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Research Area

PEBS
Long-term
Performance of
Engineered
Barrier
Systems

Final Publishable Summary Report

Table of contents

1. Executive summary

The fundamental basis of geological disposal concepts for spent fuel and radioactive wastes is generally a multi-barrier system. 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 collaborative project PEBS focused on the complex interaction of thermal, hydraulic, mechanical and chemical (THM-C) processes in clay-based EBS, associated with the evolution of the near field around a heat emitting waste canister. The investigations focused on the following periods and parameters:

- The early post closure period (early resaturation time), when the buffer is expected to experience the maximum temperature and is largely unsaturated and the thermal evolution of the EBS may be controlled by the effective thermal conductivity of the dry buffer material. The main source of uncertainty arises from possible scale effects in the determination of thermal conductivity.
- The resaturation period, when competing processes such as water uptake, thermal impact and the swelling of the buffer will interfere and may lead to unexpected transitory effects. Confirmation has to be gained, that the transitory effects will not influence the final equilibrated state of the EBS system.
- The pore pressure recovery period, when the EBS system is close to full water saturation and the key THM-parameters tend to reach equilibrium conditions. Statements on the uncertainties with regard to the safety relevant EBS parameters are required (spatial variability of swelling pressure, hydraulic conductivity and porosity in the buffer and in the Excavated Damaged Zone (EDZ)).

The resaturation phase and the successive pore pressure recovery period as well as the following hundreds of thousand years, which are considered in the performance assessment (PA), are sometimes addressed as “long-term” behaviour. They cannot be observed directly, but have to be accessed by extrapolation in time.

The work performed within PEBS involved several laboratory and large scale in-situ experiments, which provided the data base for the calibration and validation of the coupled THM-C simulations. New models were developed and applied for the extrapolation of the observed EBS behaviour to the long-term performance. The gained in-depth understanding of the EBS evolution was used to constrain the uncertainties in the long-term safety assessment in some important areas.

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

- deepen the knowledge and understanding of the THM and THM-C evolution of the EBS with time;
- provide a more quantitative basis for relating the evolutionary behaviour to the safety functions;
- 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, consisting of 15 partners from Europe, China and Japan, used its expertise for public information purposes and to promote knowledge and technology transfer through training.

2. Project context and objectives

The evolution of the engineered barrier system (EBS) of geological repositories for radioactive waste has been the subject of many national and international research programmes during the last years. The emphasis of the 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 early post closure period in the near field. 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. Exceptional 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 parameters in 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. The experimental data bases were extended on the laboratory and field scale and numerical simulation tools were developed. Less successful, however, was the attempt to use this in-depth process understanding for 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 is required to set-up the scientific validation procedures in a context which is relevant for the PA purposes. Thus, validation experiments are 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 should be specified by the needs of PA.

The work within the PEBS project was built on the existing knowledge and experience and aimed at providing a more complete description of the THM and THM-C evolution of the EBS, a more quantitative basis for relating the evolutionary behaviour to the safety functions of the system and a further clarification of the significance of residual uncertainties for long-term performance assessment. The importance of uncertainties arising from potential disagreement between the process models and the laboratory and in-situ experiments performed within PEBS, and their implications for extrapolation of results was reviewed, with particular emphasis on potential impacts on the safety functions.

The main aim of the project PEBS was to bridge the gap between the improved scientific understanding of THM-C processes and the actual needs of PA to specify EBS related safety function indicators. This comprised 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 processes fed into an adapted assessment of long-term safety functions of the EBS through extrapolation of the short-term effects on the long-term, including the evolution of their relative impacts and the 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) affecting 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 taking place 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,
- 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 R&D.

In order to fulfil these scientific and technical (S&T) objectives in an efficient way, a multi-disciplinary and integrated approach was applied.

In addition to the S&T objectives, the PEBS consortium

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

3. Description of main S&T results

3.1. Work Package 1

The early period of repository evolution is characterized by an elevated temperature together with strong thermal and hydraulic gradients (possibly mechanical and chemical as well). The duration of this period is very short in the view of the entire operational timeframe of the repository. However, the processes occurring during this period may have an impact on the performance of the barriers in a longer timescale. Work Package 1, titled “Analysis of system evolution during early post closure period: Impact on long-term safety functions”, had the following overall objectives:

1. Identify important processes during the early evolution of the EBS,
2. Describe the current treatment of the early evolution of the EBS in long-term safety assessments for spent nuclear fuel,
3. Discuss how the short-term transients will/may affect the long-term performance and the safety functions of the repository,
4. Identify the merits and shortcomings of the current treatment,
5. Discuss the needs for additional studies of these issues and how they can support future assessments – give directions to other Work Packages,
6. Define “scenarios” related to events in the early evolution of the EBS.

The first step towards the accomplishment of these objectives was a detailed description of the current treatment of the early evolution of the EBS in safety assessments from a number of European national programs (state of the art). Next was the identification of uncertainties in the process understanding and in the treatment of the processes in the assessment. The significance of the identified uncertainties on the evaluation of the safety functions was discussed. Despite the differences in repository concepts, the safety functions defined for the engineered clay barriers are similar. 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. The key processes identified are:

- water uptake in clay components of the EBS,
- mechanical evolution,
- alteration of the hydro-mechanical properties.

The identified key processes fed into the main outcome of WP1 – a list of cases related to the early evolution of the EBS. A “case” was defined as a combination of a configuration (the defined EBS with its initial conditions) and the description of an evolution of the EBS reflecting an identified uncertainty (e.g. by identifying case variants). The cases were identified based on the description of the early evolution of the EBS in the disposal concepts studied and their respective safety assessment methodologies and by:

- assessing the impact of this uncertainty on the evolution of the EBS by evaluating the processes,
- assessing the impact of the evolution of the EBS on the safety elements (functions, indicators and criteria).

This was done through integration of the knowledge, gained during PEBS and other recent EBS projects, in the existing process understanding of the real evolution of the EBS that is described in WP1. This definition implies that a case is likely (but not necessarily) to be repository concept (and thus host rock) specific.

Based on the outlined approach, WP4 proposed a specific set of cases that was agreed upon after discussion with Work Package leaders. These cases are:

1. Water uptake in the bentonite buffer below 100°C,
2. Performance of the bentonite buffer at temperatures above 100°C,
3. Hydromechanical evolution of the buffer,
4. Geochemical evolution of bentonite buffer.

The proposed cases served as the basis for integrating the knowledge gained from PEBS experimental and modelling studies (WP2, WP3, WP B) and as an input for the analysis of impact on long-term safety and guidance for repository design and construction performed in WP4.

3.2. Work Package 2

Work Package 2, titled “Experimentation on key EBS processes and parameters”, had the following overall objectives:

1. To evaluate the key HM, THM, and THMC processes and parameters taking place during the early evolution of the EBS.
2. To provide with a reliably good quality experimental HM, THM and THMC data bases, including different time and spatial scales, as input to the modelling and extrapolation work to be conducted within WP3.

The Work Package was structured into three different tasks.

3.2.1. Task 2.1 – Experimentation on key HM processes and parameters

Task 2.1 had the following overall objectives:

1. Evaluate the key HM processes and parameters taking place during the early evolution of the EBS.
2. Provide with a reliably good quality experimental HM data base, including different time and spatial scales, as input to the modelling and extrapolation work to be conducted within WP3.

EB in-situ experiment: long-term monitoring and dismantling

The physical and thermo-hydro-mechanical characterisation of the bentonite samples retrieved during dismantling of the EB test was performed mainly at CIEMAT. Water content, dry density, suction, thermal conductivity, pore size distribution, basal spacing of the smectite, permeability and swell-ing capacity were determined. The results are compiled in D2.1-7. Experimental results from other involved organizations (e.g. ANDRA, Nagra) are included in the EB dismantling synthesis report (D2.1-8).

Laboratory infiltration tests

The long-term permeability tests for evaluation of the evolution of permeability over time and of the influence of hydraulic gradient on hydraulic conductivity are still running. Three of them performed with the FEBEX bentonite started years ago, whereas two others performed with the MX-80 bentonite started during the PEBS project. The possible threshold hydraulic gradient for FEBEX would be around 200 or 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.

3.2.2. Task 2.2 – Experimentation on key THM processes and parameters

Task 2.2, which is divided into two subtasks, had the following overall objectives:

1. Evaluate the key THM processes and parameters taking place during the early evolution of the EBS.
2. Provide with a reliable good quality experimental THM data base, including different time and spatial scales, as input to the modelling and extrapolation work to be conducted within WP3.

Task 2.2.1 Laboratory experimentation on key THM processes and parameters

The **FEBEX mock-up** has been in operation for more than 16 years. Less than 16% of the sensors are damaged. Most of the non-operative sensors are relative humidity sensors that have been flooded. This fact, along with the converging pressures inside the bentonite, indicates full saturation in the external part of the barrier. A database on THM processes was compiled with the aim of providing parameters for the modelling work. It included an update of the information on the FEBEX bentonite supplied by recent laboratory tests. In particular, the database generated by the mock-up has allowed verifying some hypothesis about THM processes and the calibration of models in conditions close to saturation.

The performance of **long-term laboratory tests in cells** in which the conditions of the bentonite in the barrier are simulated with respect to kind and pressure of water, temperature, as well as density and initial water content of the bentonite. Several tests of this kind have been running for years, and their continuation or dismantling provided valuable information on the evolution of the barrier at the transient stage.

The two TH tests in cells performed with FEBEX bentonite run for almost 12 years and provided online information about the temperature and relative humidity inside the bentonite. In one of them the column of bentonite was hydrated under thermal gradient (GT40) and in the other one at isothermal conditions (I40). 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. These tests have highlighted the influence of the thermal gradient on the hydration kinetics, the persistence of the water content and dry density modifications and the slowness of the saturation process.

Two TH tests in cells were designed to reproduce the conditions in the *in-situ* HE-E test and are being carried out with a sand/bentonite mixture (S/B) and with MX-80 bentonite pellets (B). The heater at the bottom of the cells is set at 140°C and hydration with Pearson water takes place at a very low injection pressure. The effect of the thermal gradient on the water vapour redistribution was considerable. The two materials show a completely different behaviour, since the S/B mixture is much more permeable and does not swell. In fact, the column seems to be completely saturated after less than 2 years of hydration. The progression of hydration in cell B is very slow and accompanied by an increase in swelling pressure.

To support these tests, and in order to better understand the hydration process of low-density buffer materials, a series of infiltration tests were performed under isochoric conditions and at room temperature with measurement of the swelling pressure. Three tests were performed with the HE-E S/B mixture and two with the B pellets. In all the tests, and even under a very low injection pressure, most of the water was taken at the beginning of the experiments. Afterwards the water intake was very small. The development of swelling pressure on the pellets mixtures followed a pattern in which the pressure sharply increased at the beginning of hydration, then stabilised, and afterwards increased again, eventually reaching the equilibrium value when most of the water had already been taken. The mixtures became homogeneous upon saturation, no pellets could be told apart. In the tests with MX-80 pellets, the water content and dry density gradients along the bentonite remained even after having reached the equilibrium swelling pressure.

Mechanical properties of buffer material exposed to increased temperature during and after water saturation were investigated in the laboratory **study on stress-strain behaviour**. Buffer material exposed to repository and accelerating conditions involving increased temperature have been investigated in the project LOT at Äspö HRL, Sweden. Stress-strain behaviour in different positions in the LOT parcel and in reference material was determined by unconfined compression tests. Significant lower strain at failure was measured in the material exposed to high temperature. The studies performed within PEBS were initiated by this previously observed thermo-mechanically induced brittleness in buffer material. Further studies regarding the origin of brittleness were of importance to further understand the behaviour. The study in PEBS focused on the stress-strain properties of bentonite exposed to increased temperature but the influence of different mineral composition, different an-ions 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 between 90°C – 150°C in a laboratory oven during 24h. The heating was made after and just before full saturation. Examples of correlations seen in the test results were:

- 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.

Task 2.2.2 In-situ experimentation on key THM processes and parameters

At the end of the PEBS project, the **HE-E** had been operating for almost 32 months successfully. As of February 2014 the major outcomes can be summarized as a follows.

- 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 host rock can be attributed to condensation of vapour. The highest temperatures (>100°C) are thus prevailing in an EBS with a very low water content (below <20 %RH). This observation is of importance because under these conditions of very low water contents, chemical reactivity will be hampered by water availability. As long as high temperatures at the heater surface are maintained, these dry conditions are to prevail. The natural water inflow from the Opalinus Clay is occurring slowly. Although pores become saturated fairly rapidly (more so in the sand/bentonite than in the bentonite), after 32 months only at distances in the Opalinus Clay > 1 m from the tunnel wall a 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, although it cannot be fully excluded that the overpressures are influenced by the presence of the tunnels nearby acting as a constant pressure boundary at 1 bar.
- 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 no clear link between the seismic parameters and the physical phenomena could be established.

3.2.3. Task 2.3 – Experimentation on key THM-C processes and parameters

Task 2.3 had the following overall objectives:

1. Evaluate the key THM-C processes and parameters taking place during the early evolution of the EBS.
2. Provide with a reliably good quality experimental THM-C data base as input to the modelling and extrapolation work to be conducted within WP3.

The THM-C mock-ups (GAMEs)

Since May 2012, the THM-C mock-ups are running under the following conditions: the heater 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: well damaged during the water injection events, well damaged 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, consequently corrosion processes must be going on inside the structures.

It was considered that their main usefulness would be the post-mortem information gathered upon dismantling, and this would be more interesting the longer the time the materials are subjected to the operation conditions. The minimum duration of three years operation before their dismantling foreseen in the DoW will be barely reached before the end of the project, and in any case the post-mortem results would not be ready before the end of the project.

It was proposed and accepted, to provide alternative information related to the concrete-bentonite and corrosion products bentonite interactions that were expected to be seen in the GAMEs. This new information come from the analysis of tests in cells of different duration (up to 3 years) that were performed during NF-PRO but had not been reported neither analysed jointly so far. This provides modellers with a database on THM-C processes and their evolution over time.

Key processes at the canister/compacted bentonite/concrete interfaces

Studies on the small cells dismantled within the project show that in general, the absence of mortar produces a relative high final water content and low density which can be related also with a relative high total porosity. Sections of bentonite in contact with mortar seem to have lower total intruded (Hg) porosity than sections far from the interface. This correlates with low SSA values, which means that particles may have been cemented and aggregated thus showing low available surface area by means of pore clogging. There is a negligible impact of magnetite into the bentonite in terms of porosity or SSA.

Chloride migration by backwards diffusion from the bentonite into the hydration reservoir has been observed, selectively, when the mortar interface was absent. In fact, both, mortar and magnetite interfaces acted as sinks of chloride and sulphate, which limited, in the case of mortar, the migration of sulphate to the bentonite. Small quantities of sulfoaluminates and carboaluminates (Aft and Afm like phases) which can allocate chloride were determined near the mortar-bentonite interface. Gypsum and green rust (Cl-Fe) phases were detected at the magnetite interface.

The magnetite interfaces showed a Fe penetration front of < 0.1 mm. This front is very small and has been possibly influenced by the difficulty to establish the exact position of the interface. Otherwise, a calcium front was developed from the mortar towards the bentonite, in which C-S-H phases formed. Portlandite dissolved in mortar near the bentonite interface. The dissolution was higher in natural bentonite experiments than in the pre-treated bentonite. Aluminum penetrated in the mortar from the bentonite in accordance to the Aft and Afm type phases, detected either by SEM-EDX or XRD. Mg concentrated at the interface (1-2 mm) with mortar in the natural bentonite, however, this was not observed in the pre-treated bentonite. The precipitation of Mg-phases (MgSH) in the natural bentonite may buffer the C-S-H front, which is more developed in pre-treated bentonite (up to 3 mm). This means that natural bentonite has potentially higher buffer capacity to attenuate the calcium alkaline front than the pre-treated one. Then, the degree of exchangeable K+ uptake from cementitious materials, affecting initially the bentonite hydration and swelling, has to be evaluated precisely.

When dismantling the **medium test cells**, full saturation of the bentonite block was not achieved. The simultaneous heating and hydration of the bentonite block led to the redistribution of exchangeable cations along the bentonite column: Increase of Mg and K in areas close to the heater (iron interface) (70%) and Na near the hydration. There are also saline fronts moving towards the heater which drove to the concentration of chloride and sulphate, relevant to iron corrosion. Concrete and iron interfaces act as a sink of soluble salts (Cl, S) coming from the clay formation porewater or migrated through the bentonite.

The concrete/bentonite interface shows the precipitation of gypsum, CASH gels, MSH gels and carbonates (calcite and aragonite), affecting <2 mm thickness of bentonite. However, the alkaline alteration produces changes in the redistribution of exchangeable cations in the bentonite. Considering this aspect the alteration thickness is larger and it is characterized by drastic magnesium depletion due to its precipitation in alkaline porewater. This effect can be followed in a 20 mm wide region of the bentonite from the concrete interface in the medium scale cells.

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 iron alteration zone has an average thickness of 1 micron and the Fe-influenced zone was estimated to be 20 μm. The alteration zone consisted of a mixture of corrosion products (nanoparticles) and bentonite enriched in chloride and sulphate, probably due to the compression effect of bentonite swelling on Fe powder. No newly-formed Fe-rich clay phases were identified. Precipitation of Ca phases (gypsum-anhydrite) has been identified on Fe powder, as well as evidences of thermally-induced mineralogical changes such as silica precipitation at the iron/bentonite interface (600 µm): Cristobalite beads (size around 100 nm) were found in cells dismantled after 54 and 82 months of operation.

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, 100ºC) has also been identified.

3.3. Work Package 3

Work Package 3 “Modelling of short-term effects and extrapolation to long-term evolution” has the following overall objectives:

1. To perform coupled HM, THM, and THMC analyses to provide a sound basis for the interpretation of the various tests planned in the frame of the PEBS WP2.
2. To develop new or improved models as demanded by the calibration of computation results with the actual measured data.
3. To use the data and improved models for extrapolation to long-term evolution of the repository taking into account the scenarios defined in PEBS WP1 and to investigate model uncertainty and its impact on long-term prediction, thus providing input to PEBS WP4.

The Work Package was structured into five different tasks with specific objectives.

3.3.1. Task 3.1 - HM modelling of the Mont Terri Engineered Barrier (EB) Experiment

Task 3.1 had the following overall objectives:

1. The hydromechanical (HM) modelling of the EB experiment aims at providing a satisfactory scientific representation and a sound basis for interpretation of the EB hydration phase and of the dismantling data.
2. New or improved constitutive laws adjusted with the experimental data will be developed.

The EB experiment has been modelled using the computer code CODE_BRIGHT. Because the test is run under isothermal conditions, only the hydromechanical component of the full THM formulation is considered in the analysis. An important feature of the experiment is that most of the barrier material is made up of pellets. Therefore, it is a double porosity material where the microporosity is enclosed inside the pellets and the macroporosity corresponds mainly to the voids between pellets. To take this into account, a double structure (porosity) constitutive model has been adopted to describe the mechanical behaviour of the barrier material. The two structural levels (macro and micro) are explicitly considered in the model; the microstructure is governed by a nonlinear elastic law whereas the macrostructure is governed by an elasto-plastic law that encompasses both unsaturated and saturated states. Interaction functions are defined that account for the interplay between the two structure levels. Importantly, permeability for liquid flow is related to the macroporosity and not to the total porosity.

The numerical modelling of the experiment has included the full period of hydration as well as the dismantling operation. The analysis has tried to simulate, as closely as possible, the hydration conditions that have been applied during the tests. This is not straightforward as there were some episodes in the experiment in which the process of hydration was not fully controlled.

It has been observed that the results obtained from the modelling are consistent with the dismantling observations. For instance, an important degree of dry density homogenization is obtained between the blocks under the canister and the pellets above the canister. The observed lateral higher porosity of the barrier is also an outcome of the analysis. It is also predicted that the barrier is almost fully saturated throughout, again consistent with observations.

It should be noted that uniform initial conditions of the barrier have been assumed, the observed material segregation during emplacement has not been considered. Therefore, the computed degree of heterogeneity at the end of the test arises solely form the test geometry, initial material distribution and pattern of hydration. Initial non-uniformity of the material would of course lead to somewhat different results but no information on this initial distribution is available. It can thus be stated that the progression of homogenization and the degree of heterogeneity at the end of the test is adequately represented by numerical modelling.

3.3.2. Task 3.2 – THM modelling of the heater test HE-E

Task 3.2 had the following overall objectives:

1. The THM modelling focuses on the design modelling as well as prediction and interpretation of the HE-E heater test performed in the VE microtunnel.
2. Constitutive models developed in earlier projects, such as NF-PRO, will be validated.

The progress and achievements in Task 3.2 included calibration and interpretative modelling of the HE-E as well as the integration and comparison of the modelling results produced by TK Consult, GRS and CIMNE. Main outcomes are:

The temperatures in the buffer materials and in the OPA near field (<2 m) are reasonably well reproduced with the various model approaches. Modelled temperatures are highly sensitive to the relationship between thermal conductivity and water saturation especially for low water saturation. Detailed characterisation of this aspect of the materials at hand is recommended.

There is reasonable agreement between models and measured TH parameters in early resaturation. The most advanced THM models are capable of reproducing the dry-out zone which is developing over almost half the radial thickness of the bentonite. This is less the case for the TH models.

An important effort has been devoted to the characterization of the thermo-hydraulic properties of the materials involved, in particular, buffer materials. A compilation of several laboratory tests, site measurements and some additional back-analysis have been carried out for this purpose. However, some uncertainties regarding the water retention curve of the granular bentonite materials and the dependence of their thermal conductivity and water permeability on the degree of saturation still remain. The correlation between the parameters complicates the calibration process.

Models that differentiate in their setup between the initial state of the emplaced materials and their properties are capable of capturing the evolution of these materials at the start of the experiment. However, the homogenisation in temperatures and relative humidities across the material boundaries that develop after a certain time (approximately 1 year) cannot be reproduced in detail as the model results are determined by the initial material parameters.

The resaturation in the OPA including the build-up of hydraulic pressures is slow and the area close to the tunnel surface is still in suction. It will require some years of monitoring to adequately test the models for resaturation.

The size and the trend of the hydraulic overpressures can be reasonably well reproduced with various models. To obtain satisfactory results the hydraulic conditions in the OPA at a larger scale prior to the experiment initiation need to be established, which is not trivial in a URL as its presence causes an important disturbance of the hydraulic field compared to a natural (hydrostatic) regime.

Although, due to the complexity of a full-scale field experiment, it is always difficult to match all the measurements with the numerical outcomes, the numerical results are in good agreement with the measurements, which demonstrates the model capability of capturing the evolution of the heating experiment during its initial phase. The overall conclusion is that the tested TH(M) models have been shown to perform adequately for modelling this high temperature URL experiment, the performance of the barriers is well reproduced and the confidence it the longer term calculations, beyond the experimental timescale, is reinforced.

3.3.3. Task 3.3 – THM modelling of bentonite buffer

Task 3.3 had the following overall objectives:

1. The THM modelling of the bentonite buffer will provide a continuing interpretation of the long term FEBEX mock-up test as well as analysis for the long term THM tests performed in cells in the CIEMAT laboratory.
2. An extrapolation to the real scale will be undertaken.

CIMNE has completed analyses of the FEBEX mock-up test that, in addition to the conventional formulation, incorporate the following new processes: i) threshold hydraulic gradient, ii) thermo-osmosis, iii) double structure formulation, and iv) combination of double structure formulation and thermo-osmosis. In all cases, the analyses have been taken to quite long times, of the order of 30 years. It has been found that the conventional formulation reproduces satisfactorily the early stages of the test but it fails to model the slow rate of hydration that occurs at later times. Discrepancies start to show after about three years, when the average degree of saturation of the barrier is about 90%. The three hypothesis (and the combined one) used in the enhanced formulation are able to model quite accurately the hydration of the mock up tests at all stages. Although the PEBS project is not designed to establish experimentally the potential existence and effects of those three phenomena, the performance 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 quite good agreement with observations. However, numerical analysis, on its own, is unable to identify with certainty what is the phenomenon (or combination of phenomena) underlying the observed slowing down of hydration. Yet there are noticeable differences between the predictions of the different hypotheses for the long-term situation (30 years). Therefore, availability of long-term observations of the mock-up test may help in identifying the relevant phenomena at the later stages of hydration.

Inverse modelling of the FEBEX in-situ experiment using iTOUGH2 was performed. The joint inversion of the whole set of measurement data results in parameter estimates of permeability, porosity, relative permeability and capillary pressure functions for both, host rock and bentonite buffer. Comparisons of model simulations with the observations show different degrees of agreement depending on the output quantity. 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 flow 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 then neglected/simplified processes and, thus, refer to the TH modelling approach, solely. In addition, the inverse model provides uncertainty estimates of the resulting parameters in form of standard deviations which were subsequently applied in WP 3.5 in order to assess the uncertainty of long-term predictions related to Case 1.

3.3.4. Task 3.4 – Modelling of THM-C experiments

Task 3.4 had the following overall objectives:

1. Most of the THC modelling work performed in the NF-PRO Project was carried out within the context of performance assessment. On the other hand, most of the lab experiments performed within NF-PRO on canister corrosion, corrosion-bentonite interactions and concrete-bentonite interactions have not been interpreted numerically. There is a clear need to test the models used in performance assessment analyses with data of recent laboratory experiments. The main objective here is to develop advanced multiple-continua THC(m) models for clay barriers and test them with lab and in-situ tests.

An improved model has been tested with data from the FEBEX mock up test. The model reproduces the measured cumulative inflow for the last 14 years. The fit of relative humidity, however, shows some discrepancies possibly caused by some model limitations such as the consideration of a single porous space.

Further testing of coupled THMC models with data from heating and hydration experiments conducted by CIEMAT was performed, including:

- The CG experiments performed on 60 cm long bentonite columns with durations ranging from 0.5 to 7.5 years. The numerical model reproduces the observed temperature, saturation degrees, porosities and dissolved an exchanged chemical data. Geochemical predictions improve when the changes in porosity caused by swelling are considered and when some parameters such as vapour tortuosity, heat dissipation and cation selectivities are estimated.
- 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. The models were calibrated with water content and dry density data measured at the end of the experiment. The kinetic parameters of magnetite precipitation were calibrated by using Fe weight content data which are representative of the precipitation of Fe(OH)2(s). For the most part, simulations agree well with experimental data. Model results indicate that: 1) The main properties of the bentonite remain unaltered; 2) There is a sequence of corrosion products, Fe(OH)2(s) and magnetite being the end members; 3) Fe2+ is sorbed by surface complexation; 4) Fe2+ cation exchange is less relevant than Fe2+ sorption; and 5) Corrosion products penetrate a few mm into the bentonite.
- The HB experiments to study the interactions of concrete and bentonite. These tests include a 30 mm layer of concrete which is in contact with the hydration system and a 71.5 mm thick layer of bentonite. The model was calibrated with the water content and dry density data measured at the end of the experiment and with temperature and relative humidity data measured during the test. For the most part, the model reproduces 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 are 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.
- The double interface tests, 2-I 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.

3.3.5. Task 3.5 – Extrapolation to repository long term evolution

Task 3.5 had the following overall objectives:

1. To use the data and improved models from WP3.1-WP3.4 for extrapolation to long-term evolution of the repository taking into account the scenarios defined in PEBS WP1.
2. To investigate model uncertainty and its impact on long-term prediction, thus providing input to PEBS WP4.

In order to provide input to WP4, several long-term simulations were planned and agreed upon. The finalized task table comprised the following simulation tasks:

1. Isothermal buffer evolution: Long-term extrapolation of the EB experiment configuration to investigate seal performance.
2. Thermo-hydro-mechanical evolution of the buffer at temperatures up to 100 °C: This involves long-term extrapolation of the FEBEX in-situ test with two variants – one using a constant heater temperature of 100 °C and the other using a heat decay curve representative for real HLW.
3. Thermo-hydro-mechanical evolution of the buffer (T > 100 °C): Long-term extrapolation of the HE-E using a realistic source term: Three modelling teams will be involved (CIMNE, NAGRA/TKConsult, GRS).
4. Geochemical evolution, especially at interfaces: Involves studies of the canister/bentonite interface and the concrete/bentonite interface and the long-term evolution in granite.

CIMNE has performed long-term 2-D numerical analyses of simulation tasks 1 to 3. In simulation task 1 (isothermal buffer evolution), the double structure model for the barrier material has been adopted. For simulation task 2 (THM evolution of the buffer T<100 °C) the enhanced models incorporating double porosity and thermo-osmosis as well as the conventional formulation have been used. For simulation task 3 (THM evolution of the buffer T > 100 °C) the conventional formulation for elastic and elasto-plastic models has been employed. For all the cases analysed, the results of the analysis provide relevant information on the likely state of the engineered barrier in the long term.

Nagra/ TK Consult also used axisymmetric models based on the Spanish repository concept – a proposal for disposal of spent fuel canisters surrounded by a high-density bentonite buffer in granite host rock – for the task 2 simulation. Rather than the coupled thermo-hydro-mechanical approach (THM) the computationally more efficient TH-code iTOUGH2 was applied, thus, neglecting mechanical processes as induced e.g. by bentonite swelling.

Prior to prediction, the involved model parameters were derived from inverse modelling of the FEBEX in-situ experiment at the Grimsel Test Site located in the Swiss Alps. This 1:1 physical model of the mentioned repository concept provides pressure, temperature, and saturation data from a heating experiment measured in more than 600 installed sensors for a period of over 15 years. The joint inversion of the whole set of measurement data results in parameter estimates of permeability, porosity, relative permeability and capillary pressure functions for both, host rock and bentonite buffer, so that model simulations are in good agreement with the observations.

Based on the optimized parameters, long-term evolution of pressure, temperature and saturation in the granite and the bentonite has been simulated with very similar results obtained from other THM-modelling studies. Propagating the parameter covariance (an additional outcome of the inverse study) by means of a linear error analysis relative narrow error ranges of e.g. the maximum temperature in the host rock (less than 10 °C) are predicted which reflect the high sensitivity of the computed model parameters to the observed performance measures.

For simulation task 3, TK Consult developed a specifications document for the extension modelling to be used as a benchmark for the different modelling teams. For this, the relevant property information from the HE-E experiment was defined as input into a simplified repository model (based on the Nagra SF/HLW repository concept) to simulate the long-term temperature, saturation, and pressure evolution without being noticeably affected by boundary conditions. In addition, the prescribed heat generation was based on the decay heat from a MOX and UO2 canister.

The TOUGH2 code for TH simulations was used, neglecting possible coupled mechanical effects. In a reference case simulation, the relevant thermo-hydraulic phenomena associated the resaturation of the bentonite buffer of a SF/HLW emplacement cavern and heat generation associated with the decay heat of the SF/HLW were examined. A series of sensitivity simulations were conducted to assess the impact of relevant parameters, which included: (a) thermal conductivity of the bentonite buffer (as a function of saturation), (b) permeability and capillary pressure of the bentonite (c) pore expansivity of the Opalinus Clay, and (d) permeability of the Opalinus Clay. The result were evaluated in terms of peak temperatures in the buffer and in the surrounding Opalinus Clay, and in terms of pore pressure build-up in the near field associated with the differential thermal expansion of the pore water relative to the rock framework (pores). The spatial and temporal evolution of the pressures, temperatures, and saturations were analysed to delineate the extent and duration where the buffer near the waste canister exceeds 100°C and the buffer was near full saturation.

GRS used a three-dimensional model for long-term TH simulation of the simplified repository model based on Nagra's repository concept, similar to TK Consult, but used CODE_BRIGHT instead of TOUGH2. Results of a first base case calculation were comparable to those of TK Consult, although there were minor differences in terms of maximum temperature and time to full saturation. Alternative cases were considered assuming a different initial saturation of the tunnel surface at emplacement time, since this is a major uncertainty in initial conditions. The effect, however, was less significant.

UDC performed numerical models for the long-term hydrochemical evolution of the bentonite barrier of a spent-fuel, carbon-steel canister repository in granite. The model accounts for canister corrosion, the chemical interactions of corrosion products and bentonite, mineral dissolution/precipitation, Fe^{2+} and H^+ surface complexation reactions on three types of sorption sites and cation exchange reactions of Ca^{2+}, Mg^{2+}, Na^+, K^+ and Fe^{2+}. The model considers the generation of $H_2(aq)$ which is allowed to diffuse through the bentonite. Sensitivity analyses were performed for: 1) The corrosion rate; 2) The effective diffusion coefficient, De, of the dissolved species in the bentonite; 3) The water flow through the granite at the bentonite/granite interface; 4) The cation selectivities and 5) The chemical compositions of the bentonite and granite porewater. Model results indicate that canister corrosion causes a marked increase in pH and the concentration of dissolved Fe^{2+} and a decrease in Eh. Most of the released Fe^{2+} diffuses from the canister into the bentonite where it precipitates mainly as magnetite and to a lesser extent as siderite. Fe^{2+} sorbs by surface complexation on weak sorption sites and undergoes cation exchange. Sorption plays a relevant role in the geochemical evolution of bentonite. The competition of Fe^{2+} and H^+ for the sorption sites near the canister/bentonite interface causes several sorption fronts which induce fronts on pH, Eh, the concentration of dissolved Fe^{2+} and mineral dissolution/precipitation. Model results lead to significantly high $H_2(g)$ pressures. The reduction of bentonite porosity due to mineral precipitation near the canister/bentonite interface could be large and result in the clogging of the bentonite pores. The main conclusions of the sensitivity analyses include: 1) The larger the corrosion rate, the larger the pH, the larger the concentration of precipitated magnetite near the canister/bentonite, the larger the zone where corrosion products precipitate and the larger the $H_2(g)$ partial pressure; 2) The De of bentonite affects the concentration of the dissolved Fe^{2+} and the precipitation of the corrosion products; 3) The computed concentrations of dissolved species, the sorption fronts and the concentrations of precipitated magnetite and siderite are very sensitive to the water flow in the granite; 4) The thickness of bentonite affected by pore clogging is sensitive to all the investigated parameters; 5) The cation selectivities affect mostly the concentration of exchanged cations. However, the computed pH, Eh and the concentrations of dissolved and precipitated species lack sensitivity to the selectivities; and 6) Model results are sensitive to the chemical compositions of the bentonite and granite porewaters. The general patterns of pH, Eh, H_2(g) pressure and magnetite precipitation, however, are similar to those of the reference run. The results of the long-term modelling are reported in Deliverable 3.5.3.

The thermal transient (accounting for the temperature effect on chemical reactions) produces a decrease in pH and silica dissolution/precipitation. Magnetite precipitation is almost similar to the isothermal case. Therefore, the thermal transient does not have a significant effect on the overall geochemical evolution of the EBS and does not affect the thickness of the altered bentonite. Model simulations performed by UDC indicate that the uncertainty in the effect of temperature on the corrosion rate does not have a large impact. Accounting for the dependence of the corrosion rate on the chemical conditions (pH, Eh, Fe concentration) leads to an important change in the patterns of pf the corrosion products. The thickness of the altered zone is doubled. The long-term effect of the kinetic dissolution of smectite on bentonite porosity and on the thickness of altered bentonite is small. A kinetically-controlled smectite dissolution rate leads to analcime precipitation. Model results indicate that this reaction is not relevant because only 0.2% of the smectite dissolves after 1 Ma. Model predictions are sensitive to the kinetic law of magnetite precipitation and to the reactive surface area used for magnetite. The thickness of the altered zone decreases when kinetics are considered.

UDC performed also long-term THCm simulations of the geochemical evolution of a repository in clay using an axisymmetric two-dimensional model. Magnetite precipitates near the canister. The thickness of the magnetite precipitation zone in the presence of the high pH plume is significantly smaller than that of a repository in granite. pH in the concrete increases due to portlandite dissolution and 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 near the bentonite-concrete interface. No pore clogging is predicted, although model predictions for the reduction of porosity contain large uncertainties. No major alterations of the bentonite are foreseen due to the interactions with concrete. Most of the chemical reactions, dissolution/precipitation of mineral phases occur in the concrete. Model results indicate that smectite dissolution in the presence of a concrete liner in a repository in clay is about 4 times more relevant than in the case of the repository in granite. The long-term effect of the kinetic dissolution of smectite on bentonite porosity and the thickness of altered bentonite is small. The hyperalkaline plume from the concrete only extends to a distance of 0.7 m in the host clay rock after 1 Ma.

Clay Technology performed a literature study on thermo-mechanical continuum theory of mixtures in order to approach long-term evolution from a different point of view. In the Milestone M3.3-2 a description of and motivation for the study were given. The objective was to give an overview of “thermomechanically” based mixture theory and a relevant material model within the theory that is applicable for systems consisting of bentonite (montmorillonite), water and air. The work was reported as an addendum to Deliverable D3.5-4 on schedule.

One important conclusion in the report was that studies of the more general framework may give new perspectives of the theoretical foundation of “engineering” soil mechanics formulations and the concepts/quantities used therein. Assumptions used in the “engineering” formulations, not easily visible when looking from within the theory itself, become clear when having the more general mixture formulation as a reference. Studies of general theoretical frameworks and existing valid constitutive relations in mixture theory therefore very much enhance the understanding of our current numerical tools based on “engineering” formulations.

The work contains a new concept of non-associative immiscibility which gives a mixture with immiscibility on different levels. Using this concept, an attempt to schematically formulate a material model, suitable for representing compacted bentonite at different levels of saturation, is made. In this formulation, porosities belonging to different levels, which may be connected to different “scales”, are obtained.

Here follows a list of other conclusions:

- The chemical potential is a fundamental part of both classical and modern mixture theories.
- To allow for general and mechanism-based models, jump conditions (discontinuities in fields) should be possible.
- Miscible and immiscible formulations are possible. Immiscibility leads to adopting a material structure represented by volume fractions (porosity, degree of saturation).
- Pore pressures defined for fluid phases are generally not ”physical” pressures, they are scaled chemical potentials.
- ”Capillary pressure” (suction) is difference of scaled chemical potentials.
- Darcy’s law and Fick’s law are obtained from reducing linear momentum of the phase or constituent, respectively. Chemical potential and temperature are the driving forces.

3.4. Work Package 4

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

1. Obtain an overview of the findings of WP2 and WP3.
2. 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 WP1.
3. It is expected that this will provide a
    a. more complete description of the thermo-hydro-mechanical-chemical evolution of the near field,
    b. a more quantitative basis for relating the evolutionary behaviour of the EBS to the safety functions of the system and
    c. a further clarification of the significance of residual uncertainties for long-term performance assessment.
4. Finally, the outcomes will be used to give some guidance regarding repository design, by clarifying the link between long-term safety criteria and design criteria of the EBS.

At the start of the project a review was concluded on how the transient phase is currently being treated in safety assessment based on recently completed safety cases or safety assessments in France, Switzerland, Sweden, Spain and Germany (see WP1). Remaining areas of uncertainty were identified for each and grouped along four cases.

- Case 1: Uncertainty in water uptake in buffer (T< 100°C).
- Case 2: Uncertainty in temperature evolution and impacts on the buffer (T >100°C).
- Case 3: Uncertainty in hydraulic-mechanical evolution of buffer.
- Case 4: Uncertainties in chemical evolution potentially resulting in property changes.

Each case was further developed. The current understanding was described, and extrapolation modelling (either numerical on conceptual) was performed to assess the impact of the phenomena specific for the case over the whole transient period up to the point where the safety functions are assumed to be in place for a specific disposal concept.

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 early stage of the repository evolution with a focus on the saturation processes. Once emplaced, the buffer takes up water from the surrounding bedrock and starts swelling. 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 lower 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 saturation (double porosity, thermo-osmosis, Darcy threshold). Results, however, do not clearly permit identification of the processes actually relevant.

However, 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% 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 is to understand how the early stage transient of high temperatures and low degree of saturation affects subsequent long-term performance of bentonite after full saturation 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 allowed gaining insight in the expected evolutionary path of the buffer during and after the initial transient and allowed 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 can be 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. A decrease in plasticity of bentonite and a slight decrease in hydraulic conductivity and swelling pressure while at full saturation 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 the formation of some Fe-silicate alteration products at the inner surface of the 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 > ~ 125°C.

In **Case 3** the focus is on the hydro-mechanical evolution of the EBS and the remaining uncertainties related to that. 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 (EB) experiments show that dense bentonite pellets evolve to a swelled material indistinguishable from swelled block material

from a hydro-mechanical perspective, while 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 and the effects of temperature on the mechanical properties.
Uncertainties in the description of the 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, 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 in PEBS (and other results) with respect to the implications of the geochemical evolution on the long-term performance and safety functions of the engineered barrier system (EBS). The major conclusions from the integrated analysis were the following. 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 THM behaviour of the barriers as a consequence was integrated in the assessment of the barrier performance for the various safety cases and disposal concepts.

It can be concluded that uncertainties for 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. Improvements are in the areas of evolution of materials properties and model development and testing. Existing in-situ experiments (FEBEX; HE-E; FE) may play an important role in further confirming bentonite behaviour over periods of 10-20 years.

3.5. Work Package B

Work Package B “China-Mock-up Test on Compacted Bentonite-Buffer” had the following overall objectives:

1. Investigation of the THM-C behaviour of the Gaomiaozi (GMZ) bentonite under relevant repository conditions,
2. Study of the bentonite-canister interaction,
3. Examination of possible displacement of a HLW container in the bentonite-buffer,
4. Provision of input data for future design of engineered barrier system.

The large scale China-Mock-up was built according to the preliminary concept of HLW repository in China, with the intention to study the THM-C behavior of GMZ bentonite under relevant repository conditions. The China-Mock-up is the first large-scale THMC coupled experiment in China, and its successful operation plays an important role, not in the investigation of the EBS behavior, but also in demonstrating the technical feasibility, and providing a reliable database for numerical modeling and further investigations.

The China-Mock-up was constructed as a vertical cylindrical tank of 900 mm internal diameter and 2,200 mm internal height, filled with compacted GMZ-bentonite with total dry density of 1,600 kg/m^3. A heater of 300 mm diameter and 1,600 mm length, which simulates the HLW canister, is placed inside the compacted bentonite blocks and pellets. The installed hydration system on the exterior surface simulates the supply of groundwater, which is sampled at the depth of 500 m at the Beishan site. More than 160 sensors have been installed within the experiment to measure the key parameters, including the temperature, pore pressure, relative humidity, water injection pressure and the total pressure.

The operational phase of the experiment started on 1st April 2011 and is continuing until today. Based on the recorded experimental data, several aspects could be observed and interpreted, including the THM behavior of the compacted bentonite, and the displacement of the electrical heater. The saturation process of the compacted bentonite is strongly influenced by the competing mechanisms of drying effects induced by the heater and the wetting effect by the water penetration. As a result, the desiccation-saturation process was observed in the zone close to the heater. An upward displacement of the heater was also noticed, which verified potential influence of buffer material on the stability of canister.

The work performed in Work Package B included also numerical modelling of the THM coupled processes in the China-Mock-up and other experiments using the code LAGMINE. The results suggest that the proposed model is able to reproduce the mechanical behaviour of the GMZ-Na bentonite, and to predict moisture motion under coupled THM conditions.

The main progress and achievements in WP B included:

- The China-mock-up operations are running very well and better than proposed. Most of the sensors run very fine and thus provide valuable data.
- 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.

4. Potential impact, dissemination activities & exploitation of results

4.1. Potential impact

Strengthening the scientific-technical basis for geological disposal

The near field of a geological repository consists of the conditioned waste or spent fuel, the engineered barrier system (EBS) and the excavation disturbed zone (EDZ) and therefore represents a complex sub-system of the geological repository. In the near field, numerous coupled thermo-hydromechanical and geochemical interactions take place among the waste forms, the different components of the EBS system and the host rock. The long-term barrier performance of the near field of a geological repository for HLW 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 were inadequate to reproduce the complexity of the spatial and temporal development. The PEBS project aimed at the assessment of 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.

The 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

Previous and ongoing national and European research programmes have led to the detailed understanding of waste package alteration processes as well as of individual processes taking place in the near field (e.g. the projects GLASTAB, CORALUS, SFS and CONTAINER CORROSION in the 5th Framework Programme (FP), and the NF-PRO project in the 6th FP). Furthermore, the EC supports a large number of projects studying near field processes by in-situ testing in URLs (SELFRAC, BAMBUS, FEBEX, PROTOTYPE, and the Mont Terri experiments EB, VE, HE). In the field of PA, the BENIPA project was dedicated to evaluate the treatment of bentonite barriers in Integrated Performance Assessment. The expertise on the individual processes in the EBS is spread out over different organisations within the EU and abroad, including waste management agencies, R&D organisations, regulatory bodies and universities. The knowledge base is also obtained by different scientific approaches (e.g. experimental studies, process modelling, and safety and performance assessment).

At the beginning of the PEBS project in the 7th FP the main challenges included the integration of knowledge on the individual near field components, the active processes and their couplings. Progress in this domain could only be achieved by studying key processes and evolution scenarios for the near field subsystems in an integrated and multidisciplinary way.

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

- the creation of high-quality research teams performing cutting-edge research in thematic priority areas on the various subsystems and subsystem interface areas;
- 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 under-ground 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 contributes to these policy objectives, as its prime target is 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 and 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 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.

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

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 system behaviour of the near field. This underscores the strategic impact of the project PEBS which:

- integrated research in the EU on the near field 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 co-operation 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 near field will therefore contribute to the acceptance of geological disposal facilities and may also increase acceptance of nuclear power as an essential component of the energy mix within the EU.

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 thus 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.

4.2. Exploitation of results and dissemination activities

The outcomes of the PEBS project are of high relevance to the national repository development programmes in the EU Member States, China and Japan. The project consortium consists of research organisations as well as implementing organisations/radioactive waste management agencies. Within PEBS, the implementing organisations were playing a key role in defining RTD priorities. This ensured that the results generated by PEBS are of

- direct relevance to their waste management programmes and are

- exploited at the national level.

The PEBS project is structured in several Work Packages, one of which is specifically dedicated to dissemination, exploitation and training. A strategy regarding the exploitation and the dissemination of the use of project results was implemented as follows:

1. Information of stakeholders, researchers and the interested public via
    a. project website,
    b. dissemination of all public deliverables,
    c. biannual PEBS Newsletter.
2. Presentation and discussion of interim and final results during
    a. two workshops for representatives of regulatory authorities,
    b. the projects meetings with the members of the High Level Expert Committee,
    c. the “International Conference on the Performance of Engineered Barriers” – the final workshop of the PEBS project.
3. Organisation of a Bentonite Training course with a laboratory workshop and an excursion to a bentonite mine and production facility.
4. Presentation of results at international conferences.
5. Publications of results in international journals.

In addition to the above mentioned dissemination activities, several workshops were organized to present and discuss interim and final results of the PEBS project to various target groups:

1. First Regulatory Workshop – a closed workshop for representatives from the regulatory authorities.
2. Bentonite Training – a workshop at BGR’s laboratories and excursion to a bentonite mine and production facility.
3. Second Regulatory Workshop – a closed workshop for representatives from the regulatory authorities.
4. International Conference on the Performance of Engineered Barriers – the final workshop of the project. Used to present the final results of PEBS with the scientific community, put the outcomes into the context through presentations from other research projects and to discuss future activities.

4.3. Project website

The PEBS website is the central tool for the dissemination of general information on the project and announcements of latest news and upcoming events. It was especially used for all announcements and organisational issues related to the International Conference on the Performances of Engineered Barriers – the final workshop of the PEBS project. Furthermore, the project website is the platform for dissemination of the public reports. All completed public deliverables are available for download on the PEBS website.

www.pebs-eu.de