, pressure exerted by canister corrosion products and thermal expansion of the buffer porewater.

The swelling can be conceived as being caused by a force of repulsion between the montmorillonite layers. If there is a limited supply of water in a free specimen, the swelling is counteracted by a negative pressure in the porewater. If a specimen is water-saturated, i.e. all pores are filled with water; the swelling is counteracted by the formation of a negative pressure in the porewater in the water menisci on the surface of the specimen. The negative pore pressure is equal to the swelling pressure if no external pressure is applied. If the specimen is unsaturated, the water menisci develop inside the specimen as well. The negative pressure in the porewater is chiefly a function of the water ratio in the specimen, i.e. the quantity of water per unit weight of dry material. This negative pressure is called suction potential. When water is added to an unconfined specimen, the water ratio increases and the repulsion forces and the suction potential decrease. This causes the specimen to swell until a new equilibrium is established with a lower internal swelling pressure. If the volume is kept constant, a portion of the internal swelling pressure is instead transferred to an external swelling pressure, which can be measured. When a specimen with constant volume is completely water-saturated and the porewater pressure is kept positive, the entire swelling pressure becomes an external pressure. At water saturation, the swelling pressure and the porewater pressure are independent quantities and give a total pressure that is the sum of the pressures (effective stress theory).

Modelling of the large-scale tests and comparison with measurements confirm that the material model of unsaturated bentonite blocks and the calculation technique used are relevant for modelling the homogenisation process. The uncertainties concern mainly the highly complex material models, and the respective parameter values. Although the models have been verified for the one-dimensional case of swelling and homogenisation of the bentonite rings and pellets between the canister and the rock, the two-dimensional case involves more degrees of freedom for the variables and more interactions like the friction between the bentonite and the rock or canister.

Swelling pressure reduction that arises from hydro-chemical alteration is likely to occur over many tens of thousands of years, as a result of the slow dissolution and alteration processes at the canister-buffer and liner-buffer interfaces. The degree to which this reduction is compensated for by convergence of a clay host rock and the rate of the convergence are unclear and remain to be determined in modelling and experimental studies.

Corrosion products of metal components are expansive and could develop pressure on the geological medium. The expected expansion coefficients for these types of product, and the residual space inside the cell, are in principle sufficient to prevent unfavourable mechanical action.

For the seals and the clay based engineered barrier, the safety analysis requires inclusion of the risk of imperfect installation of the swelling clay elements. The effect of these contact faults is attenuated by the swelling and plasticity of the bentonite. The final homogeneity of the seal, in hydraulic terms, depends on the possibility of filling in the voids during swelling.

A non-homogeneous installation or a heterogeneous swelling of the buffer could result in excessive constraints on the spent fuel container. Its mechanical dimensioning should be sufficient to bear them.

The advantageous physical properties of a clay buffer, principally swelling pressure and low hydraulic conductivity, are determined by the capacity for water uptake between the montmorillonite layers (swelling) in the bentonite. Montmorillonite can transform into other minerals of the same principal atomic structure but with less or no ability to swell in contact with groundwater.

The transformation processes usually consist of several basic mechanisms. At the physico-chemical conditions expected in a repository, the following possible mechanisms have been identified:

- Congruent dissolution, montmorillonites will not necessarily be in chemical equilibrium with repository groundwater. As mineral solubility is low, no significant mass loss is expected from this mechanism. However, solubility is temperature and pH dependent.
- Reduction/oxidation of iron in the mineral structure, this process alters the layer charge and may destabilize the mineral structure. Corrosion of metallic iron or bacterial activity could promote the process.
- Atomic substitutions in the mineral structure; this process alters the layer charge by e.g. Al replacement of Si in the tetrahedral sheets, or Al replacement by Mg.
- Octahedral layer charge elimination by small cations, at high temperatures, e.g. Li^+ may penetrate into the octahedral sheet, which reduces the layer charge.
- Replacement of charge compensating cations in the interlayer, i.e. ion-exchange.

If montmorillonite transformation occurs the buffer functions will alter. Layer charge changes in the montmorillonite lead to changes in the interplay with water and thereby affect the swelling pressure. The hydro-mechanical properties of the clay could also be affected by other processes, generally referred to as “cementation”.

These processes need to be considered separately, since they may depend on different boundary conditions, temperature, groundwater composition, engineering materials, etc, but the combined effect of all processes need to be accounted for in the assessment.

The interaction process of corrosion products and bentonite remains uncertain, and current models should be tested with data from laboratory experiments and improved by:

1. incorporating the dependence of corrosion rates on environmental and geochemical conditions,
2. selecting the most appropriate set of secondary minerals,
3. solving uncertainties in the thermodynamic data,
4. obtaining data for mineral reactive surfaces,
5. accounting for illitization, saponization and dissolution/precipitation of clay minerals,
6. including gaseous phases, and
7. considering inhomogeneous corrosion.

Other uncertainties relate to the choice of original material.

2.5. Summary and future perspective

The product of WP 1 was a list of cases related to the early evolution of the EBS that was an integration of the entire study. Based on the outlined approach (section 2.4), WP 4 proposed a specific set of cases (see section 5.3) that was agreed upon after discussion with Work Package leaders. The proposed group of cases served as the basis for integrating the knowledge gained from PEBS experimental and modelling studies and served as an input to the analysis of impact on long-term safety and guidance for repository design and construction that was performed in WP 4.

3. WP 2 – Experimentation on key EBS processes and parameters

3.1. Objectives

The main objectives of Work Package 2 were:

- To evaluate the key thermo-hydro-mechanical and chemical parameters and processes taking place during the early evolution of the EBS;
- To provide with a reliable good quality experimental HM, THM and THMC data base for the model calibration and validation process.

The key thermo-hydro-mechanical-chemical processes and parameters were identified in WP 1. WP 2 provided a reliable good quality experimental data base, including different time and spatial scales, as input to the modelling and extrapolation performed within WP 3 and to the analysis of the impact of residual uncertainties on long term safety conducted within WP 4.

The overall approach was based on performing experiments including different time and spatial scales, according to the needs for additional studies on the identified key processes during the early EBS evolution. WP 2 made use to the extent possible of ongoing experiments being conducted by the PEBS team (both in the laboratory and in-situ). The experimental work conducted within the WP 2 of the PEBS project builds on this existing knowledge and experience and contributes diverse aspects to the understanding of the short term evolution of the EBS system.

Work Package 2 was organized in three separate tasks which focus on different key EBS processes and their couplings. For all three tasks, different time and spatial scales were envisaged.

3.2. Beneficiaries involved

The beneficiaries involved in Work Package 2 were most of the PEBS project partners, namely: BGR, Nagra, SKB, CLAY TECHNOLOGY, GRS, Aitemin, CIEMAT, ENRESA, ANDRA, UAM, GOLDER (formerly DM IBERIA), and SOLEXPERTS.

ENRESA was in charge of the scientific and technical coordination of this Work Package. BGR, as the project coordinator, was involved in this WP additionally with management duties.

3.3. Execution of work

3.3.1. Task 2.1 – Experimentation on key HM processes

Laboratory infiltration tests

Two kinds of laboratory infiltration tests under laboratory temperature have been performed:

- Long-term permeability tests for evaluation of the evolution of permeability over time and of the influence of hydraulic gradient on hydraulic conductivity. Three of them are being performed with the FEBEX bentonite and two others with the MX-80 bentonite. The hydraulic gradients applied were between 200 and 7500, and the injection pressures lower than 2.4 MPa. The bentonite was compacted at dry densities between 1.4 and 1.7 g/cm³. The diameter of the samples was 5.0 cm and their height 2.5 cm. The three tests performed with FEBEX bentonite started before the beginning of the PEBS project, and have been running for between 7 and 9 years, whereas the tests performed with the MX-80 bentonite have been running for 3 years. None of them has been dismantled.
- Infiltration tests under isochoric and isothermal conditions, applying low water injection pressures. Three of these tests were performed with the pellets mixture used in the EB in-situ experiment (Figure 3); three with the sand/bentonite (S/B) mixture used in the HE-E in-situ experiment; and two with the HE-E MX-80 pellets. All the materials were prepared in the same state with respect to dry density and water content as in the in-situ tests. The nominal length of the samples was 5 or 10 cm and the diameter 10 cm. In the tests performed with the HE-E materials Pearson synthetic water was used to saturate the specimens, as in the in-situ test. The water intake and the vertical stress developing upon saturation, as well as the small vertical deformation were measured. In one of the tests the hydraulic conductivity was measured after saturation. After dismantling, water content and dry density were determined along the specimens and in some tests, other post mortem determinations related to the analysis of the bentonite microstructure were performed. The duration of the tests was between 1 and 5 years for the EB materials and between 40 and 450 days for the HE-E materials.

Figure 3: Appearance of the EB mixture after compaction and of the specimen after saturation.

The EB in-situ experiment

The EB experiment was a full-scale demonstration test designed to represent the end of the transient phase (almost full saturation of the bentonite barrier and temperature approximately that of the host rock prior to repository construction). It was installed in a 6 m long section of a gallery (2.6 m high and 3.0 m wide) excavated in the Opalinus Clay of Mont Terri (Figure 4). A dummy canister (similar dimensions as the ENRESA and Nagra reference canisters) was installed on the top of a bed of bentonite blocks and the remaining air volume (approx. 28.4 m^3) of the section (finally sealed with a concrete plug) filled with a Granular Bentonite Material (GBM). An average dry density of about 1.36 t/m^3 of the emplaced GBM was obtained. The experiment ran for more than ten years, under isothermal conditions and with artificial hydration during the first approx. 5 years. It was dismantled in the period October 2012 – January 2013 with more than 500 samples of the bentonite taken for on-site and laboratory analyses: dry density and moisture content; suction; pore size distribution; basal spacing; thermal conductivity; hydraulic and gas conductivity; swelling strain and swelling pressure, and microbial analyses.

It should be noted that in the EB experiment there were inherent difficulties in emplacing the GBM because of interference due to the hydration tubes, thus the density achieved is lower than would be expected in a more ideal situation and the variation in density is probably significant.

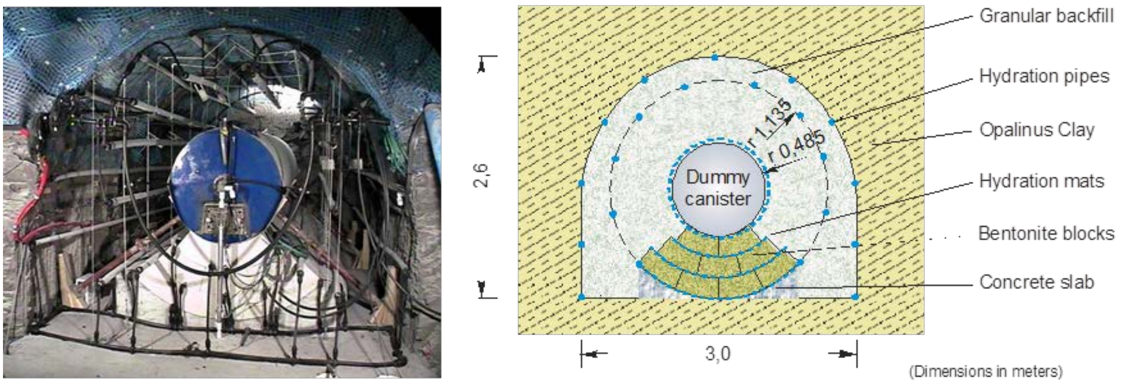

Figure 4: EB in-situ experiment at Mont Terri.

The evolution of the GBM and the bentonite blocks were on the other hand characterized with geophysical parameters. The Excavation Damaged Zone and Excavation disturbed Zone features (EDZ / EdZ) were of special interest particularly during the final dismantling process.

Seismic long-term monitoring

The evolution of the Opalinus Clay (OPA) and the backfill material FEBEX bentonite (Almeria, Spain) was characterized with the help of seismic parameters. It was a unique opportunity to observe changes in seismic parameters over 12 years. After 8.6 years a seismic array consisting of 24 piezoelectric transducers could be reactivated (see Figure 5, left). It was used between April 2002 and November 2003 over 576 days for a seismic monitoring on a daily basis (phase 1). The seismic array covers a volume of 1 m x 1 m x 2 m in the OPA and a part of the backfill. It is located at the eastern wall of the niche. During this first phase the EDZ created by the excavation of the EB niche was on the way to recover (sealing of EDZ) according to the seismic parameter changes. The resumption of the seismic long-term monitoring started on July 12th, 2012 five month before the complete dismantling of the EBS (phase 2) and is still ongoing. Potentially 112 different propagation paths of the seismic wave filed can be used.

Geoelectrical monitoring

After excavation of the EB niche three electrode profiles were installed in 2001 (see Figure 5, right), one horizontal profile at the eastern wall and two circular profiles in a distance of 2.65 m and 3.65 m to the face of the niche, respectively. The 45 electrodes of the circular profiles located every 8° (measured from a central point of the niche). The installations were used to investigate the change of resistivity distribution due to the stress relaxation in the OPA in three campaigns. After emplacement of the canister, filling the excavation and closing the niche with a concrete plug, two additional measurements were performed in 2002 under full space conditions. In July 2012 the electrode arrays were reactivated successfully. As an add-on to the seismic investigations it was decided to attend the dismantling procedure by a monitoring using circular profile 2 which provide a 2D information perpendicular to the niche axis. The geoelectrical monitoring covers the period between September 27th, 2012 and May 24th, 2013 by a daily measurement, 240 data sets in total.

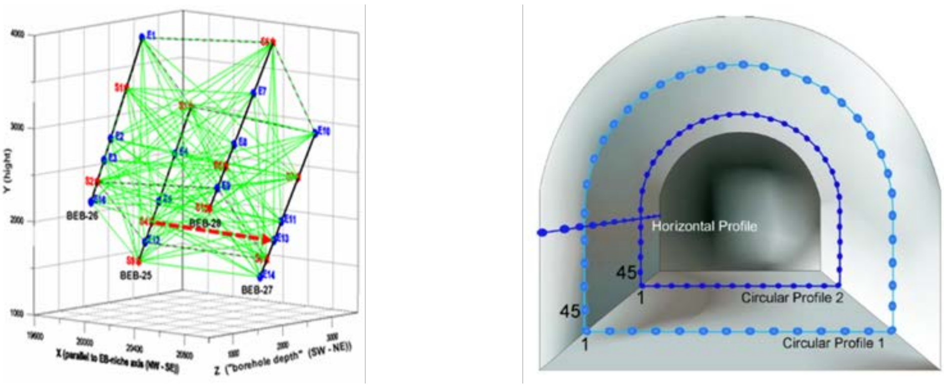

Figure 5: Geophysical installations in the EB niche. Left: Four boreholes and theoretical ray coverage of the seismic transmission experiment. Right: Sketch of the three electrode profiles installed in 2001.

3.3.2. Task 2.2 – Experimentation on key THM processes

Subtask 2.2.1 – Laboratory experimentation on key THM processes

The FEBEX mock-up

The FEBEX mock-up test is a demonstration experiment of a clay engineered barrier at almost full scale and under controlled boundary conditions (Figure 6). Its main components are: the confining structure (CS; steel with inox internal lining) that simulates the gallery, through which hydration took place; the heating control system that simulated the heat generation of the waste canisters by two electric heaters (0.17 m diameter, 1.625 m long) concentric to the CS; the hydration system that supplied granite-type water to the bentonite at controlled pressure (about 0.5 MPa) through inlets in the CS and a geotextile layer as interface to assure homogeneous water distribution; the engineered barrier (0.63 m thick around the heater, dry density 1.65 g/cm³) that is composed of compacted FEBEX bentonite blocks surrounding the heaters; the instrumentation that monitored the boundary conditions and the system behaviour.

The test was instrumented with more than 500 sensors installed in the clay barrier, the hydration system, the heaters and the confining structure. The main measured variables (and sensors) were temperature (368 Pt100), relative humidity (40 capacitive transmitters Vaisala HMP237), total pressure (50 load cells KULITE BG0234), strains (19 extensiometric gauges), and fluid pressure (20 pressure sensors KULITE HMK375). More than 85% of the sensors remain operative despite the fact that their operation expectancy was exceeded.

Sensors were installed along 25 vertical sections located every 0.25 m: a central section divided the setup in two symmetrical modules, each around one of the heaters.

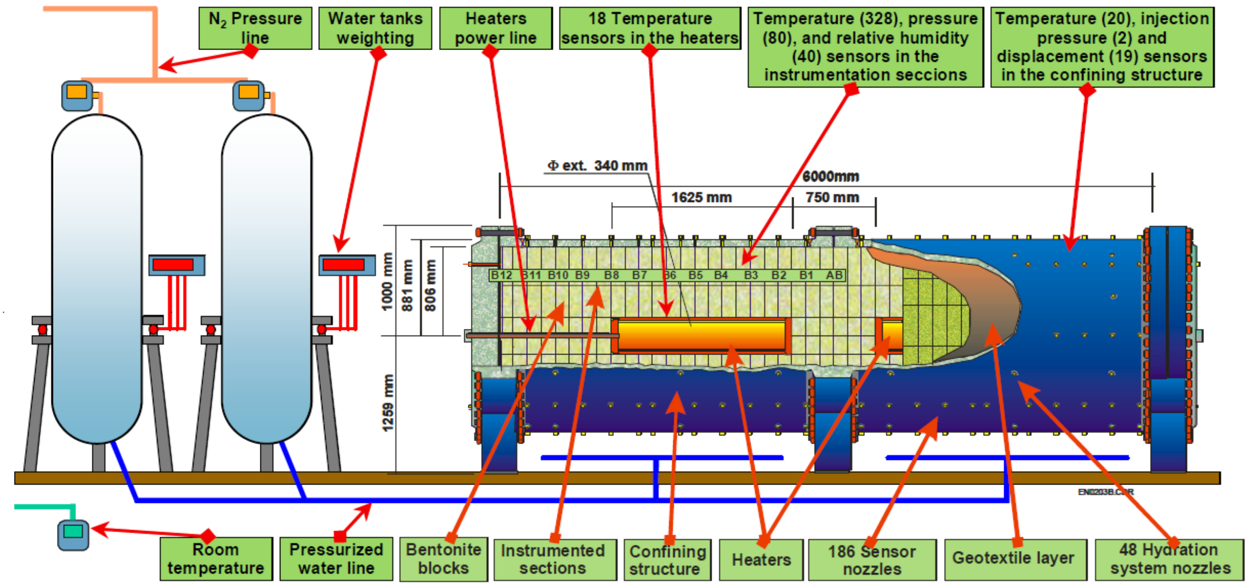

Figure 6: FEBEX mock-up experiment at CIEMAT (Spain).

The operational stage – simultaneous hydration and heating – started in February 1997. The test started with an initial flooding stage with the purpose of closing the gaps between bentonite blocks. The heating power was adjusted to supply a constant temperature at the heater control surface (100 ºC), while the bentonite buffer was hydrated at controlled pressure of around 0.5 MPa. After 5 years of operation, the power supply was fixed at 700 W/heater, hereby maintaining the surface temperature of the heaters close to 100 ºC. From that time, the test is still running under stable conditions. The temperature of the test room is 20±4 ºC.

Today, the buffer is practically saturated and hydration goes on at the inner buffer closer to heaters. The total volume injected was 1153.5 L on 31/12/2013 that corresponds to an average water content of 22.9%.

Long-term tests in cells simulating particular disposal concepts

Two series of tests in thermo-hydraulic cells have been running during the project:

- the first series consisted of two tests performed with FEBEX bentonite that were set before the beginning of the PEBS project and were dismantled before the end of it;
- the second series consisted of two tests performed with the materials used in the HE-E in-situ test, a sand/MX-80 bentonite mixture (cell S/B) and MX-80 bentonite pellets (cell B). They were launched during the PEBS project and are still running.

All the tests were performed in the same kind of setup, with some improvements for the second series. Basically they are performed in cylindrical cells of nominal internal diameter 7 cm and variable height. The cells have a heater at the bottom and a system allowing water injection on top. Three sensors measured relative humidity (RH) and temperature along the columns during the tests.

The two TH tests in cells performed with FEBEX bentonite compacted at a dry density of 1.69 g/cm^3 run for almost 12 years and provided online information about the temperature and relative humidity inside the bentonite. The length of the columns was 40 cm. In one of them the column of bentonite was hydrated under thermal gradient (GT40), since the heater was set at a temperature of 100 °C, and in the other one at room isothermal conditions (I40). In both cases deionised water injected at a pressure of 1.1 MPa was used. They were dismantled in November and December 2013 and the physical state of the bentonite was analysed. In both cells there were water content and dry density gradients along the column, sharper for cell GT40 (Figure 7).

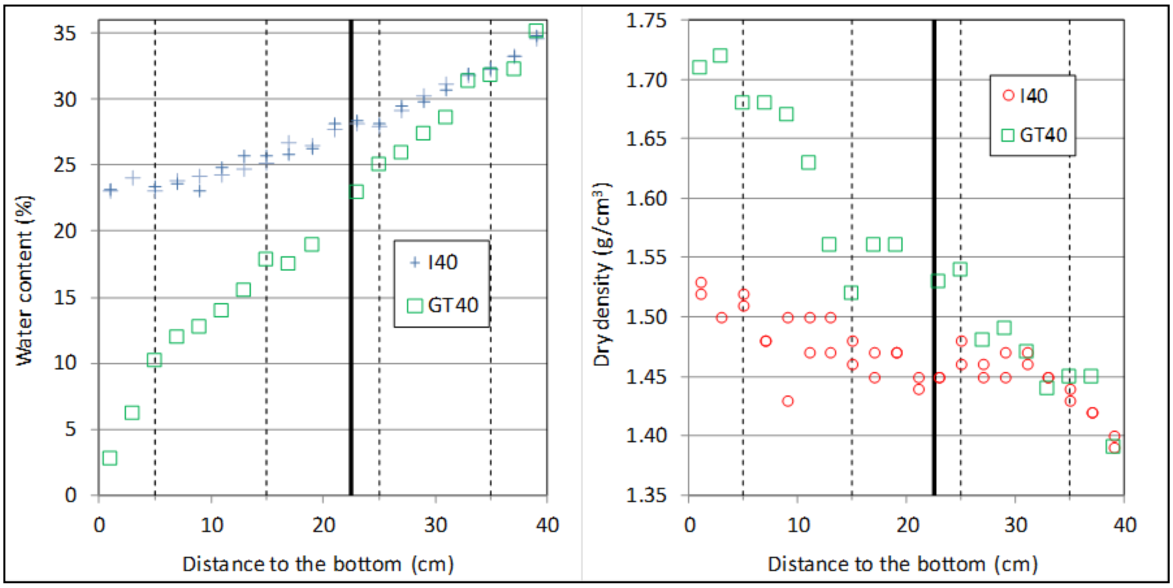

Figure 7: Final water content and dry density along the bentonite columns after 12 years of hydration. Test GT40 performed under thermal gradient, test I40 at isothermal conditions.

The two materials used in the in-situ HE-E tests are being tested in thermo-hydraulic cells in which the length of the material columns is 50 cm, which is the thickness of the GBM barrier in the in-situ test. The initial conditions of the sealing materials inside the cells with respect to dry density and water content were the same as those in the in-situ test (1.45 g/cm^3 and 3.6% for cell S/B and 1.53 g/cm^3 and 6.4% for cell B). The water intake and the heater power were measured online. In addition, cell B was instrumented with a ring load cell located on the top of the cell to determine the axial pressure generated during the test.

The temperature of the heaters placed at the bottom of the columns was increased to 100 °C and then to 140 °C during the heating phase, during which hydration did not take place. Hydration with Pearson water through the upper surface of the columns started after RH stabilisation inside the materials. Only a small pressure, given by a 40 cm high water column, was applied to the saturation water.

Studies on stress-strain behaviour

The study on stress-strain behaviour was prompted by previously observed thermo-mechanically induced brittleness in buffer material. Additional studies regarding the origin of brittleness was of importance to further understand the behaviour. The study was focused on the stress-strain properties of bentonite exposed to increased temperatures but the influence of different mineral composition, different anions and different preparation methods were also studied.

The stress-strain behaviour was determined by unconfined compression tests. In the unconfined compression test a cylindrical specimen is compressed axially with a constant rate of deformation with no radial confinement or external radial stress. The dimensions of the specimen are often a height which is double the size of the diameter but in the present study the height was equal to the diameter. To minimize the end effects of the short specimens the end surfaces were lubricated. A constant deformation rate of 0.16 mm/min was used for the tests.

The heated specimens were exposed to an increased temperature between T = 90˚C - 150˚C during 24 h in a laboratory oven. The heating was made either after or before full saturation of the specimens. In case of heating after saturation a water pressure of 600 kPa was applied to the specimens during the heating. The specimens heated before full saturation were water supplied during a couple of minutes and then placed into the oven where the specimens were sealed to avoid evaporation and without water pressure control. After the heating, water with atmospheric pressure was supplied to all specimens.

In series where specimens were exposed to heating the stress-strain behaviour was complemented by determination of swelling pressure and hydraulic conductivity. These determinations were made in a combined test in a swelling pressure device with constant volume condition. The hydraulic conductivity was determined by applying a water pressure gradient between 3900 and 10600 m/m over the specimens during measurement of the volume of the outflowing water. The hydraulic conductivity was calculated according to Darcy´s law.

The bentonite used in the majority of the test series was MX-80 which is a Wyoming bentonite product from American Colloid Co. In some tests the FEBEX bentonite was used which is a Mg-Ca bentonite extracted from Almería in Spain, exploited by the major Spanish bentonite producer, Minas de Gádor S.A. (now Süd-Chemie Espana).

Subtask 2.2.2 – In-situ experimentation on key THM processes

The HE-E experiment, designed and constructed as part of PEBS, is a 1:2 scale heating experiment considering natural resaturation of the EBS at a maximum heater surface temperature of 140 °C. The experiment is planned initially to run until 2014. The experiment is located at the Opalinus Clay (OPA) of the Mont Terri URL (Switzerland) in a 50 m long microtunnel of 1.3 m diameter (Figure 8). The test section of the microtunnel has a length of 10 m and has been characterised in detail during the Ventilation Experiment which took place in the same test section.

The aims of the HE-E experiment are elucidating the early non-isothermal resaturation period and its impact on the thermo-hydro-mechanical behaviour, namely: (1) to provide the experimental data base required for the calibration and validation of existing THM models of the early resaturation phase; (2) to upscale thermal conductivity of the partially saturated EBS from laboratory to field scale (pure bentonite and bentonite-sand mixtures).

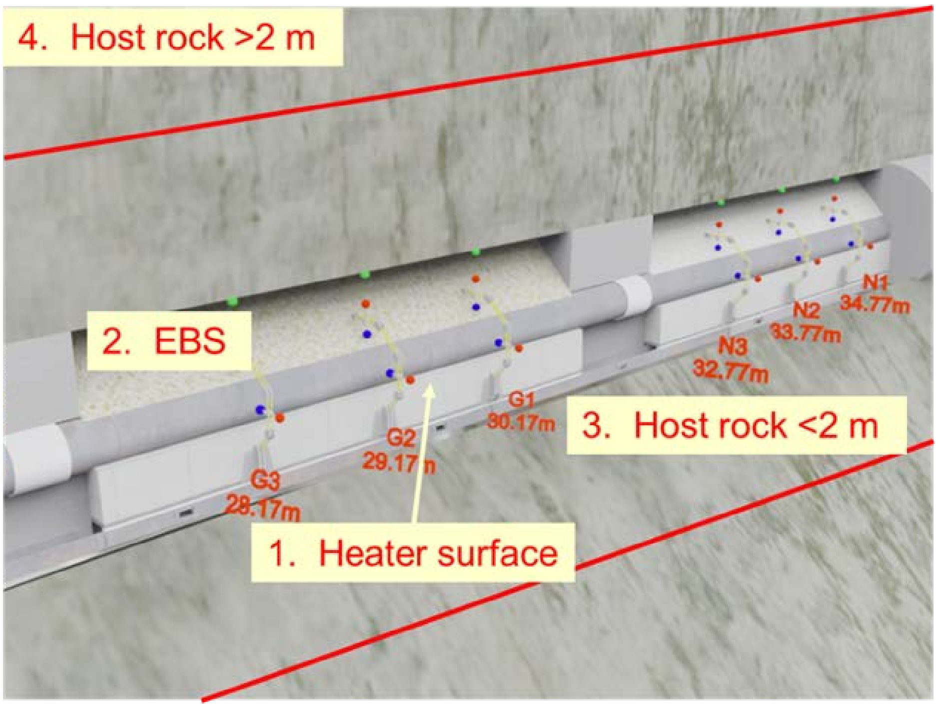

Figure 8: HE-E in-situ experiment at Mont Terri.

The construction of the HE-E experiment took place between December 2010 and June 2011. In a first step a U-profile railway was installed in the 50 m long tunnel. Subsequently the host rock was instrumented. The EBS instrumentation modules were then towed into the tunnel leading to the connection of the heater liner elements into one continuous liner. An auger, adapted to the 1.3 m diameter of the tunnel, was used to emplace the granular EBS material. Emplacement densities, established during off-site tests for the MX-80 ranged around 1.45 g/cm^3 while for the sand/bentonite mixtures the densities were estimated to be 1.50 g/cm^3. The test sections in the tunnel were separated by three concrete plugs containing also thermal insulation and a vapour barrier. Finally, in the last step, the two 4 m long heaters were emplaced in the central liner.

The instrumentation concept is targeting four zones:

1. the heater surface where the temperature is measured;

2. the EBS itself and the interface with the Opalinus Clay with very dense measurements of temperature and relative humidity;
3. the Opalinus Clay close to the microtunnel, which was under the influence of the ventilation before and during construction where temperature, humidity, hydraulic pressure and displacement are monitored;
4. the Opalinus Clay at several meters from the microtunnel, where hydrostatic conditions were less disturbed by the activities in the microtunnel and where hydraulic pressures are monitored.

In the design phase it was assumed that no significant swelling pressure would develop in the EBS. During the early resaturation phase the permeability of the granular-like buffer materials is still high, but resaturation rate is limited by the low permeability of the rock, resulting in low inflow rates. Differential thermal expansion of water and solid skeleton is likely to induce hydraulic overpressures in the saturated Opalinus Clay at some distance from the EBS-rock interface. The measurement and assessment of these overpressures became an additional objective of the experiment.

3.3.3. Task 2.3 – Experimentation on key THM-C processes

Subtask 2.3.1 – The THM-C mock-ups (GAMEs)

THM-C mock-ups are running under the following conditions: the heaters' temperature is being kept at 40 °C and hydration is taking place under periodic low-pressure pulses, due to the fact that, after several trials to improve the system, the water leaks could not be stopped. In addition, most of the sensors are out of order: they were damaged during the water injection events, or by the saline water. Due to the bad performance of the sensors, the GAMEs could not provide on-line information. Before failure the transmitters indicated high RH values and the expected temperatures. The post-mortem analyses upon dismantling of the GAMEs will provide useful data. It was decided to let the experiment run and provide alternative information related to the concrete-bentonite and corrosion products-bentonite interactions from other experiments. Although considering a different experimental scale, this provided a valuable database for the numerical modelling of the THM-C processes and their temporal evolution.

Subtask 2.3.2 – The THM-C tests on key processes at the interfaces

Key processes at the canister-bentonite-concrete interfaces

A series of six **small cell** experiments were designed to reproduce the repository conditions prevailing 1000 to 3000 years, when the bentonite is fully saturated. For a repository in an argillaceous formation the interfaces mortar-FEBEX bentonite-magnetite were studied and the system was hydrated with synthetic argillaceous type water. The cells were in operation for 18 months and the materials were dismantled simultaneously and the post-mortem analysis of the material was conducted.

Experiments in the **medium cells** were performed to simulate the operational, early post-closure and transient phases of the repository, i.e. the state before achieving full saturation of the EBS, characterised by oxic to suboxic conditions. The experiments considered the interface between FEBEX bentonite and iron powder with hydration by granite type water collected at the Grimsel Test Site (for a repository in granite) and the interface between concrete and FEBEX bentonite with hydration by synthetic argillaceous type water (for a repository in an argillaceous formation). The experiments were designed to establish the evolution, through sequential dismantling at different times from 6 months to 7 years, of the chemical processes from the unsaturated to the saturated conditions, both at the concrete-compacted bentonite and the iron-compacted bentonite interfaces separately. Therefore, a number of identical experiments were assembled simultaneously already by mid-2006 in the frame of the NF-PRO project and were sequentially dismantled. During the PEBS project duration four of these set of cells were dismantled, two with the concrete/bentonite interface that were in operation for 4.7 and 7 years, and two with the iron/bentonite interface that were in operation for 4.6 and 7 years (details in PEBS D2.3.3-1). During the project the materials from the cell dismantling were analysed.

3.4. Main results

3.4.1. Task 2.1 – Experimentation on key HM processes

Laboratory infiltration tests

Some laboratory tests suggest that the possible threshold hydraulic gradient for FEBEX bentonite might range from 200 to 1400, depending on the dry density and injection pressure. The preliminary data indicate that the threshold hydraulic gradient for MX-80 could be of the same order. No clear evolution of permeability over time has been observed.

In the infiltration tests, most of the water intake took place in a short period of time (Phase 1 of saturation). In contrast, the subsequent water intake (Phase 2 of saturation) was very small and slow. The contrast between the two saturation phases is more pronounced in low-density bentonite, in which Phase 1 is shorter and coincides with a sharper development of swelling pressure. In the bentonite pellet mixtures tested the swelling pressure sharply increased at the first stage of hydration, then stabilised, and afterwards increased again, reaching practically an almost-equilibrium value when most of the water had already been taken up. The sand/bentonite mixture did not develop any swelling pressure upon saturation.

After saturation the pellets became a homogeneous material, with hydro-mechanical properties in the range of those for the saturated powder material of the same dry density. However, the water content and dry density gradients along the bentonite can remain even after having reached the equilibrium swelling pressure. In the long term, the water content and dry densities could become more uniform, although this is not evident for the parts of the sample columns saturated quickly in which very high water contents and low dry densities were soon reached, since this large deformation could be irreversible. Also, the analyses of the microstructure of the pellets mixtures at the end of the tests showed that most of the porosity was of diameter less than 7 nm.

The EB in-situ experiment

According to the monitoring of the experiment during its more than 10 year lifetime, the following main observations were made:

- Due to the artificial hydration system used, most of the bentonite saturated fairly quickly: in the first 1.5 year period, the water intake was equal to 15.2 m^3 (while the estimated air volume before the water injection was 12.5 m^3), although some initial water leakage was observed in the bottom of the concrete plug. Also, in this period, total pressures in the barrier as high as 1.7 MPa were recorded (while for a mean dry density of 1.36 t/m^3 a maximum swelling pressure of only 1.3 MPa was expected). All the hygrometers (except one) showed full saturation.
- After the relatively short first period (1.5 years), during the remaining lifetime of the experiment (approx. 9 years), water intake was very slow (and no additional water was artificially injected after 5 years); and the recorded swelling pressures increased also very slowly, up to a recorded maximum value of 2.2 MPa.

After the experiment dismantling, the visual observations and the on-site and laboratory tests results have confirmed that the bentonite barrier was highly saturated and the bentonite blocks and GBM, which initially had significantly different dry densities, had developed rather similar average densities. More specifically, from the on-site density and moisture content determinations, done at the experiment site and as soon as possible after taking the samples, the following can be concluded:

- The average degree of saturation is higher than 95%. Moreover, during the dismantling operation it has been observed that, due to the time spent handling the samples (even if as short as possible), some drying and also some deformation (due to the non-confined conditions) of the bentonite could not be avoided before the tests were performed. The observed increase in the dimensions of the bentonite blocks placed under the canister indicates that they have swelled not only during the experiment´s life but also along the dismantling operation. Then, it might be assessed that the actual degrees of saturation are even higher than those calculated from the on-site test results. It has been estimated that very probably the actual degree of saturation varies from 98% to 100%.
- Although some degree of homogenization of the bentonite materials occurred (in the sense that the large initial density contrast between blocks and GBM has greatly diminished), the overall density range is still significant. There is also a clear trend for the moisture content to increase towards the bottom of the section (while the dry densities are lower than in the upper part).

On the other hand, the results of the tests performed in CIEMAT's laboratory have provided the following most relevant data for the characterization of the dismantled bentonite barrier:

- It has been confirmed that the bentonite was almost fully saturated. The obtained average degree of saturation is approximately 98%.
- Most of the water content average values determined in the different GBM parts and blocks range between 33% and 44%; and of the dry density between 1.24 and 1.42 g/cm^3.

- One of the main objectives of the EB experiment was to determine if the hydraulic conductivity of the GBM (after saturation) is low enough, even if emplaced with relatively low average dry density (1.36 t/m^3 in this case). The permeability tests performed on fifteen samples do confirm that, after saturation, the barrier had a low hydraulic conductivity (K_w): the values of K_w are equal to or lower than 5×10^{-12} m/s, except one (8×10^{-12} m/s), obtained with a very low dry density sample (1.18 t/m^3), less representative of the overall barrier.
- The measured thermal conductivity values are relatively high (as expected due to the saturation degree), ranging from 0.90 to 1.35 W/(m·K).
- Although the samples were almost fully saturated, they still exhibited some suction (remaining capacity to absorb distilled water). Values ranging from 2.1 to 4.7 MPa have been measured. It is noted that also saturated samples can have suction (below air entry value).
- According to the pore size analyses, a relevant percentage of the porosity of the GBM samples was in the microporosity range (diameter smaller than 7 nm), although a macropore family (sizes between 3 and 35 μm) has also been detected, which did not exist in the original GBM pellets. Also, macroporosity is predominant for samples with dry density lower than1.30 t/m^3.
- The dismantled bentonite still keeps some swelling potential: in the tests performed, swelling strain values as high as 22.5% and swelling pressures up to 0.69 MPa have been measured.
- It is noted that, after the additional water intake in the permeability and swelling tests, in general saturation degrees higher than 100% (in some cases higher than 110%) have been calculated, assuming that the pore water density is 1.00 t/m^3.

The characterization of geophysical parameters has produced the following results:

- Seismic parameters like P-wave velocity (v_p), amplitudes and the frequency content of seismic traces were derived. As a result of the dismantling the gradual recreation of an EDZ / EdZ was observed with the help of these seismic parameters. Depth levels of 38 cm, 138 cm and 208 cm were selected for a closer analysis. As can be seen in Figure 9 the evolution is different at different depth levels with different intensities.

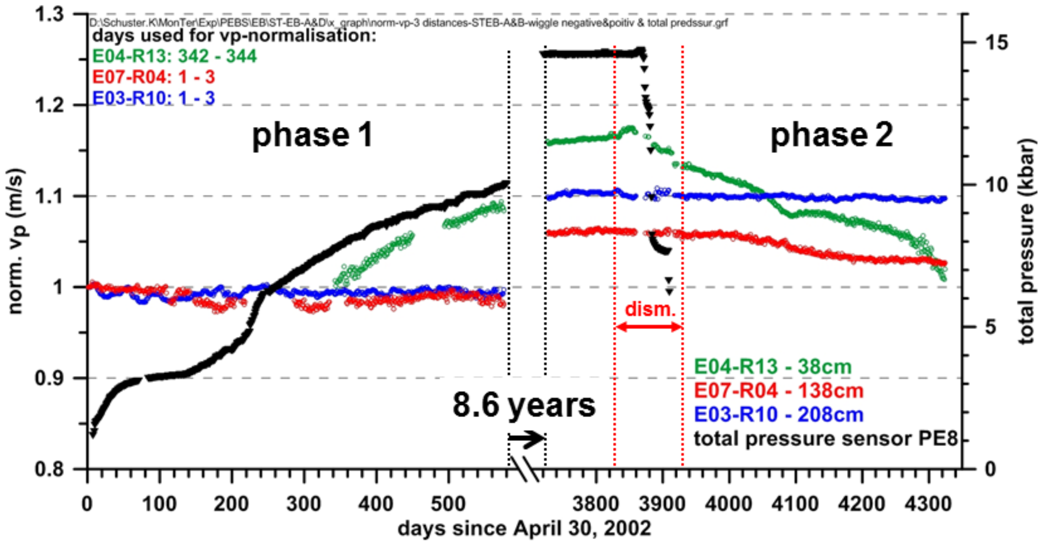

Figure 9: Normalized seismic P-wave velocities for three distances from the interface. Data were normalized with the mean values from phase 1.

- In phase 1 a normalized v_p increase from day 340 on can be interpreted as an ongoing sealing of the EDZ. The rock mass at 138 cm and 208 cm depths seem to be unaffected by the excavation of the niche and the later hydration of the bentonite. Seismic P-wave velocities jumped by about 10 % between the end of phase 1 and the restart after 8.6 years (phase 2) whereas the total pressure values, measured nearby, jumped by about 40 %. The dismantling work (start at day 3830) affects the OPA at 38 cm remarkably from the beginning. At 138 cm depth the v_p decrease starts delayed around day 4020 with a slower gradient. The v_p at 208 cm seems to be unaffected. Several derived seismic parameters are in good accordance with results gained in the initial phase of the EB Experiment and from other experiments performed by BGR.
- The results of the geoelectrical investigations for the monitoring period have to be distinguished in two parts: a) filled niche (full space conditions) and b) dismantled niche (open space conditions). The left picture of Figure 10 displays the spatial resistivity distribution before the start of the dismantling.

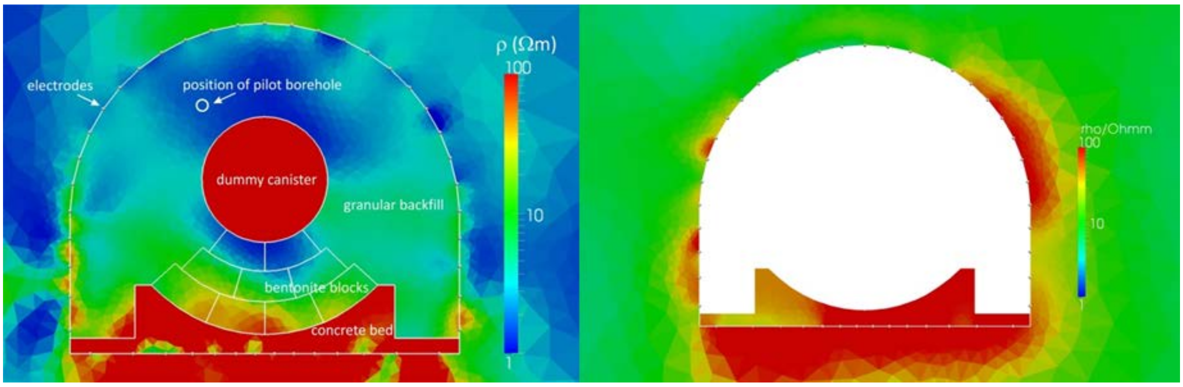

Figure 10: Model of spatial resistivity distribution, left: on September 30th 2012 (before dismantling), right: on May 23th 2013 (after finished dismantling).

- As both the concrete floor and the canister are reconstructed as high resistive structures, the lowest resistivities (below 3 Ωm) of the granular backfill are displayed above and directly below the canister. There is only a small variability of resistivity seen in the horizontal direction within the bentonite, but there is obviously a vertical gradient present with higher resistivities (~ 10 Ωm) at the floor. No contrast can be seen at the border between the bentonite blocks and the granular material. The resistivity distribution reflects qualitative the distribution of water content as a result of sample analysis while dismantling at a close section. Additional resistivity measurements of original bentonite samples in the BGR lab confirm the positive correlation of electrical resistivity and water content.
- In the open niche (see Figure 10, right) the OPA around the niche is characterized by resistivities of about 10 Ωm, except of two regions (upper right and lower left wall) where higher resistivities (>40 Ωm) are visible. These high resistive regions increase in extension as well as in resistivity contrast with time. These positions correspond to regions of high deviatoric stress, so the resistivity model shows the effect of the stress distribution building EDZ structures after dismantling the niche.

3.4.2. Task 2.2 – Experimentation on key THM processes

Subtask 2.2.1 – Laboratory experimentation on key THM processes

The FEBEX mock-up

The experimental observations on THM parameters show good homogeneity throughout the test and have revealed several features of interest – related to the specific thermal load and geometry of the mock-up – among which:

- Temperature calculations produce good fits to data. Strongly coupled hydro-mechanical (HM) processes could explain the influence of temperature on the fluctuations of the relative humidity values at equilibrium, the swelling pressure and the fluid pressure.
- The transient effects of evaporation (drying) and condensation (wetting) indicate the redistribution of water. Vapour migration through the barrier occurs even at medium-high degrees of saturation.
- Experimental measurements confirm that the water inflow (and water vapour outflow) is radial and homogeneous. The saturation of the bentonite is apparently controlled by the hydraulic properties of the bentonite and the local temperatures and/or thermal gradients imposed by heating, confirming significant differences between the “hot” and “cold” zones of the buffer as hydration progresses.
- The initial mechanical pressures depend on the specific location and installation of the sensor, the dry density of the block, and/or the development and concentration of local stresses. With time, values become homogeneous and stable as the buffer material saturates. Values for the different directions are converging to the swelling pressure values of the bentonite previously measured in the laboratory.

- The indicators of quasi-saturation are the following: high stable average values for swelling pressure and relative humidity, a positive trend in fluid pressure values, and very low water intake. All of them are occurring in most parts of the barrier, but not in the closest zone around the heaters. Although most the buffer is practically saturated, full saturation close to the heaters has not been reached yet.

From above, the following relevant conclusions may be drawn:

- The total saturation time is longer than foreseen by standard THM models.
- The buffer achieves the required performance even prior to full saturation, as shown by the sufficient and homogeneous swelling pressures developed and the homogeneous high thermal conductivity achieved.

Long-term tests in cells simulating particular disposal concepts

The two tests performed with FEBEX bentonite highlighted the influence of the thermal gradient on the hydration kinetics, which was much slower in test GT40; the persistence of the water content and dry density modifications, which remained after 12 years of testing; and the long duration of the saturation process.

The heating phase of the tests performed with the HE-E materials showed that the thermal conductivity of the dry materials is low, what caused a high thermal gradient near the heater, and low temperatures in the rest of the columns. Since the initial degree of saturation was low for both materials, the vapour phase could move inside the columns as a result of the thermal gradient. The movement of water in the vapour phase was evinced by the sharp increase of relative humidity recorded by the sensors closest to the heater – followed by a continuous decrease – and the slower increase recorded in the upper part of the columns. This pattern was also observed in test GT40.

The behaviour after hydration started was very different in columns S/B and B. In cell S/B the temperatures kept the same as before hydration for some days. Later, as the water front approached the sensors, the temperatures started to increase. The increase in RH was very sudden once the water front reached the area where the sensors were placed. The water intake was also very large until the bottom sensor became flooded, after that the water intake rate decreased.

However, in the case of cell B, the temperatures kept the same after hydration started for more than 500 days. The lower permeability of the pellets was again highlighted when hydration started, because the sensors started to record RH increases much later than in cell S/B. In fact, after more than 500 days the sensor located at 10 cm from the heater recorded a relative humidity below the initial value, and the average bentonite water content and degree of saturation, according to the water intake measurements, were only 15.4% and 53%, respectively. Hydration caused a clear increase of the pressure recorded by the load cell located on the top of the cell. This pressure seems to have stabilised at a value of 1.4 MPa, which is still far from the equilibrium swelling pressure value of MX-80 bentonite compacted at dry density 1.53 g/cm^3.

Studies on stress-strain behaviour

The study was focused on the stress-strain properties of bentonite exposed to increased temperatures. However, the influence of different mineral composition, different anions and different preparation methods were also studied. The influence of the different treatments was quantified by measurements of stresses and strains during the unconfined compression test and from some of the series also by measurements of swelling pressure and hydraulic conductivity.

In the test series with increased temperature the specimens were exposed to short-term heating in a laboratory oven during 24h. Specimens of MX-80 were exposed to 90 °C, 120 °C and 150 °C and specimens of FEBEX were exposed to 90 °C. The heating was made both after and before full saturation where heating after full saturation meant heated with a controlled water pressure to a maximum of 600 kPa while heating before full saturation in this study meant heating at a high degree of saturation without control of the water pressure but under sealed conditions.

The following observations were made in this study:

- A tendency of increased deviator stress at failure with increased temperature after short-term heating but significant deviations only after heating to 120 °C and 150 °C;
- Significant decrease in strain at failure only after short-term heating to 150 °C;
- Small decreases in swelling pressure and hydraulic conductivity after short-term heating;
- Significant influence on deviator stress and strain at failure for specimens with old fractures;
- Small but no significant influence on deviator stress and strain at failure after circulation with solutions of CaCl2 or Na2SO4;
- No influence on deviator stress and strain at failure of grinding or washing the material at preparation. However, small influence of sampling technique was seen.

Subtask 2.2.2 – In-situ experimentation on key THM processes

The observed temperature increases in EBS and Opalinus Clay are in line with those predicted by the design calculations (slight variations are attributed to differences in model setup and conceptualization).

The EBS is characterized by a very strong temperature gradient owing to its low thermal conductivity of its very dry state especially in the inner part of the buffer. At the OPA interface a temperature of below 50 °C is registered. The heat pulse causes a further drying of the inner part of the buffer, whereby the initial water content is further reduced, below the water content at emplacement for both the granular material and the blocks. A complex development of the humidity profiles takes place which is strongly determined by the different water contents and densities of the materials at installation, high sensitivity to changing two-phase flow parameters and the impact of vapour diffusion in a changing porous matrix. The vapour is driven out, in a most likely radial pattern and part of the increase in relative humidity at the interface between the EBS and the hostrock can be attributed to condensation of vapour. The highest temperatures (above 100 °C) are thus prevailing in an EBS with very low water content (below 20 % RH).

The natural water inflow from the Opalinus Clay is occurring slowly. After 32 months only at distances in the Opalinus Clay above 1 m from the tunnel wall a positive hydraulic pressure is registered. The hydraulic pressure front is progressing toward the EBS, but how long this will take and when an equilibrium state will be reached if keeping the 140 °C constant cannot be determined from the current dataset. This can only be assessed using modelling.

The measured temperatures and relative humidities in the blocks and the granular materials are dominated by the distance of the measurement point to the heater and not by the differences in material properties although conditions at emplacement where somewhat different. This rapid homogenisation can also (partly) be explained by vapour movement and is observed for the first time in the HE-E, as this is the first large scale, high temperature, experiment with different materials.

As predicted by the models, a hydraulic pressure increase, associated with the differential thermal expansion of the Opalinus Clay and the porewater, is observed in the saturated Opalinus Clay at a larger distance from the tunnel. The porewater pressure increase, which started developing shortly after switching on the heaters, developed further after the heater temperature was held stable at 140 °C and was maximal at about 3 m from the tunnel wall where an overpressure of 1 MPa developed, slowly flattening off a couple of months after the heater temperature stabilised. These overpressures were within the expected range.

Based on the seismic transmission measurements, a variation of the derived P-wave velocity evolution was observed with pronounced dependencies on the orientation of the travel paths to the bedding (anisotropy) and their distances from the S/B–OPA interface. A sequence of decreasing and increasing P-wave velocities points to the creation and sealing of invisible microcracks within the first 50 cm from the S/B–OPA interface, most probably caused by desaturation, the thermal pulse and the saturation and porewater pressures changes. Seismic methods have been shown to be a very sensitive tool for the continuous characterization of changes in rock properties although a clear link between the seismic parameters and the physical phenomena is yet to be established.

3.4.3. Task 2.3 – Experimentation on key THM-C processes

The main results from the experiments on small cells are:

- At the concrete-bentonite interface, bentonite in contact with mortar seems to have lower total intruded (Hg) porosity than sections far from the interface. At the iron-bentonite interface, there is a negligible impact of magnetite into the bentonite in terms of porosity or SSA;
- Mortar and magnetite acted as sinks of chloride and sulphate;
- The Fe penetration front into the bentonite is less than 0.1 mm;

- A calcium front was developed from the mortar towards the bentonite, in which C-S-H phases formed. In accordance to the Aft and Afm type phases detected, aluminum penetrated in the mortar from the bentonite. According to the experimental results natural bentonite has potentially higher buffer capacity to attenuate the calcium alkaline front than the pre-treated (depleted in Mg) one.

The main results from the experiments on medium cells are:

- Concrete and iron interfaces act as a sink of soluble salts (Cl, S). Besides, concrete acts as Mg and inorganic carbon filter;
- Inside the concrete the reaction path follows the dissolution of portlandite and precipitation of CSH (of low C/S (0.8) ratio), calcite and ettringite (near the bentonite interface). The reaction pathway for iron corrosion starts with the formation of iron hydroxide ($Fe(OH)_3$), then lepidocrocite and goethite (oxy-hydroxides), and finally hematite and maghemite (Fe_2O_3) when the system is depleted in oxygen;
- The concrete-bentonite interface shows the precipitation of gypsum, CASH gels, MSH gels and carbonates (calcite and aragonite), affecting less than 2 mm thickness of bentonite. The iron alteration zone has an average thickness of 1 micron and the Fe-influenced zone was estimated to be 20 µm;
- Redistribution of exchangeable cations in the bentonite is characterized by drastic magnesium depletion due to its precipitation in alkaline porewater. This effect can be followed in a 20 mm wide bentonite from the concrete interface;
- There are evidences of thermally-induced mineralogical changes such as silica precipitation at the iron-bentonite interface (600 µm): Cristobalite beads (size around 100 nm). The possible formation of very small amounts of random interstratified phases in the vicinity of the iron/bentonite interface due to long-term exposure to high temperature (7 years, 100 ºC) has also been identified.

3.5. Summary and future perspective

The in-situ and laboratory tasks carried out during the project – considering a wide range of time and spatial scales – have accomplished the following general objectives:

- Confirm, integrate and improve the existing knowledge of the THM-C processes in the early time evolution of bentonite barriers. More reliable and better understood information about the saturation rates, swelling, homogenization, thermo-mechanical, microstructural, microbiological and geochemical aspects and coupled processes of the bentonite (in different states, such as blocks, GBM and mixed with sand) has been obtained.
- This information is a good data base for future interpretation of large scale experiments and modelling works. Numerical models can now be better formulated, and the predictions of the behaviour of bentonite barriers improved. The uncertainties of models could be reduced.

- The findings of this Work Package provide more clear criteria to be conservatively applied in the Performance Assessments of engineered barriers.

A more specific summary per task within WP 2 is presented in the following sections.

3.5.1. Task 2.1 – Experimentation on key HM processes

The hydro-mechanical behaviour of bentonite-based sealing materials was tested under room temperature. Particularly, the hydration rate, its relation to the development of swelling pressure, and the material permeability have been studied, mostly under low hydration pressures. The state of the material after saturation has been also analysed. Full saturation of these materials takes long times, and the microstructural processes taking place are not yet fully understood. The effect of the water salinity on the observed behaviour has not been evaluated.

The EB experiment has shown that the values of the key safety relevant parameters (dry density, swelling pressure, permeability) that can be achieved with an emplacement technique using a granular bentonite material in the upper part of the barrier and bentonite blocks at the bottom, might fall between the acceptable limits considered in the Performance Assessment of the repository concepts.

Even though the conditions in the EB test section are now not considered as representative of a true demonstration under repository like conditions (the density achieved is lower than would be expected in a more ideal situation and the variation in density is probably significant), the permeability tests on dismantled samples do confirm that after saturation the barrier had a low hydraulic conductivity (equal to or lower than 5×10^{-12} m/s).

It has been shown that geophysical monitoring is a useful tool for the characterization of continuously ongoing changes of rock properties, although not all correlations and dependencies between varying geophysical parameters and related rock property changes are completely understood until now.

3.5.2. Task 2.2 – Experimentation on key THM processes

Subtask 2.2.1 – Laboratory experimentation on key THM processes

More than seventeen years after the start of the operational phase of the mock-up test, it could be deduced from the most recent data available that most of the barrier has achieved high degrees of saturation. The observed THM behaviour shows good homogeneity throughout the test and has revealed several features of interest, such as the underestimation of saturation times and the major implications of the thermal aspects. The FEBEX mock-up test supports the evidence of the slowing down of hydration, under a specific thermal load and geometry. The long-term evolution of the test may provide a better understanding of the latest stage of the saturation (average saturation degree above 90%).

Two TH tests in cells run for 12 years to compare the hydro-mechanical behaviour of bentonite saturated under thermal gradient and at room conditions. Although the saturation rate was very slow in both cases, the thermal gradient clearly delayed the process, which was enhanced by the fact that the cells did not remain hermetic during the tests.

The two tests in cells designed to reproduce the conditions of the two materials used in the in-situ HE-E test (sand/bentonite mixture and bentonite pellets) showed a completely different behaviour, since the S/B mixture is much more permeable and does not swell. The effect of the thermal gradient on the water vapour redistribution was considerable, which had been observed in test GT40. The progression of hydration in cell B is very slow and accompanied by an increase in swelling pressure. The fact that the water injection pressure is very low can contribute to this long duration of the hydration process.

The two series of tests have provided a database of online results very useful for model calibration and verification. The complete post mortem analyses of the samples of tests GT40 and I40 remain to be conducted, as well as the dismantling and post mortem analysis of cells S/B and B.

With respect to the studies on stress-strain behaviour, the results from specimens exposed to short-term heating to 120 °C and 150 °C showed deviations of deviator stress and strain at failure compared to the reference specimens. The tested specimens of bentonite were saturated or almost saturated. Further tests on specimens heated in a clear unsaturated state are suggested.

Subtask 2.2.2 – In-situ experimentation on key THM processes

The HE-E experiment at the Mont Terri URL was one of the key elements of the PEBS project and was designed, constructed and operated successfully within the project timeframe. Considering the high density of the instrumentation characterising this experiment, the combination of a consistent dataset with the explanatory insights provided by the various models marks and achievement both from an experimental and modelling viewpoint.

At the end of the PEBS project, the HE-E experiment continued as a Mont Terri partner project and its extension is decided upon on an annual basis by the partners (BGR, GRS, ENRESA and Nagra). Both its continued monitoring, but also the dismantling of the EBS finally will continue to provide essential information on the behaviour of the EBS in this very hot and dry early saturation phase.

3.5.3. Task 2.3 – Experimentation on key THM-C processes

The GAMEs dismantling has not yet been accomplished. However, concrete-bentonite and corrosion products-bentonite interactions from other experiments provided modellers (UDC) with a database on THM-C processes and their evolution over time similar (although considering a different experimental scale) to that expected from the GAMEs.

Laboratory experiments on small and medium cells provided to modellers very useful data about parameters and main processes at the concrete-bentonite and iron-bentonite interfaces considering the operational phase and the transient (1000-3000 years) stages of a HLW repository.

Future work should make emphasis in aspects relevant to porosity and transport processes at the interfaces. In this sense, the clogging of porosity at the concrete-bentonite interface should be precisely evaluated, as well as the thermally-induced mineralogical changes at the iron-bentonite interface. The possibility of formation of silica or new tri-octahedral clays in small quantities should be further confirmed in the long–term experiments and with more SEM or TEM studies. A deeper characterization of the CSH or CASH phases present at the concrete-bentonite interface and the iron corrosion products should be made. Therefore, some studies at high resolution scale should be conducted in order to determine the extension of Mg-silicate phase formation. Finally, an effort to integrate the results from different experimental approaches in terms of upscaling (spatial and temporal) should be made.

4. WP 3 – Modelling of short-term effects and extrapolation to long-term evolution

4.1. Objectives

The overall objectives of this work package were

- to perform coupled HM, THM, and THMC analyses to provide a sound basis for the interpretation of the various tests planned in the framework of WP 2,
- to develop new or improved models as demanded by the calibration of computational results with the measured data, and
- to use the data and improved models for extrapolation to long-term evolution of the repository taking into account the scenarios defined in WP 1 and to investigate model uncertainty and its impact on long-term prediction, thus providing input to WP 4.

The work package is structured into five different tasks.

Task 3.1 – "HM modelling of the Mont Terri Engineered Barrier (EB) Experiment", aimed at providing a satisfactory scientific representation and a sound basis for interpretation of the EB hydration phase and of the dismantling data, by using new or improved constitutive laws adjusted to the experimental data.

Task 3.2 – "THM modelling for the planned heater test HE-E", focused on design modelling as well as predictive and interpretative modelling of the HE-E heater test and the validation of constitutive models developed in earlier projects, such as NF-PRO.

Task 3.3 – "THM modelling of bentonite buffer", has the objective to study various aspects of buffer behaviour in different experiments and disposal concepts. This involves numerical studies on buffer evolution in the Swedish concept, the set-up and use of an inverse modelling framework for the analysis of the FEBEX in-situ test, and a continuing interpretation of the long-term FEBEX mock-up test as well as analyses for the long-term THM tests performed in cells in the CIEMAT laboratory.

Task 3.4 – "Modelling of THM-C experiments on bentonite buffer", had the objective to develop advanced multiple-continua THC(m) models for clay barriers and test them with lab and in-situ tests performed in the frame of PEBS and NF-PRO. The emphasis is on the numerical interpretation of container-bentonite interactions and concrete-bentonite interactions.

Task 3.5 – "Extrapolation to repository long-term evolution" had the objective to use the data and improved models from Task 3.1- Task 3.4 for extrapolation to long-term evolution of the repository and to investigate model uncertainty and its impact on long-term prediction, thus providing input to WP 4. This involves

- Critical assessment of the results of the other WP 3 tasks regarding their implications for different time and space scales including long-term conditions;
- Identification of the significant processes in the resaturation phase and after resaturation;
- Development or modification of the available HM, THM and THM-C formulations to incorporate phenomena and processes deemed to be relevant for long-term predictions;
- Performance of coupled numerical analysis for long-term evolution of the engineered barrier system in the repository, with different degrees of abstraction and different focuses according to the different modelling teams;
- Evaluation of the model uncertainty and its implications for long-term prediction and safety analysis.

An additional objective of Task 3.5 was the compilation and evaluation of the usefulness of natural analogues for providing support, testing and validation of long-term predictions of current THMC models. Furthermore, a study of the thermo-mechanical continuum theory of mixtures was included in Task 3.5, in order to approach long-term evolution from a different point of view and to provide a relevant material model applicable for systems consisting of bentonite (montmorillonite), water and air.

4.2. Beneficiaries involved

The beneficiaries involved in WP 3 were Nagra (Task 3.2, 3.3, and 3.5), SKB (Task 3.3 and 3.5), GRS (Task 3.2 and 3.5), ENRESA (all tasks), CIMNE (Task 3.1, 3.2, 3.3 and 3.5), UDC (Task 3.4 and 3.5), TK Consult (Task 3.2, 3.3, and 3.5), and Clay Technology (Task 3.3 and 3.5).

GRS was in charge of the scientific and technical coordination of this Work Package. BGR, as the project coordinator, was involved in this WP with management duties.

4.3. Execution of work

4.3.1. Task 3.1 – HM modelling of the Mont Terri Engineered Barrier (EB) Experiment

Modelling of the EB experiment (described in Section 3.3.1) addressed both the buffer behaviour during the hydration phase and the state of the buffer at the end of the test, as established during the dismantling operation. The coupled hydraulic-mechanical analyses were performed by CIMNE using the computer code CODE_BRIGHT with a plane-strain geometry. The mechanical behaviour of the compacted bentonite blocks was described by a thermo-elastoplastic model, commonly known as the Barcelona Basic Model (BBM). The main advancement in this task was the development and application of a double porosity model for the bentonite pellets. The macrostructural behaviour is described by equations for unsaturated non-expansive soils (like the BBM). For the microstructural behaviour, saturation and reversible deformation are assumed to be independent of macrostructural effects. Coupling between the two structural levels takes into account irreversible macrostructural strains when elastic microstructural strains take place; that means elastic microstructural strain (swelling or shrinking) leads to irreversible macrostructural strain. The functions describing the coupling between the structural levels are dependent on the “degree of openness” of the macrostructure relative to the applied stress. The parameters required for the double-structure model were calibrated from the numerical modelling of wetting-drying tests at constant vertical load and wetting tests at constant volume. The complete model description can be found in Deliverable D3.1-1/D3.1-2.

The new model was successfully used to simulate the granular buffer evolution. An alternative approach additionally taking into account a variable density for the liquid phase had also been considered, but was not required in the end.

4.3.2. Task 3.2 – THM modelling for the heater test HE-E

Three teams participated in the modelling of the HE-E experiment in the framework of PEBS. The Nagra team used TOUGH2 with a thermo-hydraulic (TH) approach and a three-dimensional model. GRS used CODE_BRIGHT with a thermo-hydraulic-mechanical (THM) approach and a two-dimensional plane-strain model. CIMNE also used CODE_BRIGHT with the full THM approach and a two-dimensional axisymmetric model; for some considerations, also a plane-strain model was used. The history of the HE-E tunnel, which had formerly been used for the Mont Terri Ventilation Test, involving a complicated series of drying/wetting cycles of the surrounding rock, was accounted for by suitable simplifications leading to a reasonable initial pore pressure.

In a first step, scoping calculations were performed with preliminary material data prior to the installation of the HE-E. The objective was to give a first idea of the response to heating that could be expected and to find out whether the planned instrumentation was suitable to measure this response. While there were considerable deviations in the results of the three teams, they agreed that an early pore pressure increase was to be expected not in the close vicinity of the HE-E tunnel, but a few metres away. Consequently, the instrumentation was supplemented accordingly. Details on the scoping calculations are found in the HE-E design report, Deliverable D2.2-2.

While performing the first predictive simulations of the HE-E, a modellers’ database was developed, compiling all the material data needed for the simulations. This involved existing data on the THM behaviour of the buffer materials and the rock as well as laboratory testing results obtained in PEBS Work Package 2, especially regarding the bentonite pellets and the granular sand-bentonite mixture.

With the completed database interpretative calculations were performed and compared to the actual measurement results, in terms of temperature, relative humidity in the buffer, and pore pressure in the rock. The models and assumptions used in thee simulations are described in detail in the combined Deliverable D2.2-11/D3.2-2 “The HE-E Experiment: Lay-out, Interpretation and THM Modelling”.

4.3.3. Task 3.3 – THM modelling of bentonite buffer

Task 3.3 was dedicated to the investigation of various aspects of buffer THM behaviour. A special emphasis was on the use of approaches exceeding standard views and applications.

Clay Technology studied eleven modelling tasks involving the bentonite buffer for the Swedish disposal concept. An overview of these tasks is given in Deliverable D3.3-2, including information about the objective, models used, some main results, and uncertainties. The tasks with higher relevance regarding the PEBS framework were described in more detail, namely: Analysis of time scale of buffer hydration, analysis of moisture redistribution in dry rock scenario, and buffer homogenization. The respective simulations using CODE_BRIGHT and ABAQUS were performed early in the project and made use of the data available at that time.

TK Consult and Nagra studied, whether TH inverse approaches can be applied for interpreting long-term THM experiments, neglecting mechanical processes as induced e.g. by bentonite swelling, but profiting from the computational efficiency introduced by the reduction of complexity. In order to ensure predictive reliability, the study derived the involved parameters from inverse modelling of the full-scale FEBEX in-situ test which provides pressure, temperature, and saturation data from a heating experiment for a period of 15 years. A series of models had to be maintained, each representing one phase of the experimental setup, which includes, (1) excavation and installation, (2) isothermal hydration, (3) first heating phase, (4) cooling down of first heater, (5) dismantling of first heater, and (6) second heating phase. The initial conditions being transferred in each case from the previous phase, the six models differed in geometry and boundary conditions but were driven by the same set of model parameters. Details are given in the PEBS Deliverable D3.3-1. The joint inversion of the whole set of measurement data resulted in parameter estimates of permeability, porosity, relative permeability and capillary pressure functions for both, host rock and bentonite buffer. In addition, the inverse model provided uncertainty estimates of the resulting parameters in form of standard deviations which can be applied in following modelling steps in order to assess the uncertainty of long-term predictions.

CIMNE simulated two long-term infiltration cell tests (an isothermal cell test and a thermal gradient cell test) and the FEBEX mock-up test using CODE_BRIGHT with a full THM formulation. Earlier analyses had shown that there were some discrepancies between modelling results and observations, especially regarding the rate of water uptake of compacted bentonite. In the framework of PEBS, enhanced constitutive laws were taken into account in order to explain the deviations. Four types of analyses were carried out:

- Reference analyses, using the conventional THM formulation (BBM);
- Analyses assuming non-Darcy flow due to the existence of a threshold gradient in the liquid flow law;
- Analyses incorporating thermo-osmosis;
- Analyses incorporating the evolution of micro-fabric by means of a double structure constitutive law (compare Section 4.3.1).

Details are given in Deliverable D3.3-3.

4.3.4. Task 3.4 – Modelling of THM-C experiments on bentonite buffer

Starting from an existing THC formulation, UDC incorporated mechanical and geochemical couplings in order to account for porosity changes caused by swelling phenomena (THCm). In addition, reactive gaseous species, such as O_2, CO_2, and H_2 were incorporated. The improved model was tested with the data from the FEBEX mock-up test. Further tests were performed using different experiments performed at CIEMAT (see Chapter 3):

- The CG experiments performed on 60 cm long bentonite columns with durations ranging from 0.5 to 7.5 years;
- Corrosion experiments to study the corrosion products generated at the canister-bentonite interface under repository conditions and analyse how the corrosion products affect the properties of the bentonite. These experiments were performed on samples of several lengths (25 mm for SC tests and 100 mm for FB tests) and temperatures (25 ºC, 50 ºC and 100 ºC);
- The HB experiments to study the interactions of concrete and bentonite, including a 30 mm layer of concrete which was in contact with the hydration system and a 71.5 mm thick layer of bentonite;
- The so-called double interface tests which include a 3 mm thick layer of cement mortar which is in contact with the hydration system, a 18 mm thick layer of bentonite and a 2 mm layer of powder magnetite.

Although some uncertainties remain, many aspects of the different experiments were successfully reproduced with the improved model (Deliverable D3.4-1).

4.3.5. Task 3.5 – Extrapolation to repository long-term evolution

One of the major exercises of Task 3.5 was to define and numerically model a set of simulation cases relevant for the repository long-term evolution, building on the insights from the other PEBS tasks and providing input to WP 4. In order to have a maximum benefit from this exercise, it was concluded that

- The processes which exhibit uncertainties were the most relevant for the extrapolation consideration;
- Substantial data to improve their description should be provided within PEBS;
- The modelling cases to be considered should be of interest to more than one of the partners.

With these criteria in mind, the following long-term simulation cases were defined:

- Simulation Case 1 – Isothermal buffer evolution;
- Simulation Case 2 – Thermo-hydro-mechanical evolution of the buffer at temperatures up to 100 °C;
- Simulation Case 3: Thermo-hydro-mechanical evolution of the buffer with temperatures temporarily exceeding 100 °C;

- Simulation Case 4: Geochemical evolution at canister-bentonite and bentonite-concrete interfaces, including a long-term simulation of a repository in granite.

The description of the cases and the simulation results are found in Deliverable D3.5-4.

Simulation Case 1: Isothermal buffer evolution

For the numerical simulation of the long-term isothermal buffer evolution CIMNE extrapolated the EB experiment over a period of 100 years. The model assumptions and parameters were the same as described in Section 4.3.1. In particular, the new double structure model was used for the simulation. In contrast to the other simulation cases, no thermal effects had to be considered, so that a pure hydro-mechanical formulation could be used.

Simulation Case 2: Buffer THM evolution up to 100 °C

This case is based on the Spanish disposal concept in granitic rock as described by the ENRESA Performance Assessment exercise "ENRESA 2000" (ENRESA, 2001) and the R&D programme on bentonite material, particularly the FEBEX project (ENRESA, 2006). The repository concept in granite considers the disposal of spent fuel in carbon steel canisters in long horizontal disposal drifts. Canisters are surrounded by high-density bentonite. A canister measures 4.54 m in length and 0.90 m in diameter, and contains 4 PWR or 12 BWR fuel elements in a subcritical configuration. The thermal power at the beginning of the geological storage thermal power amounts to 1220 W per canister. Two case variants were considered, one being a long-term simulation with constant thermal output after reaching a maximum temperature of 100 °C, which is not realistic but included for reference, the other incorporating a realistic thermal output of the emplaced canisters.

CIMNE performed full THM long-term simulations of the two case variants over 1000 years of emplacement using CODE_BRIGHT with an axisymmetric geometry. For the bentonite buffer behaviour, three formulations were compared to each other:

- Reference analyses, using the conventional THM formulation (BBM);
- Analyses incorporating thermo-osmosis;
- Analyses incorporating the evolution of micro-fabric by means of the new double structure constitutive law.

A detailed description of new processes included in long-term simulations is given in Deliverable D3.5-2, "Formulation of a model suitable for long-term predictions".

TK Consult and Nagra simulated the case variant with realistic thermal output using the code TOUGH2 with a TH formulation over 100 years. The geometric model was again axisymmetric and represented the centre of a disposal drift. An additional model representing the end of the drift was also investigated.

The parameters for the different materials were taken from the inverse modelling of the FEBEX experiment described in Section 4.3.3. With the inverse framework provided by the code iTOUGH2, also confidence intervals for the modelling results could be given. Beside the statistic parameter uncertainty and the geometry effect, two additional conceptual uncertainties were investigated by alternative simulations, namely an increased initial fluid pressure in the rock of 5 MPa corresponding to 500 m depth below surface of the disposal drift and a lower initial saturation of the buffer.

Simulation Case 3: Buffer THM evolution above 100 °C

Three teams (Nagra, GRS and CIMNE) were involved in the simulation of this case, which is based on the Swiss reference concept of drift disposal, with waste canisters resting on compacted bentonite blocks and the remaining void backfilled by bentonite pellets. The heat power per canister is 1500 W at emplacement. All teams simulated a disposal cell covering a single canister, making use of the obvious symmetry boundaries, and different additional simplifications.

Nagra and GRS both used a three-dimensional model, giving a realistic geometrical representation of the repository cell, but reduced the complexity of the problem by performing thermal-hydraulic simulations, neglecting mechanical effects. Nagra used TOUGH2 and simulated various cases in order to get an insight into modelling uncertainties: A reference case with the material parameters from the HE-E database (see Section 4.3.2) and variants with reduced thermal conductivity of the buffer, reduced pore expansivity of the clay rock, altered hydraulic parameters of the bentonite blocks, the pellets, or the clay rock. GRS used CODE_BRIGHT and simulated the reference case. Due to very high calculation times (months), only an altered initial saturation profile of the rock was considered beside the reference case. An additional difference between Nagra's and GRS' models was Nagra's consideration of a 0.7 m wide excavation damaged zone (EDZ) with increased permeability in the rock.

CIMNE also used CODE_BRIGHT, but with full THM coupling and the simplification of a two-dimensional axisymmetric geometry. Since the heterogeneous buffer composition (bentonite blocks and pellets) cannot be represented in such a model, two variants were considered: a pure pellet buffer and a buffer where the canister is completely surrounded by blocks. Adjacent emplacement drifts had to be neglected due to the geometry. A 0.6 m wide EDZ was considered. Due to long calculation times, only the reference case using the database parameters with the conventional THM formulation could be simulated.

Simulation Case 4: Geochemical evolution at interfaces

For the simulation of the geochemical evolution at the canister-bentonite and bentonite-concrete interfaces UDC used the THCm formulation introduced in Section 4.3.4.

For the long-term simulation of the canister-bentonite interface, a one-dimensional axisymmetric model of the Spanish disposal concept in granitic rock as described in "ENRESA 2000" (ENRESA, 2001) was used, including the steel canister and the surrounding bentonite blocks. Granitic porewater was supplied from the outer boundary of the model. The model considered canister corrosion, the interactions of corrosion products with bentonite and the pH buffering mechanism, with the reaction types of aqueous complexation, acid/base reactions and redox reactions. The model accounted for dissolution/precipitation of calcite, gypsum, quartz, magnetite, siderite and goethite. The model also accounted for cation exchange of Na^+, Ca^{2+}, Mg^{2+}, K^+ and Fe^+ and surface complexation reactions, which were modelled with a triple sorption site model in the bentonite. All reactions were assumed at equilibrium in the reference model. In the frame of an uncertainty analysis, some simulations were performed accounting for kinetically-controlled precipitation of some minerals or including new minerals such as smectite.

Simulations were performed for a time span of one million years at a constant temperature of 25 °C, neglecting the early post-closure temperature transient. Simulations considering the temperature gradient were, however, also performed to explore the temperature influence on the geochemical evolution. Most of this work is described in Deliverable D3.5-3, an update is found in Deliverable 3.5-4 with the other cases.

The bentonite-concrete interface was modelled with a one-dimensional axisymmetric model representing the Spanish disposal concept in clay rock, including in the base variant three material zones: The bentonite buffer, concrete, and clay formation. Initially, the buffer is unsaturated with a water content of 14 vol.%. Clay pore water infiltrates into the concrete, interacting with the cementitious materials and producing hyper alkaline pore water, which then diffuses into the bentonite. The bentonite is saturated, but the high pH fluid interacts with the bentonite minerals as it diffuses, inducing the dissolution of the primary minerals and the precipitation of secondary minerals in the bentonite and the concrete. Until full saturation, mechanical effects (porosity reduction from swelling) are considered. Water flow is negligible once the bentonite buffer is saturated. Then, solute transport occurs entirely by molecular diffusion.

The minerals considered in the base variant were calcite, gypsum, quartz, portlandite, brucite, sepiolite, tobermorite, and gyrolite. In an enhanced model, canister corrosion was considered additionally. This resulted in adding dissolved iron and oxygen to the chemical components and solid iron, magnetite, siderite and goethite to the minerals. A further enhancement also considered smectite dissolution, which extended the list of minerals by smectite, analcime, saponite and cronstedite. Temperature evolution was considered in the simulations; for the variants with corrosion a constant corrosion rate of 2 μm/y was assumed.

Besides the four long-term simulation cases, additional effort was made in different directions. The usefulness of natural analogues for providing support, testing and validation of long-term predictions of current models was investigated. The possibility of deriving scaling laws by integrating available data for bentonites from different scales and using them for extrapolation was explored. A long-term simulation of a repository in granite (Spanish concept) was performed. The thermo-mechanical continuum theory of mixtures was studied in order to approach long-term evolution from a different point of view.

Natural analogues

One of the activities carried out by UDC in Task 3.5 was the compilation and evaluation of the usefulness of natural analogues (NA) for providing support, testing and validation of long-term predictions of current THMC models. Several NA projects were studied in this regard. The results are summarized in the PEBS Milestone 3.5-3 document.

Scaling laws

A large number of hydrodynamic, geochemical and thermal data has been collected for compacted bentonites during the last 30 years to characterize their properties and evaluate the suitability of compacted bentonite for EBS in a HLW repository. Past and on-going experiments cover a wide range of time and spatial scales. Their durations range from a few months in the case of the CT cells to more than 14 years in the case of the FEBEX mock-up and in-situ tests. The size of the experiments ranges from 10 cm in CT cells to more than 10 m in the in-situ test. An integrated analysis of the hydrodynamic, thermal and chemical data from several space and time scales was performed by UDC in terms of dimensionless variables. This work is documented in Deliverable D3.5-1.

Mixture theory

Clay Technology performed a review of thermomechanical continuum mixture theories potentially applicable for EBS materials. It was motivated by several limitations or inadequacies of common material representations, such as the lack of coupling retention to mechanics, the uncertainty in the actual mechanism of water transport or the limited validity of mechanical representations which were developed for typical geomaterials instead of clayey swelling materials.

Following the study, a concept of non-associative immiscibility which gives a mixture with immiscibility on different levels was developed. An attempt to schematically formulate a material model using this concept was described. Deliverable D3.5-4a summarizes the related work.

4.4. Main results

4.4.1. Task 3.1 – HM modelling of the Mont Terri Engineered Barrier (EB) Experiment

The progress of hydration, as observed in the evolution of relative humidity (in the buffer and in the rock) and pore pressure (in the rock) is generally satisfactorily reproduced by the numerical model. Larger discrepancies concern the time evolution of relative humidity in the buffer, which is a likely consequence of the complexity of the artificial hydration system as well as a lack of control in some of the early hydration stages.

Dismantling revealed that the barrier was at or very close to full saturation throughout, and that a significant degree of homogenization was been achieved, although some heterogeneities persisted. Again, the numerical model achieved a very good representation of the state of the buffer at dismantling. A practically fully saturated barrier was predicted and the degree of homogenization is also well reproduced. Even the pattern of heterogeneities in the cross section of the barrier is well reproduced.

It has been considered likely that part of the heterogeneity observed upon dismantling may be caused by an initially heterogeneous barrier due to emplacement difficulties and possible segregation of the granular bentonite. It should be noted, however, that the numerical analyses assumed an initially homogeneous granular bentonite. Therefore, the modelling suggests that at least some of the observed heterogeneity at the dismantling stage is a direct consequence of the layout and geometry of the test.

4.4.2. Task 3.2 – THM modelling for the heater test HE-E

Nagra's thermal-hydraulic 3D simulations resulted in a good representation of the temperature field. A sensitivity study on the effect of the relation between thermal conductivity and saturation of the buffer showed that a significant impact is restricted to the vicinity of the heater. Regarding the evolution of relative humidity as a measure of saturation of the buffer, there was some deviation between the measured data and simulation results. Desaturation in both sections of the granular buffer was restricted to the close vicinity of the heater, and no desaturation of the bentonite blocks was observed in the simulation, as opposed to the relative humidity measurements. In order to reproduce pore pressure evolution in the rock, the thermal expansion of the grains in comparison to the thermal expansion of the pore water was investigated numerically. With an additional adaption of the pore compressibility as a compensation for transverse anisotropy which cannot be considered in TOUGH2, a reasonable representation of pore pressure evolution could be obtained.

GRS used CODE_BRIGHT with plane-strain geometry, full THM coupling, and simple elastic models for rock and buffer in order to explore their performance in simulating the HE-E. As a consequence of the plane geometry, temperature was overestimated in the buffer, since the axial heat flow component is neglected. For the relative humidity evolution in the sand-bentonite buffer, a satisfying representation was obtained with a square-law retention curve which represents the measurement results in the relevant saturation range better than the alternatively considered van Genuchten curve. In the bentonite pellet buffer, the elastic model proved to be inadequate. The pore water pressure evolution in the rock was underestimated in these simulations.

Most of CIMNE's simulations were carried out using an axial symmetric model which is not capable of catching the difference between the bentonite blocks and the granular buffer materials, but avoids the thermal overestimation introduced by a plane strain model. Consequently, satisfying modelling results of the temperature field were obtained. Using an elastoplastic model (Barcelona Basic Model) for the buffer and retention curves of a modified van Genuchten type which represented well the laboratory and additional back-analysis results, the simulation of relative humidity in both buffer types was also reasonable. Still, some uncertainties regarding the retention curves of the granular buffer materials remain. The initial state of pore pressure in the rock could not be simulated adequately with the axial symmetric model; an additional plane-strain model produced a better match. On the other hand, the axial symmetric model gave better results in terms of the impact of heating on pressure evolution.

As an overall conclusion of the HE-E simulations one can state that turning the attention to different aspects of modelling, as the different teams did, led to good results regarding these aspects. The shortcomings could be attributed to accepted simplifications in considered processes, geometry or constitutive models. In particular, the buffer behaviour can be simulated in an adequate way, although uncertainties concerning the retention curves of the granular buffer materials and the dependence of their thermal conductivities and permeabilities on the degree of saturation remain.

4.4.3. Task 3.3 – THM modelling of bentonite buffer

The results of the Clay Technology team studying THM behaviour of the bentonite buffer in the Swedish disposal concept are described in Deliverable D3.3-2. One finding was that the saturation time for the buffer is affected by changes in the retention curve. Buffer permeability was less important for the adopted hydraulic conditions in the rock. Thermodynamics as well as experiments suggest that retention is stress dependent. Therefore, the evolution of the actual stress state should be coupled to the retention. Stress dependence is, however, not included explicitly in the normally used van Genuchten formulation. Furthermore, it can be concluded from Clay Technology's studies, that existing models like the Barcelona Basic Model do have difficulties simulating buffer homogenization behaviour in a system such as the Swedish concept, with large initial density differences between highly compressed bentonite blocks and an outer slot backfilled with bentonite pellets. A thermodynamically/chemically based model might be of benefit (see Section 4.4.5).

For TK Consult's inverse modelling of the FEBEX in-situ experiment (Deliverable D3.3-1), comparisons of model simulations with the observations show different degrees of agreement. While the pressure fit obtained in the granite boreholes is suffering from the unconsidered heterogeneity and potential measurement errors the agreement of relative humidity in the buffer and temperature in both, buffer and rock is remarkable, taking into account the simplicity of the axisymmetric model. Moreover, the estimated thermal and two-phase parameter values fit well into the range of available laboratory measurements. Other parameter estimates (e.g. the low porosity of the bentonite) include the influence of neglected/simplified processes and, thus, refer to the TH modelling approach, solely.

The three enhanced models (taking into account threshold gradient, thermo-osmosis or microfabric evolution) used by CIMNE for the simulation of the long-term infiltration tests and the FEBEX mock-up are all able to model reasonably accurately the hydration of the mock-up test at early and later stages (Deliverable D3.3-3). Although the PEBS project was not designed to establish experimentally the potential existence and effects of those three phenomena, the results of THM modelling of the FEBEX mock-up test (16 years of observations) gives some useful information on the effects likely to be associated with each one of the individual hypotheses considered. Numerical modelling has shown that each of these possibilities is capable of providing results in reasonable good agreement with observations. However, numerical analysis, on its own, is unable to identify with certainty which is the phenomenon (or combination of phenomena) underlying the observed slowing down of hydration. However, there are noticeable differences between the predictions of the different hypotheses for the longer-term situation. Therefore, availability of long-term observations of the mock-up test may help in identifying the relevant phenomena at the later stages of hydration.

4.4.4. Task 3.4 – Modelling of THM-C experiments on bentonite buffer

With the enhanced model, the cumulative inflow measured in the FEBEX mock-up for the last 14 years could be reproduced. The fit of relative humidity, however, shows some discrepancies possibly caused by some model limitations such as the consideration of a single porosity model.

Regarding the 60 cm long (CG) experiments, the numerical model reproduced the observed temperatures, saturation degrees, porosities and dissolved an exchanged chemical data. Geochemical predictions improved when the changes in porosity caused by swelling were considered and when some parameters such as vapour tortuosity, heat dissipation and cation selectivities were estimated.

With respect to the corrosion experiments, simulations agreed well with experimental data for the most part. Model results indicated that

- The main properties of the bentonite remain unaltered;
- There is a sequence of corrosion products, $Fe(OH)_2$(s) and magnetite being the end members;
- Fe^{2+} is sorbed by surface complexation;
- Fe^{2+} cation exchange is less relevant than Fe^{2+} sorption;
- Corrosion products penetrate a few mm into the bentonite.

For the most part, the model also reproduced the reactions observed at the concrete-bentonite tests, including calcite and brucite precipitation in the hydration contact and the dissolution of portlandite and precipitation of CSH, calcite and MSH near or at the bentonite-concrete interface. The model predictions for ettringite and gypsum were less accurate. The precipitation of CASH phases was not accounted for in the models due to the lack of thermodynamic data. The nature of low crystal size C-(A)-S-H and M-S-H at the bentonite-concrete interface is still unclear.

4.4.5. Task 3.5 – Extrapolation to repository long-term evolution

Simulation Case 1: Isothermal buffer evolution

The simulation of the EB experiment was continued until reaching a time of 100 years to examine the long-term behaviour of an engineered barrier under isothermal conditions. Since the barrier was in a state of full saturation or near full saturation at the end of the EB field test, few changes were computed in the extended analysis. Basically, the rock mass returned to the initial state before excavation and buffer emplacement, and the barrier naturally stayed saturated.

The most relevant observation is the fact that the degree of heterogeneity remained unchanged so the distribution of porosity (or dry density) observed at dismantling remained constant. It is likely that this conclusion is quite dependent on the degree of irreversibility implicit in the constitutive model of the barrier material. Although the constitutive model and parameters used have proved very adequate when modelling the observed behaviour of the test, it is conceivable that different constitutive models could lead to potentially different results. This is an issue that probably deserves more attention in the future. It should also be noted that no creep phenomena (i.e. deformation under constant effective stress) have been considered either in the buffer or in the rock. If creep is relevant over the long period considered, it would probably lead to a higher degree of homogenization. Creep is potentially an important phenomenon in long-term predictions and should be the subject of focused research.

Simulation Case 2: Buffer THM evolution up to 100 °C

When comparing the two case variants (constant temperature and heat decay), the patterns of the early transient results in the two variants are naturally very similar. However, the long-term predictions are of course quite different.

In CIMNE’s simulations, temperatures reach a peak and start to fall after a few centuries in the heat decay variant. Temperatures have practically recovered to the initial values at the end of the analysis (1000 years). It should be stated, however, that long-term temperature predictions are sensitive to the particular model geometry, which is assuming an infinite number of deposition tunnels by using the symmetry of the system. While the effect on the temperature evolution is negligible for early times, it is obviously relevant for the long-term.

In the heat decay reference case (without thermo-osmosis or double structure of the buffer), full saturation of the barrier is achieved after approximately 8.5 years - a significantly shorter time than in the constant temperature analysis. Swelling pressure also fully develops over similar times. Observing the long-term results, it can be noted that, after achieving the maximum values, the stresses reduce somewhat, because of the contraction associated with temperature reduction.

The incorporation of thermo-osmosis changes significantly the hydration times of the barrier. In the constant temperature case it prevents full saturation indefinitely, but even in the heat decay analyses, full saturation is only achieved towards the end of the analysis (1000 years). Development of swelling pressure follows the progress of hydration, so the full final value is only achieved at the end of the analysis. Similarly, consideration of the micro-fabric evolution also delays full hydration (and full swelling pressure development) until the end of the analysis, i.e. 1000 years. As expected, temperature fields are affected very weakly by using the alternative hypotheses of the enhanced models.

The results correspond to a specific geometry and a single set of parameters. The parameters chosen have the only merit of providing a reasonable good representation of the observed short-term transient behaviour but here they are applied to long-term calculations, so a significant uncertainty inevitably remains. Even modest variations of parameters can result in significant changes in predicted THM behaviour. A sensitivity study for the long-term situation would thus be quite valuable to assess the degree of uncertainty and the reliability of the reported results.

TK Consult and Nagra received confidence intervals for their results with respect to parameter uncertainty and also performed some alternative calculations with altered initial conditions. The simplification of disregarding mechanical effects, on the other hand, led to best-fit parameters that are not in all cases reflected by measurements (e.g. bentonite porosity).

In the reference case, full saturation of the buffer was predicted to be achieved after 15 to 20 years. With increased initial pressure this time was reduced to 5 to 8 years, while it was increased to above 20 years with lower initial water content of the buffer. This variant also led to slightly increased temperatures (4 °C maximum). The model considering the end of the emplacement drift showed slightly lower temperature at later times, which can be expected as a consequence of the additional axial heat flow component. The confidence bandwidth of results coming from the confidence intervals of the parameters was rather narrow as a consequence of small standard deviations of the parameters. On the whole, the results confirmed current knowledge regarding evolution of temperature and resaturation and showed the capability of the systematic error analysis to provide additional input to the assessment of modelling results.

Simulation Case 3: Buffer THM evolution above 100 °C

With respect to the temperature evolution, all three teams predicted the peak temperature to be reached after 5 to 6 years. The 3D-models of Nagra and GRS came up with values of 141 °C and 145 °C, respectively, using the reference parameter values. After 130 to 185 years, the temperature dropped below 100 °C everywhere in the buffer. Nagra's model variations using reduced thermal conductivities of the buffer resulted in peak temperatures of 152 °C. A change in the hydraulic parameters had no significant influence on the peak temperature. The temperature evolution in the clay rock is not visibly influenced by the buffer thermal conductivity.

CIMNE's 2D models considered the canister completely surrounded by bentonite pellets or by blocks, respectively. Due to the considerably higher initial thermal conductivity of the blocks, the peak temperature amounts to 165 °C for the pellet variant and to 115 °C for the block variant.

In the reference case, full saturation of the buffer was reached after 50 years (Nagra), 27 years (GRS), 85 years (CIMNE pellet variant), or 56 years (CIMNE block variant). The low value for GRS is possibly due to a deficiency in the suction curve match, but may also be due to the disregard of an EDZ. Nagra's model variations showed that changing the buffer hydraulic parameters has only little influence, while decreasing the rock permeability prolonged the saturation time to 100 years.

Nagra calculated a maximum pore pressure in the rock of 10 MPa, reached after about 100 years. In the GRS simulation, 10 MPa pore pressure are reached already after ten years, which is another reason for the lower saturation time of the buffer in this model. In contrast to the TH calculations of Nagra and GRS, CIMNE considered different thermal expansion coefficients for the solid grains, the pore liquid, and the grain skeleton. This improvement has a direct effect on pore pressure evolution and leads to maximum pore pressures slightly below 8 MPa, reached after ten years at 15 m distance from the emplacement tunnel. It has, however, to be mentioned that, while this value is lower than those of the other simulations, CIMNE's model neglects additional parallel emplacement tunnels which will have an effect on pore pressure.

All in all, the different simulations of Case 3 led to comparable results. Where significant differences occurred, they could be explained by the different model assumptions and simplifications. The different models complemented one another, increasing confidence in the results.

Simulation Case 4: Geochemical evolution at interfaces

The canister corrosion, the interactions of corrosion products with bentonite and the pH buffering mechanisms were simulated over one million years at a constant temperature of 25 ºC for a spent-fuel carbon-steel canister repository in granite. The canister was fully corroded after $5 \cdot 10^4$ years for a constant corrosion rate of 2 μm/y. Canister corrosion caused an increase in the concentration of dissolved Fe^{2+} and pH, and a decrease in Eh. Most of the released Fe^{2+} diffused from the canister into the bentonite where it precipitated or sorbed. The largest pH in the bentonite was almost 9.5 at $2 \cdot 10^5$ years. The evolution of the concentration of dissolved Fe^{2+}, pH and Eh are determined by the generation of corrosion products, the precipitation of magnetite and Fe sorption on weak sites.

Magnetite was the main corrosion product in the bentonite. Approximately 70 mol/L of magnetite precipitated in the canister-bentonite interface before the canister was fully corroded and the precipitation stopped. Its precipitation progressed as Fe^{2+} diffused into the bentonite. The thickness of the bentonite zone where magnetite precipitated was about 7 cm. Siderite precipitation was much smaller due to the limited availability of dissolved bicarbonate. The thickness of the bentonite zone where siderite precipitated was similar to that of the magnetite. Calcite dissolved in most of the bentonite except near the canister where it precipitated due to the increase in pH induced by canister corrosion. Dissolution/precipitation of quartz and gypsum were not significant.

The precipitation of the corrosion products close to the canister led to a very relevant decrease of bentonite porosity near the canister-bentonite interface. The bentonite thickness significantly affected by porosity reduction increased with time to about 7 cm after one million years. A negligible increase of the porosity was observed in the rest of the buffer.

The interaction of the bentonite with the concrete liner was evaluated with a two-dimensional axisymmetric THCm model. Mineral dissolution/precipitation is especially marked in the concrete. Kinetically-controlled smectite dissolution leads to analcime precipitation. Model results indicate that smectite dissolution in the presence of an OPC concrete liner in a repository in clay is about 4 times more relevant than in the case of the repository in granite. Magnetite precipitates near the canister. The thickness of the altered zone at the canister-bentonite interface in the presence of the high pH plume is 4 cm. This is half of the thickness of the altered zone for a repository in granite.

The pH in the concrete increases due to portlandite dissolution. It also increases in the bentonite due to the penetration of the hyperalkaline plume from concrete. The precipitation of calcite, brucite and sepiolite buffers the hyperalkaline plume. The high pH plume extends throughout the bentonite and causes mineral precipitation, changes in the composition of the exchanged cations and a reduction of the porosity of the bentonite. The pH is about 11 after 105 years and later decreases to 9.5. The hyperalkaline plume from the concrete penetrates 1 m into the clay host rock after one million years.

Numerical models predict pore clogging in a 4 cm thick zone near the canister, 5 cm in the concrete-bentonite interface and 5 cm in the clay-concrete interface. Changes in porosity caused by mineral dissolution precipitation are significant throughout the bentonite and in a narrow band (25 cm) of the host rock.

Natural analogues

Natural analogues were used initially to improve the understanding of key processes and model/database testing. This is still a major justification for some analogue projects. More recently NA have been used to provide general support for the safety case by studying the evolution of relevant systems over geological timescales and to increase confidence in extrapolating results from lab and field experiments to the repository. Natural analogues are, however, not well defined in terms of boundary and initial conditions and model parameters. Therefore, their use as a tool for validating long-term predictions is limited.

Scaling laws

The main conclusions of the integrated analysis of water uptake data were that there is a clear difference for one-dimensional and axisymmetries, and that an upscaling of small tests was not possible. With regard to water content, initial conditions and boundary conditions were too different in the various tests. The chemical composition of the bentonite is most often derived from aqueous extract tests which must be interpreted numerically with inverse geochemical models, which adds a difficulty to the integrated analysis of chemical data. The overall conclusion was that data from different space-time scales cannot be integrated, so there is no possibility for extrapolation in time from available data using the scaling law approach. Therefore, this approach was not pursued further.

Mixture theory

Continuum mixture theory is a macroscopic representation of the thermo-mechanical behaviour of a material body consisting of a mixture of several constituents, i.e. a multi-component formulation. The framework is capable of incorporating diffusion, phase transition, and chemical reactions in the broadest sense. Miscible and immiscible formulations are possible. Immiscibility leads to adopting a material structure represented by volume fractions. Porosity and degree of saturation may be defined in terms of volume fractions. In mixture theory, the fundamental variable is the chemical potential. Pore pressures for fluid phases are generally not “physical” pressures, but scaled chemical potentials. As a consequence, capillary pressure, or suction, is the difference between scaled chemical potentials. Darcy’s law and Fick’s law are obtained as simplifications of the mass balance equations. In these laws chemical potential and temperature are the basic driving forces. A concept of non-associative immiscibility developed by Clay Technology gives a mixture with immiscibility on different levels. A schematic formulation of a respective material model led to porosities belonging to the different levels. Chemical reactions were not addressed in the review, but their incorporation seems unproblematic.

4.5. Summary and future perspective

In the framework of PEBS comprehensive numerical simulations were performed in order to interpret the experimental results, improve the basis for long-term extrapolation, predict long-term repository evolution, and quantify and reduce uncertainties in the predictions. The performed simulations covered:

- HM modelling for the interpretation of the EB experiment;
- THM modelling for design, interpretation and of the HE-E experiment;
- Investigations of various aspects of buffer THM behaviour, involving modelling of various laboratory tests, the FEBEX mock-up and the FEBEX in-situ test;
- THMC modelling of several experiments investigating the processes at the interfaces canister-bentonite and bentonite-concrete;
- Long-term extrapolation modelling of repository configurations representing the Swiss and the Spanish concepts.

Some of the simulations were performed using conventional models, but there was also considerable progress in enhancement of existing and development of alternative models.

Regarding the THM behaviour of the buffer, additional processes, like non-Darcy flow and thermo-osmosis were considered, and a double porosity model was implemented. The double porosity model proved suitable for characterizing the buffer evolution in the EB experiment. All the enhanced models were able to simulate the previously unexplained slowdown of buffer resaturation; a decision on the most likely process (or combination of processes) is, however, not yet possible. Further monitoring of the running long-term experiments will aid in the discrimination.

For reducing uncertainties in TH material data, an inverse framework was implemented for detecting best estimates of parameter combinations. This provided also uncertainty estimates of the resulting parameters in the form of standard deviations.

A new approach was taken by considering the buffer from the viewpoint of thermo-mechanical continuum mixture theory. A non-associative immiscibility concept was presented which, in the future, may provide an alternative description of buffer behaviour with the chemical potential as fundamental variable.

THMC models were developed further, taking into account porosity change by swelling and incorporating reactive gaseous species. For the most part, simulations agreed well with experimental data from corrosion experiments. This holds also for the bentonite-concrete interface, although some phases (e.g., precipitated CASH) could not be accounted for.

An approach to an integrated analysis of THMC data from different test scales proved less successful – the differences in the various geometries and test conditions was too large.

For the long-term extrapolation exercise, four simulation cases were defined.

- Simulation Case 1: Isothermal buffer evolution, an extrapolation of the EB experiment to long-term;
- Simulation Case 2: Thermo-hydro-mechanical evolution of the buffer at temperatures up to 100 °C, a simulation of the Spanish reference repository concept in granite;
- Simulation Case 3: Thermo-hydro-mechanical evolution of the buffer with temperatures temporarily exceeding 100 °C, a simulation of the Swiss reference repository concept in clay rock;
- Simulation Case 4: Geochemical evolution at canister-bentonite and bentonite-concrete interfaces, including a long-term simulation of a repository in granite.

The most important results of these simulations were the following:

- Simulation Case 1: Little change in the buffer was found during long-term extrapolation of the EB experiment, since the buffer was already close to saturation at the end of the field test. Heterogeneities in density remained as a consequence of the constitutive model – no creep had been considered. Creep is potentially an important phenomenon in long-term predictions and should be the subject of future research;
- Simulation Case 2: Including model enhancements like thermo-osmosis or double porosity in the simulation led to considerable extension of saturation time. Instead of values in the range of 10 years, buffer resaturation went on over 1000 years. The results are strongly dependent on the parameter set, even modest variations in parameters can have significant effects. A sensitivity study for the long-term situation will be useful to reduce uncertainty. In addition, further monitoring of the ongoing long-term experiments will provide more reliable data;
- Simulation Case 3: Due to problems with high calculation times, the simulation of this case could only be performed with standard models. Different simplifications were introduced by different modelling teams; taking these differences into account, the results are quite comparable;
- Simulation Case 4: THMC modelling of the canister-bentonite interface in a repository in granite led to an altered zone with a thickness of about 7 cm, where porosity is reduced due to precipitation of magnetite and siderite. In a clay repository, the thickness of the altered zone is only 4 cm, due to the different pore water chemistry. Near the concrete, pore clogging is predicted 5 cm in the concrete-bentonite interface and 5 cm in the clay-concrete interface. Changes in porosity caused by mineral dissolution/precipitation are significant throughout the bentonite and in a narrow band (25 cm) of the host rock.

The modelling exercises performed within PEBS have identified several directions most relevant for performing future studies:

- Continuation of existing long-term experiments in order to distinguish between processes potentially relevant for the long-term THM behaviour (e.g. thermo-osmosis, double porosity, creep) and to reduce uncertainty in parameter estimates;
- Calibration of enhanced models with the additional data and use of these models for long-term simulations;

- Further investigation of promising alternative models;
- Further improvement and validation of THMC models and parameters.

5. WP 4 – Analysis of impact on long-term safety and guidance for repository design and construction

5.1. Objectives

Work Package 4 "Analysis of impact on long-term safety and guidance for repository design and construction" had the following overall objectives:

- Obtain an overview of the findings of WP 2 and WP 3 and relate the results and uncertainties to the long-term safety functions of the repository components and to the overall long-term performance of the repository, as outlined in WP 1.

It was expected that this will provide

- a more complete description of the thermo-hydro-mechanical-chemical evolution of the near field,
- a more quantitative basis for relating the evolutionary behaviour of the EBS to the safety functions of the system, and
- a further clarification of the significance of residual uncertainties for long-term performance assessment.

Finally, the outcomes are used to give some guidance regarding repository design, by clarifying the link between long-term safety criteria and design criteria of the EBS.

5.2. Beneficiaries involved

The beneficiaries of WP 4 are mainly implementing organisations (Nagra, SKB, ENRESA, Andra) completed by GRS.

Nagra was in charge of the scientific and technical coordination of this Work Package. BGR, as the project coordinator, was involved in this WP with management duties.

5.3. Execution of work

The dataflow with respect to WP 4 is defined in Figure 11.

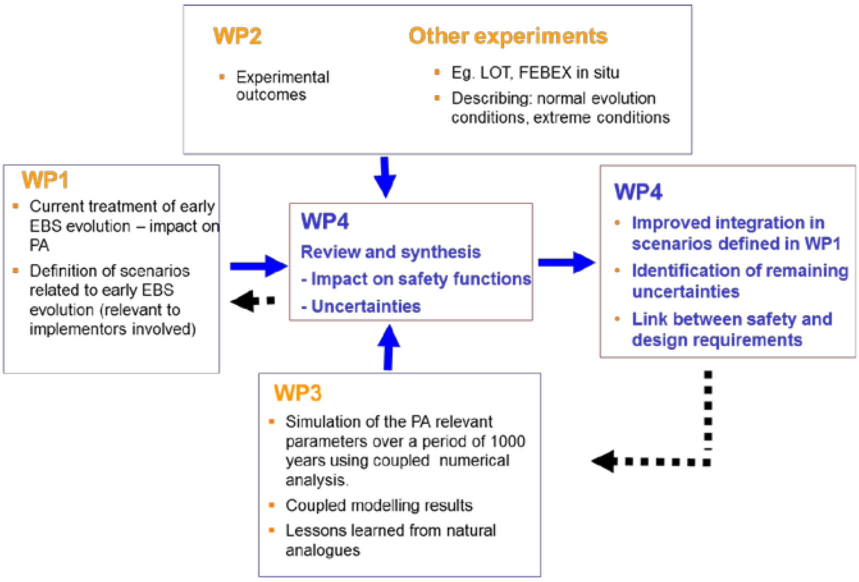

Figure 11: Data flow defined for WP 4.

The activities in WP 4 started mainly in the 2nd reporting period of the PEBS project. A joint WP 1-4 Workshop took place in Switzerland with the objective to obtain an agreement on the cases and how these could be treated in WP 4 and which input could be given to WP 2 and WP 3 with respect to the formulation of the results and the modelling activities. The reduction of the cases based on the complete list of the process and uncertainties as defined in WP 1 was discussed. The cases identified for the purpose of WP 4 and providing guidance to Task 3.5 are listed in Table 3.

Table 3: Cases related to uncertainties in the early evolution of the EBS used for the integration of project findings.

	Description	**Origin**	**Related work in PEBS**
Case 1	Uncertainty in water uptake of buffer (T < 100 °C)	Results of standard THM model vs. FEBEX observations	Enhanced models and FEBEX mock-up experiment etc.
Case 2	Uncertainty in thermal evolution in buffer (T > 100 °C)	Lack of validation of TH model for high T and low saturation rate	HE-E experiment modelling and experimental results
Case 3	Uncertainty in hydro-mechanical evolution of buffer	Lack of large-scale experiments	EB experiment results
Case 4	Uncertainties in geochemical evolution	Experimental vs. modelling results of corrosion product-bentonite and cement-bentonite interactions	GAME experiments and modelling

The expected WP 2 and WP 3 input to these cases was discussed informally after the Regulator Workshop in Mont Terri in May 2012 and consolidated by GRS in the cases table corresponding to Task 3.5 activities.

The main activities in WP 4 in the 3rd reporting period were:

- Reviewing of the findings of the WP 2 and WP 3 experiments and models in order to develop a more complete qualitative process-related description of the early evolution phase of the repository (the first several hundred years) and the residual uncertainties in the evolution structured along the four cases.
- Establishing the significance in relation to long-term safety functions of the buffer (canister and host rock) to be discussed in a quantitative fashion, including the importance of residual uncertainties, based on insights from existing safety assessment studies (e.g. SR-Can, Opalinus Clay safety case).
- Proposing an improved and more complete approach to integrating the thermal and resaturation phase of the repository with the long-term steady state phase of repository evolution. In addition, the significant uncertainties will be identified and recommendations will be made for future studies.

5.4. Main results

The PEBS activities relevant for the case were extracted and based on results also from other projects the remaining uncertainties were identified. The case analyses, each of them being particularly relevant for specific disposal concepts, were then pulled together and for relevant concepts and safety cases it was assessed how a better integration of the early transient behaviour could be integrated in future safety cases whereby remaining uncertainties and areas for further study were identified.

Case 1 describes the processes in the EBS during the early stage of the repository evolution. The emplaced buffer takes up water from the surrounding bedrock and starts to swell. During the early stage of the repository evolution, coupled thermal, hydraulic and mechanical phenomena affect the hydration process. The swelling is restricted by the rock wall and a swelling pressure develops. The process depends on the properties of the buffer as well as on the local hydraulic conditions. After final saturation, the hydraulic conductivity of the buffer will be very low and the swelling pressure will be high. This process is common for all concepts with a bentonite buffer and is also relevant for bentonite seals (without thermal effects). The timescale for the saturation process is however strongly dependent on the boundary conditions. Although there is good agreement in THM modelling between models and data for different laboratory, mock up and in-situ experiments (with high saturation rate/water supply), in a number of these experiments the progress of saturation at the later stages of hydration is slower than anticipated by the conventional coupled THM models. Although such slowing down of hydration has been observed in a variety of experiments, evidence is not totally clear cut. A detailed analysis was performed on which phenomena could explain this delayed late resaturation (double porosity, thermo-osmosis, Darcy threshold). Results, however, do not clearly permit identification of the processes actually relevant. But the context from long-term safety is clearly improved – it can be stated that even though saturation is not yet fully reached (e.g. after 15 years of FEBEX mock-up test), the safety function is achieved because sufficient swelling pressure is reached throughout the barrier at 85-90% average saturation. Thus, the uncertainty in water uptake appears to be not important from a long-term safety perspective for the Spanish disposal concept at hand for the PEBS project.

In **Case 2** the basic challenge was to understand how the early stage transient of high temperatures and low degree of saturation affects subsequent long-term performance of bentonite after full resaturation and cooling. Results that contributed to a large extend were the comparison of the results of THM models of early evolution to experimental results for a well-characterized system (column tests and 1:2 scale HE-E heater URL test). These results allowed gaining insight in the expected evolutionary path of the buffer during and after the initial transient and assessing the consequences of the evolutionary path (including uncertainties) for long-term buffer behaviour. The overall findings regarding the remaining uncertainties in the processes relevant for Case 2 are, that the reduction in swelling pressure in unsaturated conditions is significant above about 120 °C – the results from several saturated long-term heater-buffer experiments show minor thermal transient effects at up to 130 °C – and that a decrease in plasticity of bentonite and a slight decrease in hydraulic conductivity and swelling pressure might occur. The thermally-induced mineralogical transformation of bentonite is likely to be very limited even over very long times while some alteration of bentonite in contact with low pH concrete liner can be expected as well as some Fe silicate alteration products at inner surface of bentonite. In the Nagra safety assessment context, indications are that the effects of early high temperature processes in the bentonite barrier have generally low relevance to safety also because the time window of elevated temperatures coinciding with significant saturation is of the order of decades and limited to a small part of the EBS. Some uncertainties remain regarding swelling and hydraulic properties of bentonite for peak temperatures above approx.125 °C.

In **Case 3** the focus is on the thermo-hydraulic evolution of the EBS and the related residual uncertainties. Relevant results generated in the PEBS project were the EB experiment and modelling, the FEBEX mock-up and in-situ test and their modelling and the stress-strain behaviour studies in the laboratory. Laboratory and field experiments (e.g. the EB experiment) show that dense bentonite pellets evolve to a swelled material indistinguishable from swelled block material from a hydro-mechanical perspective. Furthermore, the EB experiment shows that even under non-optimum emplacement conditions swelling of mixtures of blocks and pellets with large initial density differences can achieve effective sealing. In the recent Swedish SR Site safety case the following uncertainties have been identified: mass loss due to piping and erosion in the very early evolution, swelling and homogenisation of components with different density, sealing after losses of mass, the importance of friction within the bentonite and between bentonite and other materials – also in the unsaturated state – and the effects of temperature on the mechanical properties. Uncertainties for mechanical processes occurring in the resaturation period have been better constrained through PEBS studies, the uncertainties in the long-term performance of bentonite barriers have thus been reduced in some areas, especially related to the homogenization of the installed buffer, such as the development of swelling pressure during slow wetting and the mechanical properties of a heated bentonite.

Case 4 integrates the findings of the experimental and modelling studies performed within PEBS (and other related research projects) with respect to the implications of the geochemical evolution for the long-term performance and safety functions of the EBS. The major conclusions from the integrated analysis can be summarized as follows. Thermally-induced mineralogical changes will be relevant mostly above 150 °C based on literature data. This should be confirmed in large scale long-term experiments. The interactions of corrosion products and bentonite indicate that the main properties of the bentonite remain unaltered. Under unsaturated conditions iron corrosion products penetrate << 1 mm into the bentonite. For the most part, the coupled THC numerical models reproduce the experimental data. The interactions of bentonite and concrete produce an altered layer of bentonite several millimetres thick (<5 mm) which is cemented by the precipitation of new minerals in the pore space. The hydration of bentonite proceeded in spite of this layer being present. Coupled THCm numerical models capture the main trends in mineral dissolution-precipitation. While there are still open questions regarding the conceptual geochemical model, the pore clogging processes, and the final parameters and properties of the altered zone, current models indicate that the thickness of the altered bentonite can be bounded. The potential impact on the physical properties due to the geochemical reactions studied in this case and the resulting THM behaviour of the barriers was integrated in assessment of the barrier performance for the various safety cases and disposal concepts.

5.5. Summary and future perspective

Summary

The PEBS project has been successful in developing an improved understanding of the early transients in bentonite barriers and reducing the associated uncertainties in the context of long-term safety assessments for disposal of spent fuel and HLW.

The project included a broad range of laboratory and in-situ experiments on bentonite dealing with THMC processes associated with the short-term transients in the EBS, combined with extensive modelling of the these processes. New large-scale in-situ studies included the HE-E experiment and the decommissioning, HM modelling and post-test analysis of the EB experiment. In addition, detailed modelling of the FEBEX mock-up, which started in 1997, combined with small-scale laboratory tests provided a good opportunity to validate the THM models.

In order to permit integration of a broad range of information and to put information in context, four cases were identified and the broad conclusions are briefly noted below.

Case 1 - Uncertainty in water uptake in the buffer below 100 °C

- There was good agreement in THM modelling between models and data for large-scale heater experiments (with high resaturation rate/water supply), but late stage resaturation is slower than predicted with models;
- Various model variants (double porosity, thermo-osmosis, Darcy threshold) were tested but results do not clearly permit discrimination;

- Despite this, the context from long-term safety is clearly improved – it can be stated that even though saturation is not yet fully achieved (e.g. after 15 years of FEBEX), the safety function is achieved because sufficient swelling pressure is reached throughout the barrier at 85-90% average saturation. The model uncertainty is thus not important from a long-term safety perspective.

Case 2 - Uncertainty in the thermal evolution of the buffer above 100 °C

- A new 1:2 scale URL experiment (HE-E) shows that there is reasonable agreement between models and measured TH parameters in early resaturation; the temperature field in EBS and host rock (up to 140 °C) is modelled accurately;
- Resaturation is slow (as expected; driven by host rock water supply) and so it will require some years of monitoring to adequately test models for resaturation;
- Further studies of the effects of heating bentonite above 100 °C in a partially saturated state suggest that the swelling pressure may be somewhat reduced (~25%), but will still meet the requirements;
- Review of process understanding and data support do not suggest important changes in performance in this high temperature range.

Case 3 – Uncertainty in HM evolution of the buffer

- Cementation during heating-cooling cycle can increase strength of dense bentonite; more data has been obtained, which has shown that the effects are small below 100 °C;
- The observed cementation process is not kinetic, i.e. results are basically the same for a 1 day or long duration cycle;
- Safety relevance is related to mechanical impacts on the canister (e.g. shear across a borehole); cementation also reduces swelling pressure, but has little effect on hydraulic conductivity;
- Various laboratory and field (EB) experiments show that dense bentonite pellets evolve to a swelled material indistinguishable from swelled block material from a hydro-mechanical perspective;
- The EB experiment shows that even under non-optimum emplacement conditions swelling of mixtures of blocks and pellets with large initial density differences can achieve effective sealing.

Case 4 - Uncertainty in geochemical evolution of the buffer and its interfaces with the canister and rock or liner/tunnel support

- The main effects of geochemical evolution are clearly at the interfaces;
- Based on review of published data, below about 130 °C, limited alteration of smectite will occur within the main part of the barrier based on alteration models and natural analogues - an important factor is that the thermal phase is short;
- At a steel canister interface, the bentonite alteration is very limited over periods of several years, but is difficult to estimate over long periods;

- Impacts on system interfaces can be bounded (a few cm reaction zone over the very long term), although porosity evolution clearly requires further research (both for steel-bentonite and cement-bentonite);
- It should be kept in mind that geochemical modelling provides valuable insights but is not fully predictive (especially over the long term) - a lot of model testing and supporting information is needed.

Future perspectives

Over the next years there are good prospects for resolving residual uncertainties in the performance of bentonite barriers that relate to how the thermal and resaturation period may affect the long-term performance. Some important experimental studies that will contribute to this improvement in understanding include:

- The excavation of the in-situ FEBEX experiment, which will obtain valuable information on the properties of a bentonite barrier that has been exposed to partial saturation at temperatures of up to 100 °C for 15 years;
- Continuing observations in the FEBEX mock-up test over a longer period should provide relevant information on the likely mechanisms operating at the later stages of saturation;
- The HE-E experiment provides reliable data for the validation of models simulating the TH evolution of the bentonite barriers and the near-field clay; the slow resaturation of the bentonite will be the subject of further model investigations, and the eventual dismantling will permit the properties of bentonite exposed to temperatures of up to 140 °C to be assessed;
- The first two heaters in the Prototype Repository at the Äspö HRL have been excavated and the results from the investigations are about to be published. The ABM test at Äspö, where a number of different bentonites are/have been exposed to temperatures up to 130 °C for different time periods, permits the further investigation of the mineralogical effects;
- Work on cement-bentonite and cement-host rock interfaces, in particular determination of porosity and nature of alteration is ongoing at a number of institutes and has been proposed for a European project.

In relation to lessons learned from the PEBS studies that provide relevant feedback to design, the following points are noted:

- Laboratory and field studies have shown similar performance of blocks and pellets after resaturation, which provides some confirmation that suitable design concepts are being used;
- In terms of cement-bentonite interactions, while there are improvements in the overall chemical modelling of the associated processes, it remains difficult to constrain the long-term impacts without use of low pH cement as a design measure;
- The studies performed help to define buffer design parameters such that early resaturation phase-induced heterogeneities in density are occurring within a range

that will not violate the safety function indicators related to sufficiently high swelling pressure and low hydraulic conductivity even if it is assumed that the heterogeneities do not disappear over time.

6. WP B – China-Mock-Up Test on Compacted Bentonite-Buffer

At the present stage, Gaomiaozi (GMZ) bentonite is considered as the candidate buffer and backfill material for the Chinese HLW repository. Lots of basic experimental studies have been conducted and favourable results have been achieved.

In order to understand the complex coupled THMC behaviour of the buffer and backfill material and to further study the behaviour of the GMZ Na-bentonite under relevant repository conditions, a mock-up facility, named China-Mock-Up, was proposed based on a preliminary concept for a HLW repository in China. The experiment is intended to evaluate THMC processes taking place in the compacted bentonite-buffer during the early phase of HLW disposal and to provide a reliable data base for numerical modelling and further investigations. The interaction between GMZ Na-bentonite and the canister is considered in the experiment. The vertical displacement of the canister in the KBS-3V concept is very critical for the HLW disposal repository; possible displacements of a HLW container in the bentonite-buffer are also studied.

The main objectives of the China-Mock-Up are summarized as follows:

1. To study the behaviour of GMZ-Na-bentonite under coupled THMC conditions;
2. To study the bentonite-canister reaction under coupled THMC conditions;
3. To simulate vertical placement of a container with radioactive waste;
4. To monitor the behaviour of GMZ-Na-bentonite barrier exposed to high temperatures and special water;
5. To experiment the installation method and validity of sensors;
6. To provide data for future design for engineered barrier system.

6.1. Beneficiaries involved

The China-Mock-Up experiment is an important milestone of the buffer material study for HLW disposal in China. Based on the current experimental data, several aspects are obtained, including the observed THM behaviour of the compacted bentonite, the displacement of the electrical heater, the temperature distribution of the bentonite, the stress evolution of the bentonite, and also the influenced by the competing mechanisms of drying effect and the wetting effect.

The experiment is a valuable step in establishing the viability of the reference concept, and making progress in the understanding of the behaviour of the buffer material under THM coupled condition.

BRIUG use the start-up of the China-Mock-Up experiment as an opportunity to put the spotlight on its unique technical and scientific R&D in and around the buffer/backfill material filed and to attract the attention of universities and other scientific institutions or engineering organisations, with a view to strengthening the network of future collaborations. This is also a demonstration experiment in terms of knowledge and information management for HLW disposal administrant.

The China-Mock-Up can provide with the methodology, data, knowledge and understanding of EBS properties for technical engineering. It can also give feedback and guidance for repository design and construction as well as to future R&D.

6.2. Execution of work

In order to study the behaviour of the GMZ-bentonite under simulative repository conditions, a mock-up experiment called China-Mock-Up has been proposed according to the preliminary concept of HLW repository in China since 2009. The China-Mock-Up is used to evaluate the key THMC processes of bentonite; it is performed in the laboratory of Beijing Research Institute of Uranium Geology (BRIUG).

The China-Mock-Up has been constructed with compacted bentonite blocks in a large steel tank with 900 mm internal diameter and 2200 mm height. An electric heater of 300 mm diameter and 1600 mm length, which is made out of the same stainless carbon steel as the substitute of a real HLW container is placed inside the bentonite buffer. The bentonite blocks are heated from ambient temperature to 90 °C and then cooled down. The groundwater flow is simulated by injecting the formation water (taken from the host granite rock in the Beishan site, NW China) around the outer surface of the barrier. The complex THMC processes occurring in the bentonite buffer are monitored by a number of sensors installed at various locations. The main parameters measured in the EBS include temperature, water inflow, relative humidity (suction), swelling and total pressure, as well as displacement of the heater inside the buffer.

The China-Mock-Up with is composed of eight components in a vertical configuration, namely compacted bentonite blocks, steel tank, heater and corresponding temperature control system, hydration system, sensors, gas measurement and collection system, real-time data acquisition system and monitoring system, as shown in Figure 12.

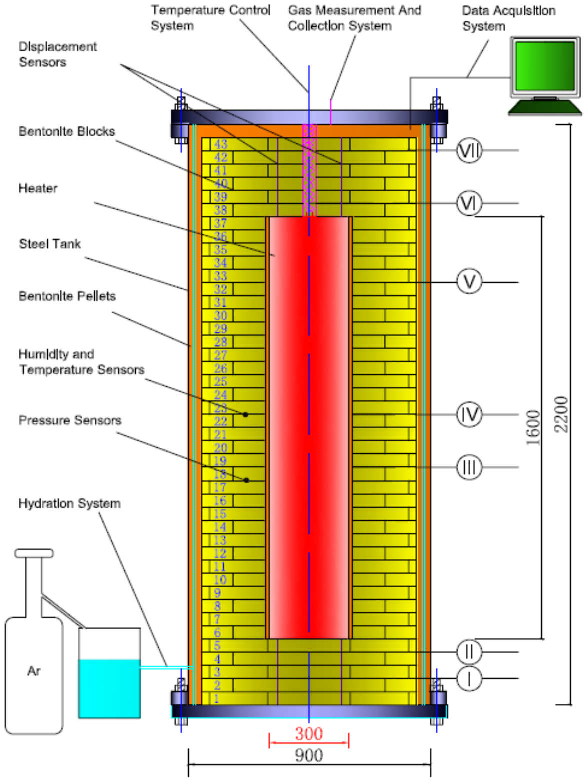

Figure 12: Sketch of the China-Mock-Up facility (unit: mm).

6.2.1. Experiment material

The bentonite used for the China-Mock-Up comes from the GMZ bentonite deposit, which is located in Inner Mongolia Autonomous Region, 300 km northwest of Beijing. The deposit, with bedded ores, was formed in late Jurassic. Clay minerals include montmorillonite and quartz, feldspar, cristobalite, etc. The reserve is about 160×10^6 tons, while with 120×10^6 tons of Na-bentonite. The major bentonite clay layer of the deposit extends about 8,150 m with thickness ranging from 8.78 to 20.47 m.

The preliminary study on GMZ-bentonite shows that it is characterized by high content of Montmorillonite (>70%) and low impurities. Various tests revealed some of other properties of GMZ-bentonite: cation exchange capacity (77.30 mmol/100g), Methylene blue exchange capacity 102 (mmol/100g) and alkali index (1.14). The properties of the compacted bentonite at dry density 1.8 g/cm^3 are: thermal conductivity (around 1.0 W/(m·K) at a water content of 8.6%), hydraulic conductivity (1×10^{-13} m/s), and swelling pressure (10 MPa, at full saturation). Those figures have shown that GMZ-bentonite is a suitable buffer/backfill material.

A computer-controlled triaxial test machine in combination with specially designed steel molds are used to compact the GMZ-bentonite into compacted blocks with five different shapes, as presented in Figure 13. The square bar-shaped bentonite blocks are subsequently crushed into small pellets in different grain sizes to fill the space between the bentonite blocks and the steel tank walls.

Figure 13: Compressive test machine and compacted bentonite blocks.

To investigate the influence of crushed pellet sizes on the density of pellet mixtures, a sensitive analysis for different pellet sizes (2 mm, 4 mm, 6 mm, 8 mm, 10 mm) is carried out via a standard orthogonal L25 (56) array. The orthogonal experiment design as a simple, systematic and efficient method enables us to investigate the relative importance of control factors and identify the best levels for different factors on a performance output; and the results can be analysed by using a common and rigorous mathematical procedure. This method can significantly reduce experimental time and research cost. Based on twenty-five experiment cases, the optimal mixture ratio of different pellet sizes was obtained from the analysis of means (ANOM) for capturing the reasonable density (1.3 g/cm³) of pellet mixtures, as presented in Figure 14.

Figure 14: Crushed pellets used to fill the space between bentonite blocks and steel tank walls.

For the China-Mock-up, 44 bentonite block sections, each with a thickness of 50 cm, are installed across the entire length of the tank. Each complete buffer section consists of two or three concentric rings, which are dependent on the space in which the heater is placed, formed by compacted bentonite blocks with different shapes and numbers. The inevitable spaces between buffer layers and blocks may provide the preferential paths for water penetration, resulting in a negative impact on the inner THM environment and sensors' working performance. To reduce or eliminate the effect of adverse penetration paths and maintain a uniform and stable water penetration rate in the bentonite, a standard layer (i.e. the bottom layer) has been designed. Once the bottom layer is determined, the second layer above the standard layer can be rotated 15° clockwise or counter-clockwise so that the potential coalescence of penetrating water between the bentonite layers can be suppressed as far as possible. Every two layers/sections follow the same principle, and the optimal overlapping layer can be found. The determination of the standard and overlapping layers provides with a basis precondition for the further layout design of sensors.

6.2.2. Sensors used in the China-Mock-Up

The China-Mock-Up is equipped with 9 different types of sensors to monitor the comprehensive performances of GMZ Na-bentonite under coupled THMC conditions. The 5 sensor types inside the China-Mock-Up include stress sensor, hydraulic pressure sensor, LVDT displacement sensor, temperature sensor and RH sensor. In addition, a series of metal corrosion samples are placed inside the bentonite blocks and crushed pellets to investigate the influence of internal environment of the mock-up on metal corrosion behaviours. Another 4 sensor types consisting of Coriolis mass flowmeter, fiber Bragg grating strain/temperature sensor, resistance strain gauge and dial gauge are located outside the mock-up. Measurements based on the 9 types of sensors are mainly carried out at seven measurement profiles located from the top to the bottom of the mock-up vertical model. The overall sensing system installed in the mock-up provides reliable data for numerical modelling and future design of EBS.

More than 160 sensors have been installed within the experiment to measure the important parameters, including the temperature, pore pressure, relative humidity, water injection pressure and the total pressure. The sensors are distributed in the seven sections in vertical direction, as illustrated in Figure 12. Different types of sensors are placed within each section to investigate the variation of temperature, hydration process and the behaviour of buffer material under the complex coupling condition. The sensors were installed within the grooves cut in the compacted bentonite blocks. Most of the sensors used were made in China except for the RH sensor (HW4) which was made in Switzerland.

According to the reference concept of HLW disposal in China, the canister is completely supported by the surrounding buffer material. Therefore, the mechanical performance of buffer material may influence the overall stability of the canister. In order to evaluate this potential influence, six LVDT sensors are installed on the top and bottom of the heater to monitor its vertical displacement.

6.2.3. Mock-up operation

The China-Mock-Up experiment was assembled completely on 10th September 2010. After a pre-operational phase, the operational stage of the China-Mock-Up test started on April 1st 2011, the date identified as “day 0” on the time scale. The heating and hydration phase with the time is illustrated in Figure 15.

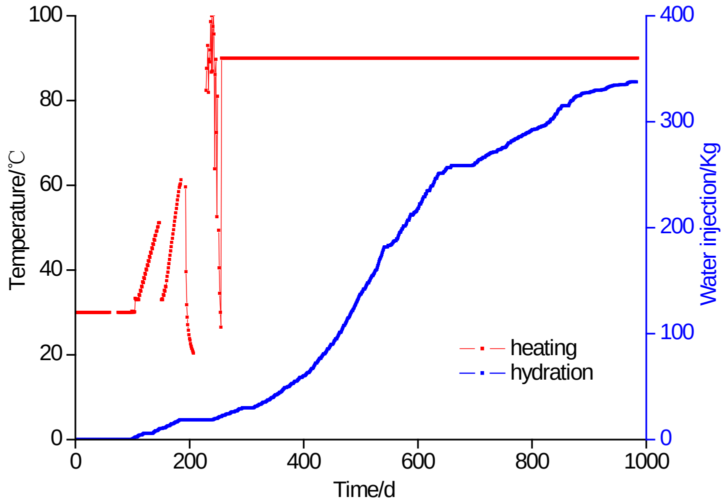

Figure 15: Mock-up operation.

Heating

The power supply to the heater has been made in four phases: during the first 2 days, the temperature of the heater was increased to 30 °C; over the next 95 days, the temperature was maintained constant to verify the reliability of the installed sensors; then, during the period 98 to 255 days, the temperature was increased progressively to approximate the final value of 90 °C which is the maximum temperature expected on the canister surface according the current disposal concept in China. Finally, the system was switched to the constant temperature control mode. The necessary electric power was adjusted to maintain 90 °C on the surface of the heater. It should be mentioned that, the heater and corresponding temperature monitoring system are controlled by the computer automatically. The electrical heater is 1.6 m high, and the effective heating length is about 1.2 m located in the central part of the heater.

Hydration

The water injection started from 8th July, 2011. In order to avoid potential damage to the sensors by a sudden saturation process, the hydration was initially controlled by a water injection rate which was increased gradually from 400 g/day to 1500 g/day in the first 700 days. Then the hydration was controlled by constant pressure at 0.2~0.7 MPa. As planned, a constant pressure of 2 MPa is to be applied when the pellets become fully saturated. To mention here, the water supply was performed artificially every day, and the platforms in the curve of water injection indicates that no water is injected during the corresponding period of time.

6.2.4. Numerical study of the China-Mock-up

A numerical study of the China-Mock-Up test, with the purpose of evaluating the performance of the compacted GMZ bentonite under coupled THM conditions, is conducted. The principal THM characteristics of the GMZ bentonite are presented at first. A THM model is then presented to tackle the complex coupling behaviour of GMZ bentonite. The model of Alonso-Gens is incorporated to reproduce the mechanical behaviour of the GMZ bentonite under unsaturated conditions. With the proposed model, numerical simulations of the China-Mock-Up test are carried out by using the code of LAGAMINE.

In order to reproduce the physico-mechanical behaviour of the GMZ bentonite aforementioned, a coupled THM model is proposed. In the model, various THM coupling phenomena are taken into account, including the transport of heat (conduction and convection), motion of liquid water, vapour diffusion, and their couplings with mechanical behaviours. The main formulations of the proposed model are presented in this part.

Diffusion models

In general, the compacted bentonite is composed of three phases, namely the solid, liquid water and gas (air and water vapour). In the simulations, the conservation mass of each phase (water or gas) is assumed. The phase exchange term thus will not be considered in the balance equations. The variables chosen for the description of the flow problem are liquid water pressure, gas pressure and temperature. The generalized Darcy's law for multiphase porous medium is adopted to simulate the motion of liquid water. The water vapour flow is assumed to follow Fick's diffusion law in a tortuous medium. In the study, the formulation proposed by the model of PHILIP & VRIES (1957) is adopted. For the pores partially filled by air, it will be more difficult to constitute pathways for water flow, the permeability is consequently decreased. The variation of permeability with the saturation degree is taken into account by introducing the variable of water relative permeability. In the context, one unique temperature variable is adopted. It means that the temperature is assumed to be homogenous in all phases. The heat transport is related to three effects: conduction, convection and vaporization.

Mechanical model

The significant influence of saturation degree on the mechanical behaviour of soil has been verified by numerous experimental studies, which should be taken into account in the mechanical modelling. Based on the experimental investigations, some constitutive models are proposed (ALONSO 1990; ALONSO 1999; TANG 2009). The BBM model is widely used because of its capacity of representing the main fundamental features of partially saturated soils in a consistent and unified manner. It should be noted that the expensive behaviour of compacted bentonite is better represented with the modified BBM model (ALONSO et al. 1999) by taking into account of the microstructural variation during wetting process. However, the formulation of the model is much more complicated, and some parameters are difficult to identify. As a preliminary study, the BBM model is adopted.

Geometry and Boundary Conditions

A 2D-axisymetric finite element simulation is realized with the help of the software LAGAMINE. The geometry and boundary conditions are illustrated in Figure 16. For simplicity, the steel tank is neglected. The fixed horizontal/vertical displacement is imposed on the nodes in contact with the steel and the heating is simulated by imposing the temperature on the nodes in contact with the heater. The hydration influence is modelled by increasing water pressure on the nodes of outer boundary. The convection transfer between the GMZ bentonite and atmosphere is simulated thanks to frontier thermal elements. In the simulations, air flow is not considered, whereas the vapour diffusion is assumed.

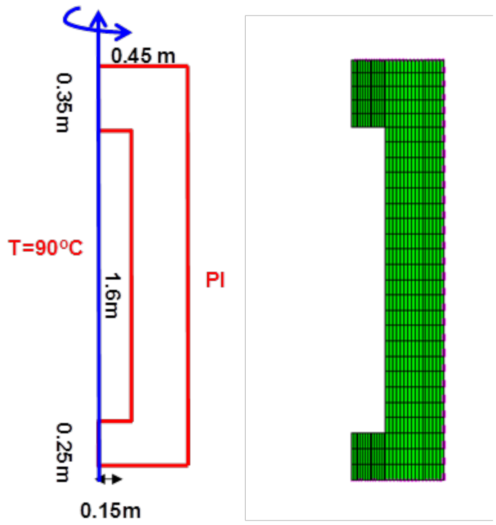

Figure 16: Boundary conditions and mesh.

The system is initially at a temperature of 20 °C. The gas pressure is assumed to be constant in order to have a better numerical convergence. The compacted GMZ bentonite has an initial water saturation of 48% and a void ratio of 0.57. According to the water retention curve determined, a suction of 80 MPa is initially employed. As aforementioned, the dissolved air will not be taken into account. Following the experimental procedure, the numerical simulation is divided into two phases: firstly, the temperature on the boundary connected to the heater and the water pressure on the outer boundary are increased respectively to 90 °C and 2 MPa in 10 hours. In the following, the boundary conditions applied previously are kept constant for 3 years.

6.3. Main results

6.3.1. Experimental results of China-Mock-up

Temperature evolution

The temperature variation with time in different sections of the facility is illustrated in Figure 17. As the beginning of the test, the temperature is increased globally with time, especially for the sensors close to the heater. It can be noticed that, the temperature has continuously increased with time, especially the sensors located in the inner rings. Moreover, the distribution of temperature is non-uniform vertically, and it is much higher in the central part. Even in section III, the temperature is still below 60 °C. In the experiment, the relatively low temperature may be partly attributed to the existence of the installation space between the heater and compacted GMZ blocks, which is 5 cm in width and filled with the pellets. It could be an important factor resulting in the higher temperature in the central part of the barrier. The temperature distribution is also influenced by a complex coupling mechanism. Besides the thermal conductivity, the specific heat and the thermal expansion coefficient, the temperature distribution is also strongly related to the saturation process within the barrier.

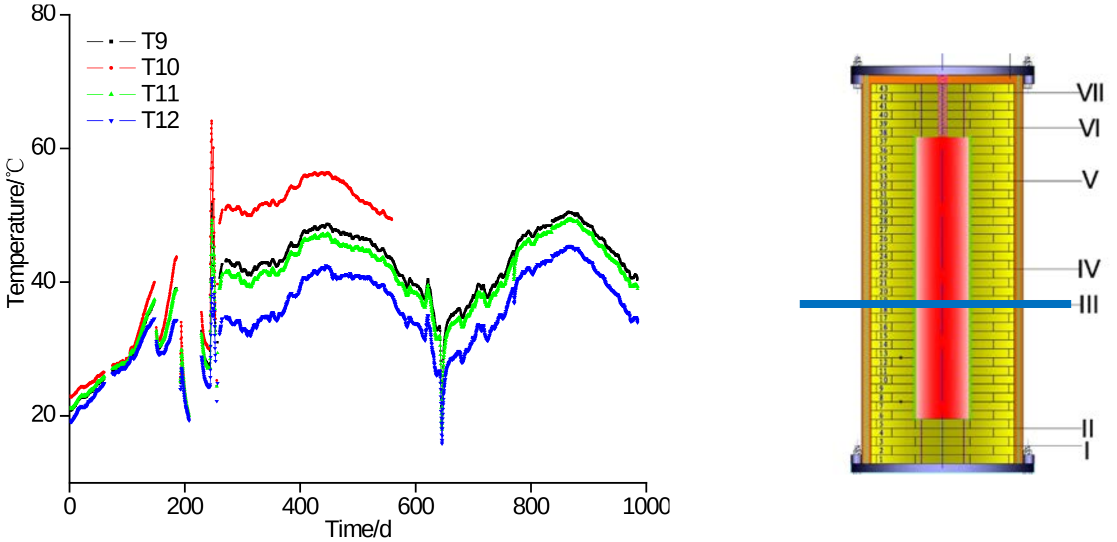

Figure 17: Temperature variation with time at section III.

Relative humidity

Figure 18 presents the evolution of the relative humidity at several distances from the heater in the relatively "cold" sections without heater. As illustrated, the compacted bentonite is progressively saturated in section I and II, and the distance to the heater has a significant influence on the saturation velocity. In the outer rings, the compacted bentonite is almost completely saturated after 200 days. However, due to the extremely low permeability of the bentonite and the drying effect by the heater, the variation of relative humidity is rather limited in the inner rings.

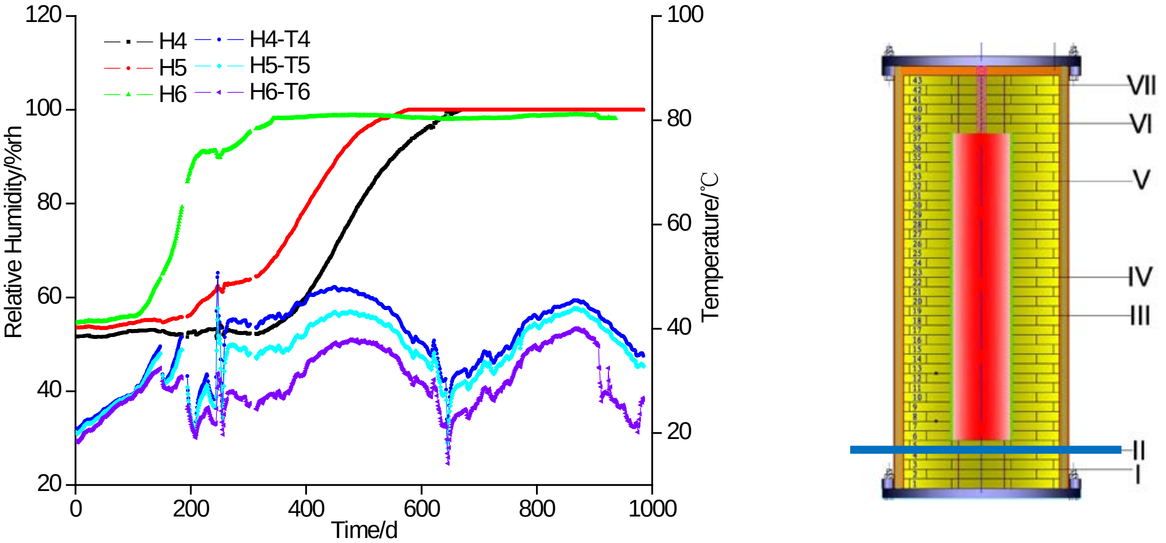

Figure 18: Relative humidity distribution at section II.

The RH evolution in the "hot" section III is illustrated in Figure 19. As noticed, the RH evolution in the "hot" sections is much more complex. With the increase of temperature, the decrease of RH can be observed, particularly in the inner rings. In the "hot" zone (inner part), the following phases can be noticed: a) the stable RH with some fluctuations in the first 250 days; b) when the temperature is kept constantly on 90 °C, continuous heat transfer from the heater leads to the drying effect that causes decreasing RH; c) after some time, hydration overcomes the drying effect and RH increases. This wetting tendency appears tightly related to the accelerated saturation process by the corresponding increased water injection rate. On the contrary, the desiccation is not noticed in the "cold" zone where the drying effect is not significant.

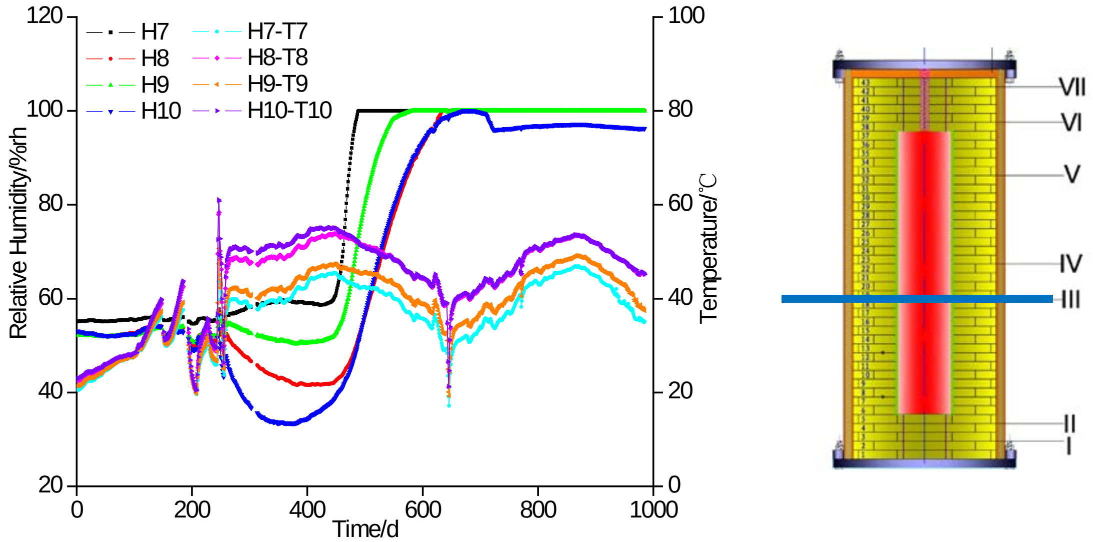

Figure 19: Relative humidity distribution at section III.

Because of the temperature change previously mentioned, some fluctuation of the RH evolution can be observed in these sections. The heating process generally leads to an increasing tendency of RH, which is probably related to the generation of vapour phase. Then, continuous heat transfer from heaters produces the drying effect that causes decreasing RH. The similar incidence and observations are also reported in other research works (MARTIN & BARCALA 2005). These unexpected fluctuations can also be considered as a validation of the reliability and sensitivity of the installed sensors.

In conclusion, the RH variation in the inner rings is found to be strongly influenced by the competing mechanisms of the saturation process induced by the water penetration and the drying effect by the heater. The experimental result indicates that, due to the low permeability of the compacted bentonite, the drying effect is dominant in these sections at the beginning of the test. Similar phenomena are also reported in other research works (MARTIN & BARCALA 2005; ALONSO et al. 2005; VILLAR et al. 2012).

It should be mentioned that, the hydration process is initially controlled by the water injection rate instead of constant water pressure, and the water injection has not been carried out continuously during the day. Considering the water supply is limited at the beginning, the injected water would be mainly concentrated at the bottom of the vertical tank due to the effect of gravity. As a result, the saturation process is non-uniform vertically. It can be another factor responsible to the smaller saturation degree in the central part of the barrier.

The RH evolution on the top section of the China-Mock-Up facility is given in Figure 20. Due to the non-uniform water supply in the vertical direction, the saturation process in this section is not as pronounced as in the sections at the bottom. The desiccation phenomenon is also observed for the sensor located in inner ring. In addition, the fluctuation of RH induced by the heating interruptions is particularly evident in this section. It indicates that the generated vapour phase is diffused in both radial and longitudinal directions.

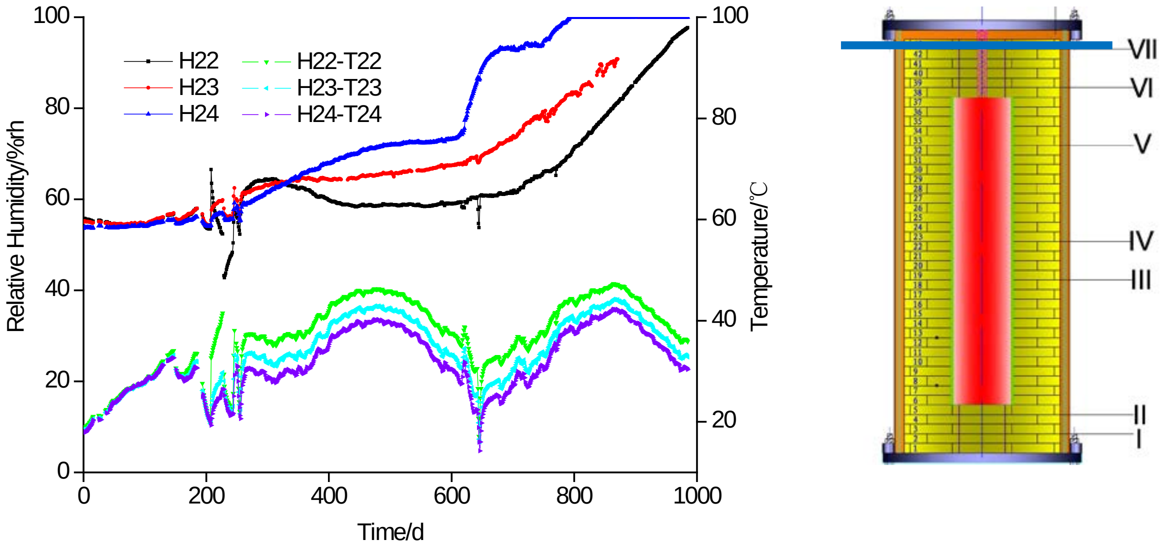

Figure 20: Variation of relative humidity with time at section VII.

Stress evolution

In the China-Mock-Up facility, the stress variation of the compacted bentonite is influenced by several mechanisms, including the thermal expansion induced by the high temperature, the swelling pressure generated by the water penetration, etc. The stress evolutions are presented in Figure 21. As illustrated, with the increase of the injection water, the saturation process is dominant, and the stress in this area is increased gradually to 2.0 MPa especially in the outer boundary. In other sections, almost no significant variation of stress in compacted bentonite is observed up to now near the heater. This could be attributed to two reasons: at first, the saturation process is relatively limited near the heater; and the second reason is the initial space between the sensors and the blocks of the compacted bentonite. It can be noticed that there are some fluctuation in hot section III-V because of the power supply incident.

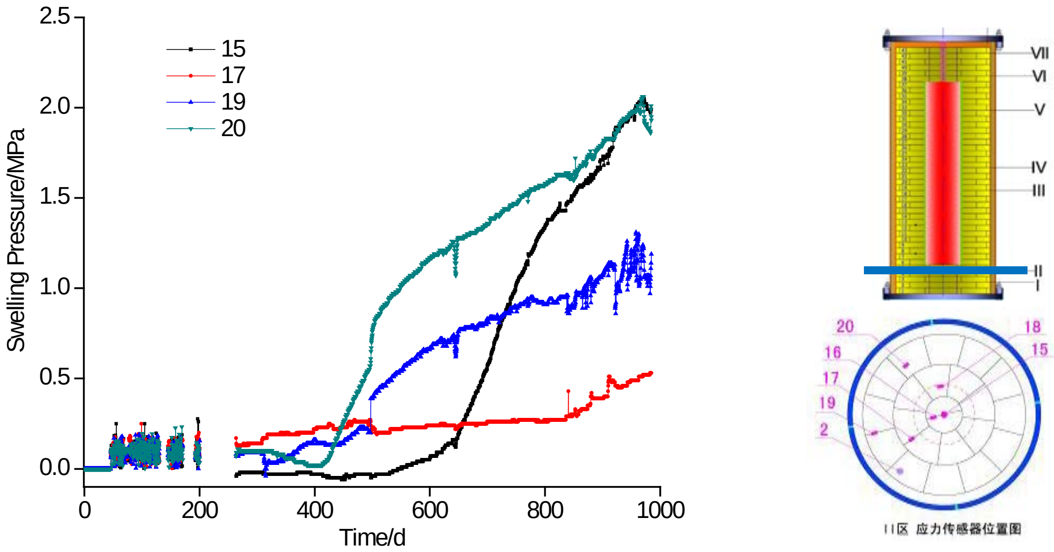

Figure 21: Stress evolution at section II.

Vertical displacement of the canister

In order to investigate the potential movement of canister in long-term, six LVDT sensors are installed in the China-Mock-Up test to monitor the vertical displacement of the electrical heater. Three of them are installed at the bottom of the heater, and the others are installed in the upper part. The variation of the vertical displacement of the heater is record in Figure 22. It can be noticed that, the electrical heater moved upward after a stable phase. This phenomenon could be attributed to the thermal expansion of compacted bentonite, and the increased swelling of bentonite induced by the water penetration from outer boundary. In the proceeding of the test, the displacement became more and more flat. This result indicates that the saturation process of the buffer material may affect the stability of the canister, which should be considered in the design of the repository project. However, unfortunately the sensors in upper part are out of work because of the harsh environment after 800 days.

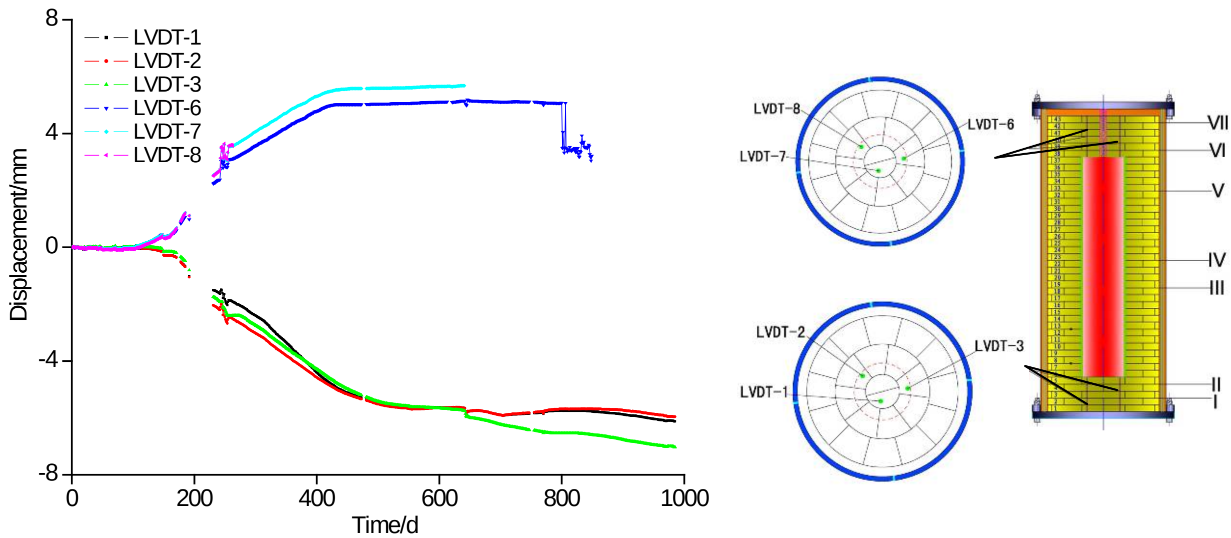

Figure 22: Vertical displacement of the heater with time.

6.3.2. Numerical results of China-Mock-up

Thermal simulation

Following the experimental procedure, the numerical simulations are divided into two phases: the temperature on the nodes of the electrical heater and the water injection on the bentonite's outer boundary are increased to 90 °C and 1200 g/day. The temperature on the outer boundary changes according to actual room temperature. The simulated temperature with time is illustrated in Figure 23. In the first few months, the temperature of the compacted bentonite increases significantly. Afterwards the high temperature area expands slowly. It can be noticed that the temperature of the steel elements remains in a low level, mainly as a result of the low thermal conductivity of the heat insulating material outside the steel tank.

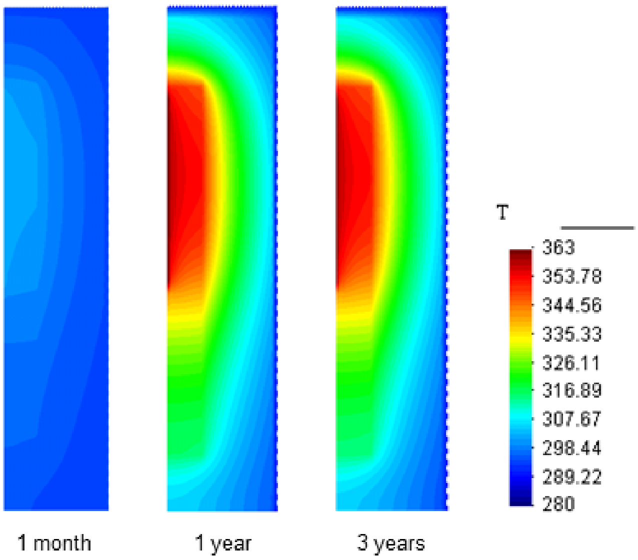

Figure 23: Distribution of temperature.

Hydro-thermal simulation

The numerical calculation of water pressure with time is analysed in Figure 24. As a result of the different water injection on the boundary, the water pressure of the bottom is higher than the other areas. It is noticed that in the field exposed to high temperature, the water pressure decreases over time. This result seems reasonable considering that the evaporation generated by high temperature is more significant in this area.

Numerical results of relative humidity at some points in China-Mock-Up are also studied. It is interesting that the saturation of the internal bentonite is firstly increased and then decreased. This can be explained by active vapour diffusion under the effect of high temperature. In contrast, the relative humidity of the area that far from the heater continues to increase over time. It indicates that the hydraulic effect is more significant in these areas.

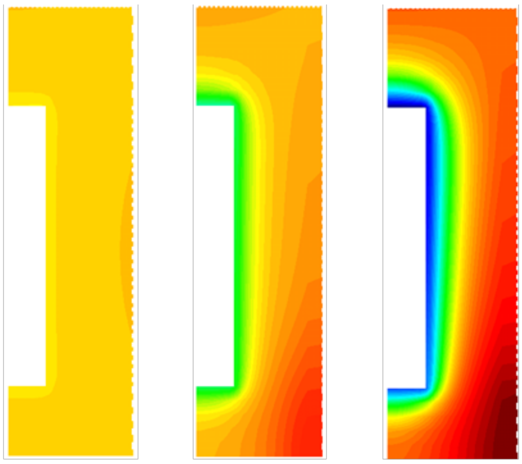

Figure 24: Distribution of water pressure.

6.4. Summary and future perspective

The buffer material is one of the main engineered barriers for the HLW repository. In order to study the behaviour of the compacted GMZ-Na-bentonite under coupled THMC conditions, a large-scale mock-up facility, China-Mock-Up based on a preliminary concept of HLW repository in China, has been designed and constructed in the laboratory of BRIUG.

The current experimental data is presented in the report, including the variation of temperature, relative humidity, stress and displacement etc. A thermo-hydro-mechanical model is proposed to reproduce the complex coupling behaviour of the compacted GMZ bentonite. With the proposed model, numerical simulation of the China-mock-up test is realized. According to the analysis of the experimental and numerical results, some conclusions are obtained and summarized as follows:

(1) The experimental data indicates that the saturation process of the compacted bentonite is strongly influenced by the competitive mechanism between the drying effect induced by the high temperature and the wetting effect by the water penetration from the outer boundary. For this reason, the desiccation phenomenon is observed in the zone close to the heater.

(2) Except for the temperature change induced by the interruption of electrical power supply, the temperature within the bentonite has increased with time. Considering the saturation may change the thermal conductivity, the temperature distribution is influenced by the coupling mechanism between the thermal conduction and the saturation process in the mock-up test. However, it is noticed that the change of seasons has a significant effect on temperature.

(3) For China-Mock-Up test the upward displacement of the heater suggests that the thermal expansion and saturation process of the buffer material may influence the stability of canister in the long-term, which should be considered in the design of the repository. It has to be mentioned here, the displacement of electrical heater is strongly influenced by the experimental configuration and boundary conditions. Considering the repository conception in China is not finalized yet, the similar weight of the canister and electrical heater cannot be

assumed. Therefore, this result is not totally representative of the real ones, and further validation is still necessary.

(4) In the China-Mock-Up facility, the stress variation of the compacted bentonite is influenced by several mechanisms, including the thermal expansion induced by the high temperature, the swelling pressure generated by the water penetration, and etc.

(5) Based on the analysis of the current experimental data, the China-Mock-Up test is considered as a source of valuable data to improve the knowledge of the THM process in the EBS, and to establish the reliable numerical method to predict the THM coupled behaviour of EBS in long-term. With the progress of the experiment, the conclusions achieved will be further examined and refined.

(6) Based on the quantitative analysis of the numerical results, it is suggested that the proposed model is capable to reproduce the principal thermal behaviour of the compacted GMZ bentonite. As a quantitative analysis of the numerical results, the numerical study for now can be considered as a preliminary stage. With the progress of the experimental test, further quantitative studies are needed.

The China-Mock-Up is the first large-scale THMC coupled experiment in China, and its successful operation will play an important role in investigating the long-term behaviours of GMZ-bentonite under relevant repository conditions. The China-mock-up operations so far are running very well and better than proposed. Most of the sensors run very fine Hence, the decision was made that BRIUG will continue to perform the experiment.

The China-Mock-Up experiment is an important milestone of the buffer material study for HLW disposal in China. The observed THMC processes taking place in the compacted bentonite-buffer during the early phase of HLW disposal provide a reliable database for numerical modelling and further investigations of EBS, and the design of a HLW repository.

7. Summary

7.1. Progress and achievements

The main scientific and technical achievements of the PEBS project are described in detail in Chapter 2 to 5. Here, only a brief summary of these achievements are given in the order of the Work Packages.

Through the work performed in **WP 1**, important processes during the early evolution of the EBS were identified and the need for additional studies was assessed. The product of WP 1 – the list of four cases – served as orientation throughout the entire project and helped to integrate the knowledge gained from the experimental and modelling studies into an analysis of impact on long-term safety and guidance for repository design and construction.

A broad range of laboratory and in-situ experiments dealing with the early evolution of the EBS were performed in the framework of PEBS. The main achievements of the experimental studies performed in **WP 2** include:

- Confirmation, integration and improvement of existing knowledge of the THM-C processes in the early evolution of bentonite barriers;
- Compilation of data for future interpretation of large scale experiments;
- Providing a reliable data base for the validation and enhancement of numerical models;
- Providing more distinct criteria to be conservatively applied in the Performance Assessments of engineered barriers;

Through the comprehensive numerical simulations performed within **WP 3** the following progress and achievements were made:

- Simulation of the laboratory and in-situ tests helped to interpret the experimental results;
- Enhancements of existing models, including threshold gradient, thermo-osmosis and double porosity, allow for the simulation previously unexplained phenomena in the EBS evolution;
- Development of new model concepts based on thermo-mechanical continuum mixture theory, allowing for an alternative description of the EBS behaviour;
- Enhancements of THMC models for the simulation of corrosion and effects at the bentonite-concrete interface, taking into account porosity change by swelling and incorporating reactive gaseous species;
- Quantification and reduction of uncertainties in the model predictions by implementing an inverse framework;

- Improvement of the basis for long-term extrapolation of the EBS behaviour and prediction of long-term repository evolution.

In **WP 4** significant progress was made in the evaluation of uncertainties in process understanding of the EBS. The work in WP 4 was based on the approach developed in WP 1 and integrated the outcomes of the other Work Packages as well as findings from outside PEBS – this permitted the integration of a broad range of knowledge and put the gained information into the context of PA. The significance of remaining uncertainties for the long-term safety functions of the EBS was elaborated, taking into account different national safety cases.

The core of **WP B**, the China-Mock-Up experiment, is an important milestone of the buffer material study for HLW disposal in China. The observed THMC processes taking place in the compacted bentonite buffer improve the knowledge of the early phase evolution of HLW repositories. Furthermore, they provide a reliable database for the validation of the numerical models, which in turn are used for the extrapolation to the long-term behaviour of GMZ-bentonite under relevant repository conditions.

7.2. Recommendations and future perspective

At the finalisation of the PEBS project, various recommendations for future scientific and technical work can be given. These are described in detail in Chapter 2 to 5. Here, only a brief summary of these recommendations are given:

- Observations from the execution and excavation of existing and new in-situ experiments will play an important role in further confirming bentonite performance over periods of 10-20 years;
- For repository concepts anticipating temperatures above 100 °C certain aspects, such as the influence on swelling pressure and strength of the EBS material, require further experimental data collection;
- A more detailed description is needed for the potential impact of very long saturation times (thousands of years) on the performance of the EBS;
- Work on the THMC processes at material interfaces (e.g. cement-bentonite, cement-host rock) will be continued, with a special focus on porosity determination and the nature of alteration;
- The continuation of the China-Mock-Up test will provide an important role in the investigation of the long-term behaviour of GMZ bentonite and in the design of a HLW repository in China;
- Although geophysical monitoring has proved to be a useful tool for the characterisation of the EBS and EDZ, further investigations are needed to better understand the correlations between the geophysical parameters and the rock properties;

- The continuation of existing long-term experiments will help to identify processes potentially relevant for the long-term THM behaviour of the EBS (e.g. thermo-osmosis, double porosity, creep) and to reduce uncertainty in model parameters;
- The enhanced numerical models, which were developed and applied within the framework of PEBS, will be further calibrated with additional experimental data and should be used for long-term simulations;
- Promising alternative models, such as the concept based on the continuum mixture theory, will be further investigated;
- Extensive model testing and supporting data is required to improve the predictive capability of geochemical modelling.

7.3. Potential impact

Strengthening the scientific-technical basis for geological disposal

The engineered barrier system represents a complex sub-system of a geological repository for spent fuel and HLW. In the near field of the repository numerous coupled thermo-hydro-mechanical and -geochemical interactions take place among the waste forms, the different components of the EBS and the host rock. The long-term barrier performance of the near field cannot be demonstrated without an adequate understanding of these coupled processes. At the beginning of the PEBS project, the present state of the art included detailed knowledge on the individual processes and material interactions as well as on relatively simple process couplings. Due to the strong simplifications of the existing models, they were often inadequate to reproduce the complexity of the spatial and temporal development. The PEBS project aimed to assess the system behaviour of the near field, focussing on the EBS and taking into account different scenarios regarding the long-term evolution a repository for HLW disposal.

One main scientific achievement of PEBS was to acquire a comprehensive insight in the system behaviour of the EBS, in particular the complex interactions between various materials and its evolution with time. This in-depth knowledge will facilitate the evaluation of the barrier performance of the near field components. With a comprehensive scientific approach, the PEBS project was able to strengthen the scientific-technical basis for geological disposal by

- Deepening the knowledge and understanding of the coupled processes in the EBS with time;
- Providing a more quantitative basis for relating the evolutionary behaviour of the EBS to the safety functions;
- Clarifying further the significance of residual uncertainties for long-term performance assessment.

Overcoming fragmentation and complementing national efforts

At the beginning of the PEBS project the main challenges included the integration of existing knowledge on the individual processes in the near field and their interaction. Progress in this domain could only be achieved by studying key processes and evolution scenarios for the EBS in an integrated and multidisciplinary way.

In the PEBS project European and non-European organisations active in the research on geological disposal brought together their multidisciplinary expertise, which was required to integrate and structure research on the EBS within the EU and abroad. The level of integration aimed at by PEBS, in particular the development of a comprehensive and phenomenological insight in the overall EBS behaviour and its spatial and temporal evolution, has not been achieved before. The envisaged integration was achieved by:

- The creation of high-quality international research teams;
- The establishment of a forum of experts in different disciplines to develop coherent approaches;
- The pooling of research facilities and infrastructures (including analytical facilities and underground research laboratories for in-situ testing);
- The optimisation of experimental tools and protocols, data treatment, reporting, transfer, and exploitation of the experimental results.

Supporting the EU policy objective on the implementation of national programmes on geological disposal

Finding a solution for the disposal of high level radioactive waste is undeniably the major concern in radioactive waste management. Accordingly, it is a key strategic policy objective of the EURATOM Programme. With the "Radioactive waste and spent fuel management directive"[1], adopted on 19 July 2011, EU Member States have to submit the first national programmes for the implementation of disposal solutions by 2015.

The project PEBS contributed to these policy objectives, as its prime target was to strengthen the scientific-technical basis for the establishment of national programmes for the geological disposal of radioactive waste and spent fuel. PEBS focused on an essential component of any geological disposal system: the engineered barrier system (EBS) which encloses the waste containing canister. The scientific advances achieved within the PEBS project will contribute to ensure high levels of safety, may accelerate practical developments required for the management of HLW, and may help to respond in a flexible way to new policy needs.

Contributing to policy developments

Over the past 25 years, national programmes within the EU pursuing geological disposal have made considerable progress. Several EU Member States have made the transition

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[1] Council Directive 2011/70/Euratom of 19 July 2011

from R&D to repository development and plans to implement geological repositories are underway in Sweden and Finland. However, the societal and scientific-technical challenges of geological disposal have proven to be substantially greater than anticipated when national programmes for the geological disposal of HLW were established several decades ago. Worldwide, no geological repository for the disposal of heat generating high-level radioactive waste has been taken in operation until now. The large and growing inventory of HLW from civilian nuclear programmes is handled in surface facilities that are intended only for interim storage. Against this background, finding clear solutions to the management of HLW is of highest importance, and is also a prerequisite for a continued use of nuclear energy sources in the EU.

Given the state of the art, geological disposal is the safest option for the long-term management of HLW. Most repository concepts under development within the EU put strong emphasis on the containment properties of the near field system in general and the EBS in particular. The near field shall ensure the containment and minimisation of the release of radionuclides over extended periods of time and is an essential factor with respect to the overall safety of a geological repository. Accordingly, the capability to demonstrate a robust near field performance is a major scientific challenge in all national programmes within the EU. National programmes must therefore have dedicated and focussed research programmes in view of developing a sound understanding of the near field sub-system. These programmes must also maintain sufficient flexibility to improve the design the EBS system and respond to new policy needs.

PEBS integrated the expertise within the EU into a collaborative project that evaluated the behaviour of the EBS. This underscores the strategic impact of the project PEBS which:

- Integrated research in the EU on the EBS of a geological repository for HLW;
- Moved the scientific basis for geological disposal beyond the state of the art;
- Strengthened interactions between various players in radioactive waste management, in particular R&D organisations, agencies/implementing organisations;
- Helped to develop a consensus within the EU on key issues for the safety of geological repositories in support of the decision making process;
- Intensified the cooperation in the scientific field, which helps to move national programmes ahead.

Addressing societal concerns about the safe disposal of radioactive waste

Public acceptance of geological repositories for HLW depends to a large extent on the ability to clarify that geological disposal is a safe long-term solution for the management of high-level radioactive waste. Strengthening the scientific basis to reduce remaining uncertainties is the key to confidence building. However, public acceptance will only be gained by actively communicating the scientific findings and their implications for the safety functions of the repository. A consensus on key issues for the safe disposal of HLW in the EU and beyond will also help increase public acceptance. Current disposal concepts within the EU put strong emphasis on the containment properties of the EBS. Building confidence in the containment function of engineered barriers will therefore contribute to the acceptance of geological disposal facilities.

PEBS may contribute to an increase of public acceptance of geological repositories by advancing the knowledge on a crucial component of the repository system – the EBS – and thereby reducing uncertainties regarding the long-term barrier performance; a key topic within PEBS was to relate the scientific finding to the safety function of the repository. One Work Package of the project was dedicated to the dissemination of results and training activities. Disseminating the scientific and technical results to various stakeholders, and making the majority of reports publicly available facilitates the development of a consensus within the EU and beyond on key issues for the safety of geological repositories, which in turn may help to raise public acceptance.

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Annex II – List of Acronyms

Aitemin	Asociacion para la Investigacion y el Desarrollo Industrial de los Recursos Naturales
ANDRA	Agence Nationale pour la Gestion des Déchets Radioactifs
BGR	Bundesanstalt für Geowissenschaften und Rohstoffe
BBM	Barcelona Basic Model
BRIUG	Beijing Research Institute of Uranium Geology
Ciemat	Centro de Investigaciones Energéticas Medioambientales y Tecnológicas
CIMNE	Centre Internacional de Mètodes Numèrics en Enginyeria
CS	Confining structure
EB	Engineered Barrier
EBS	Engineered Barrier System
EDZ	Excavation Damaged Zone
EdZ	Excavation disturbed Zone
ENRESA	Empresa Nacional de Residuos Radioactivos SA
EU	European Union
GBM	Granular Bentonite Material
GMZ	Gaomiaozi
GRS	Gesellschaft für Anlagen- und Reaktorsicherheit
HE-E	Heater Experiment
HLW	High-level radioactive waste
HM	Hydro-mechanical

JAEA	Japan Atomic Energy Agency
NA	Natural analogues
Nagra	Nationale Genossenschaft für die Lagerung radioaktiver Abfälle
OPA	Opalinus Clay
OPC	Ordinary Portland cement
PA	Performance Assessment
PEBS	Long-term Performance of Engineered Barrier Systems
R&D	Research and development
RH	Relative humidity
RTD	Research and technological development
S/B	Sand/bentonite
SF	Spent fuel
SKB	Svensk Kärnbränslehantering AB
THM	Thermo-Hydro-Mechanical
THMC	Thermo-hydro-mechanical-chemical
UAM	Universidad Autónoma de Madrid
UDC	Universidade da Coruña
URL	Underground Research Laboratory
WP	Work Package