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Long-term Performance of Engineered Barrier Systems PEBS

Definition of cases/scenarios to be studied

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PEBS



Preface

The main aim of the project PEBS (Long-term Performance of the Engineered Barrier System) is to evaluate the sealing and barrier performance of the EBS with time. The focus is to study the processes in the early evolution of the repository system and to evaluate the impact of the processes on the long-term safety functions. The final objective of the project is to improve the treatment of the early transients in long-term safety assessments for HLW/Spent fuel.

The report defines a number of cases or “scenarios” that will be assessed further within the PEBS project.

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 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

These processes will be the main topic for further assessments within the project. The details in the cases will be discussed further within the project.

This version of the report has been updated to cover comments from the HLEC.

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2 Definition of cases/scenarios to be studied

2.1 Introduction

2.1.1 Scope

In the previous sections the repository concepts from Sweden, France, Switzerland and Spain was presented. Despite the differences in repository concepts the safety functions defined for the engineered clay barriers are similar. This can be clearly seen by comparing **Fehler! Verweisquelle konnte nicht gefunden werden.** and **Fehler! Verweisquelle konnte nicht gefunden werden.** where safety function indicators for the buffer the Swedish and the Swiss concepts are documented. 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 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 are:

- Water uptake in clay components of the EBS
- Mechanical evolution
- Alteration of the hydro-mechanical properties

These will be discussed further in the next sections.

2.1.2 Out of scope

The PEBS project is focussed on the performance of a bentonite buffer or a bentonite seal in a repository for heat emitting waste. This is generally the component that is exposed to the strongest thermal and hydraulic gradients in the early repository evolution. The mechanical and chemical processes in the early phase are also of prime importance for the long-term performance of the repository.

A number of considerations and processes regarding the EBS are therefore not treated within PEBS, for example:

- Canister processes, such as corrosion and mechanical behaviour, are generally not studied within the scope of PEBS, since they are normally not regarded as “early evolution”. Reactions between corrosion products and the buffer are however treated, since they may have an impact on buffer performance.
- PEBS focuses on the “early evolution”, thus processes involving radionuclide transport are not considered. Furthermore, the processes that are unique to conditions of a a failed waste canister are not considered. No comparisons between concepts and components from different concepts are done within PEBS. It is up to the national program to justify their selections of repository systems.

2.2 Water uptake in clay components of the EBS

2.2.1 Overview

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.

2.2.2 Process description

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.

2.2.3 Uncertainties

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, being the predicted hydration rates 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 is generally deemed less important, at least in the FEBEX context.

2.3 Mechanical evolution

2.3.1 Overview

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 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.

2.3.2 Process description

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.

In a deposition position, 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 relative 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. This 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).

2.3.3 Uncertainties

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 are mainly the material models, which are very complicated, and the parameter values. Although they 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 unfavorable mechanical action.

For the seals and the clay 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.

2.4 Alteration of the hydro-mechanical properties

2.4.1 Overview

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.

2.4.2 Process description

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
- 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.

2.4.3 Uncertainties

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 Cases to be studied in PEBS

The product of WP1 was a list of cases related to the early evolution of the EBS that should be an integration of the entire study.

Cases (defined for this document): based on the description of the early evolution of the EBS in the disposal concepts studied and their respective safety assessment methodologies, cases need to be identified. A case can be 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 (eg by identifying case variants) and:

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

This is 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.

The term “cases” as it is used here is thus not identical to “cases” or “scenarios” as part of a formal safety assessment, but the meaning is similar in that it describes a system evolution making assumptions with respect to certain aspects (parameters or processes) of the system.

WP1 proposed that the cases be based on the topics 2.2-2.4, thus the main processes related to the evolution of the EBS, including the associated uncertainties, should be captured, i.e.

- Water uptake in clay components of the EBS
- Mechanical evolution
- Alteration of the hydro-mechanical properties

It should also be ensured that the cases:

- Are of general interest
- Are related to studies performed within the project
- Use data and observations from the project
- Are possible to evaluate within the project

The cases were considered likely to be disposal concept specific and therefore a balance should be struck. A standard table that describes the cases should be used. An example is given in Table 1 for one of the cases “Discrepancy in water saturation of the buffer”.

Table 1 Standard table for the cases. “Discrepancy in water saturation process of buffer” given as an potential example of a “case”

Title	Discrepancy in water saturation process of buffer
Description	
Reference disposal concept	Concepts based on bentonite as an engineered barrier
Processes involved/boundary conditions assumed	Temperature profile (eg as calculated for Nagra’s case) Permeability of the hostrock (eg Opalinus clay) The initial state of the material (eg Febex/Mx-80)
Potential impact of safety functions	Defines the initial state
Treatment in SA up to now	”standard THM model”
Potential relevant information from WP2/WP3	WP2: HE-E experiment, lab tests WP3: Prediction/Validation modelling of HE-E
Other potential relevant information outside PEBS	FEBEX mock-up and in situ test SKB experiments
Feasibility of making progress within PEBS	Will this information allow for improvement of the current understanding?

Based on the outlined approach, WP4 proposed a specific set of cases that was agreed upon after discussion with Work Package leaders. The cases are outlined in Table 8.

Table 8 Cases related to early evolution of the EBS to be used as a basis for integration of project findings in WP4

Case Number	Case description	Origin of the Case (from WP1)	PEBS activities feeding into case assessment
Case 1	Uncertainty in water uptake in buffer (T< 100°C)	Discrepancies between standard THM model and FEBEX observations	1. Modelling by Clay Technology 2. FEBEX mock-up data and modelling 3. THM Column Tests at

			Ciemat 4. EB experiment 5. FEBEX in situ test and modelling
Case 2	Uncertainty in T evolution in buffer (T >100°C)	Lack of validation of TH model for high temperature and low saturation rate	1. HE-E experiment and modelling
Case 3	Uncertainty in HM evolution of buffer	Lack of large-scale experiments	1. EB experiment and modelling 2. HE-E experiment and modelling 3. Febex mock-up and in situ 4. Stress-strain behaviour studies
Case 4	Uncertainties in geochemical evolution	Experiments vs. models of corrosion product/bentonite and cement/bentonite interactions	1. GAME experiments and modelling 2. Interface studies (WP2.3) 3. Modelling in WP3.4

The proposed group of cases serves as the basis for integrating the knowledge gained from PEBS experimental and modelling studies and should serve as an input to the analysis of impact on long-term safety and guidance for repository design and construction that will be performed in WP 4.