D7.8 BEACON
Bentonite Mechanical Evolution

# Full project report that includes the synthesis report from the WP1-6

DELIVERABLE D7.8
Report

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# 1 Introduction

The current report forms a very brief summary of the activities that have been performed within the Beacon project. All details can be found in the individual deliverables from the different work packages.

# 2 Mechanical evolution of bentonite barriers

The sealing ability is a principle safety function for bentonite-based barriers in all geological repository concepts. Sealing is achieved by the combination of a high swelling potential and a low hydraulic conductivity. The swelling potential will ensure self-sealing, but may mechanically impact the other barriers in the repository as well. The low hydraulic conductivity ensures that transport of dissolved species by advection will be very limited. Swelling pressure and hydraulic conductivity can normally be expressed as a function of dry densities of the bentonite materials. The required quantitative values thereof strongly depend on the repository concept and the environment.

The barriers are installed as blocks, pellets, and/ or granules depending on the overall repository concept and the required density. Despite the precautions taken when installing these materials, technological voids may occur and dry density variations may be observed in the structure. Therefore, bentonite barrier needs to be conceptualized such that these technical voids can be compensated for by the swelling of the bentonite and that density variations after hydration are minimized or in the range of the expectations.

Despite the high swelling potential of bentonite, full homogenization between the installed components is never expected to be reached. The key question is: "is the homogenization sufficient to reach the targets for the safety functions after saturation?" If the answer is yes, then the barrier can be assumed to have its assigned properties in the safety case. If the answer is no, then the effect of a heterogenous barrier needs to be considered (e.g. advection in the barrier) and/or the design and installation of the barrier components needs to be improved.

This makes it necessary to have predictive models that can describe the evolution of the properties of the bentonite barriers from "the installed state" to a "saturated state". The input to the models should be the design specification, including uncertainties, and the site properties, also including uncertainties. In this aspect uncertainties include variability and tolerances. The output should be the final state of the barrier, preferably expressed in distribution of dry density and evolution of stresses. The results from the models can then be compared with the indicators/targets for the safety functions to check whether they are fulfilled. The key parameter to check is the dry density, which has a direct relation to the swelling pressure and the hydraulic conductivity.

<u>The overall objective of the Beacon project has been to develop, test and improve models that are able to predict the mechanical evolution of installed bentonite components. Their application is both to support the handling of the barriers in the safety case and to give feedback to the design and the engineering of the barrier components.</u>

# 3 Beacon

The scientific-technical work in Beacon was structured in five work packages, WP1-5, dissemination is handled in two work packages, WP6-7, training in WP7 while coordination and project management is covered in WP8. The interconnections between the work packages are illustrated in
Figure 1.

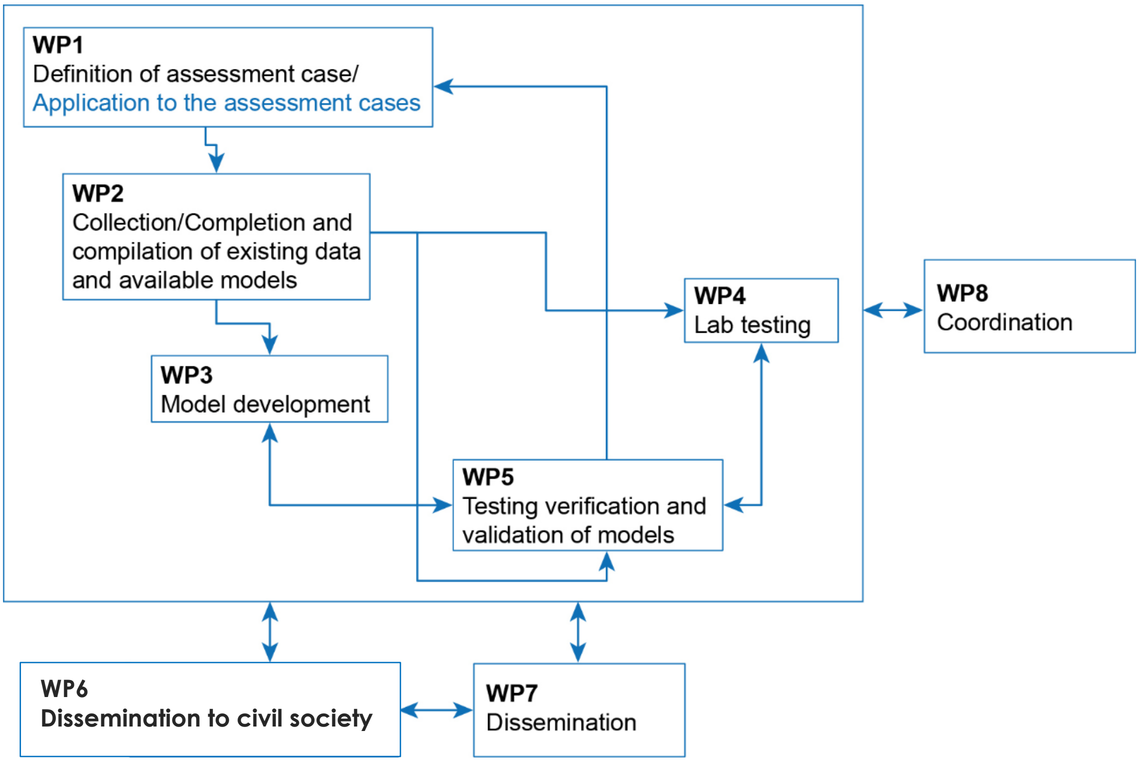


***Figure 1 Interconnections between the work packages in Beacon.***

WP1 dealt with the application of the results from the project in safety case and design. The purpose of WP2 was to collate and share knowledge on the available information about bentonite mechanical evolution. WP3 handled development of models. The objective of WP4 was do provide experimental data and observations to support model development and testing. The core activities of Beacon were however performed in the WP5 where numerical models describing the mechanical evolution of bentonite barriers were tested, verified, validated and finally applied in relevant assessment cases. The originality of work performed in this work package is to propose test cases in which heterogeneities in the bentonite-based component are present initially or to revisit large scale experiments in the perspective to follow heterogeneities evolution and the capacity of the model to predict the final state.

At the onset of the Beacon project, there were very few examples of the application of mechanical models of bentonite in a safety case. Many teams had the mechanical formulations included in their THM-codes, but the level of testing and verification of those formulations was, in general, rather limited.

## 3.1 WP1

In the framework of WP1, the needs of safety assessment regarding the evaluation of non-homogeneous backfill properties was addressed, in particular to what extent nonhomogeneous material property distributions comply with safety requirements. The outcome of this work package was a (hydro)-mechanical assessment of the case studies, given a range of uncertainties in the boundary conditions based on empirical and numerical evidence, that would, ultimately, result in a set of requirements under consideration of the host rock and the repository design. The results from WP1 is collected in deliverable D1.3. The purpose of that deliverable was to utilize all results produced in Beacon in the context of a safety case.

The key questions that should be answered were:

1. What is the probable final heterogeneity in a bentonite barrier?
2. How well can we predict this heterogeneity?
3. What are the main uncertainties regarding this prediction?
4. Will the heterogenous barrier still fulfil its assigned safety functions with acceptable margins?

The questions are discussed in detail in D1.3. There will always be a remaining heterogeneity in a bentonite barrier after full saturation. The swelling tends to decrease the inhomogeneities in the installed system, but there are examples of systems were the heterogeneity actually increases (e.g. FEBEX). The predictive capability of the final state of a barrier in well understood systems is good among the teams involved in Beacon and this capability has also increased significantly during the course of the project. The stress transients are more challenging to predict. These may however be of less concern in an actual assessment case. There are still uncertainties that will affect the results in the simulations. These are related to:

- external factors that could impact the processes of homogenization, like temperature, rate of hydration and water alimentation.
- initial boundary conditions, like geometrical configurations of installed components and material properties.
- Conceptualization of processes and phenomena, like wall friction and porosity concepts.

The assessment of whether a heterogenous barrier still would fulfil its assigned safety functions with acceptable margins was not included within the scope of Beacon. This issue needs to be handled by each national program separately.

In the framework of WP1, the needs of safety assessment regarding the evaluation of nonhomogeneous backfill properties were addressed, in particular to what extent non-homogeneous material property distributions comply with safety requirements. For this work package, three case studies were defined:

- the Andra tunnel plug
- the Nagra disposal cell
- the KBS-3 deposition tunnel backfill

Based on the outcome of the assessment cases and the evaluation method and uncertainties, the end-user may formulate design-specific requirements that can be used for a safety case or a design evaluation.

The modelling of the assessment cases proved to be rather challenging. All teams managed to produce results for the cases that they had selected. There were however rather large differences in the predicted final dry density of the barriers. It was common for all three cases. Despite the spread in results, most simulations indicated that the final dry density of the barriers would fulfil the safety functions assigned by the national programs. The assessment cases that were modelled in Beacon were selected already in the proposal for the project. At that time, it was not clear how much work that would be needed to handle these cases. In hindsight, it is clear that the number and complexity of the modelling tasks in Beacon, including the benchmarks in WP5, were over-ambitious. The modelling teams have been able to produce results for all tasks, but not enough time has been assigned to the evaluation and interpretation of the results. This is especially true for the assessment cases. The Covid-19 situation also made it impossible for the teams to meet in person to discuss the issues and the results from the assessment cases which significantly contributed to this experience.

## 3.2 WP2

The first activity in Beacon was an open workshop that was held in Kaunas, Lithuania, June 19-20, 2017. One main purpose of the Workshop was to kick start Beacon work package 2 – Collection and compilation of existing data and available models. The objective was to present and discuss the current state-of-art regarding the mechanical evolution of bentonite barriers, the information available from national and international projects at the beginning of the Beacon project which are relevant for the exploration of the role of heterogeneities in bentonite components on long term performance assessment. Another aim of the Beacon Initial Workshop was to establish a network of specialists in support of the project, and further to initiate a process leading to successful dissemination of the results.

At the beginning of the Beacon project information available about mechanical processes in bentonite was collected in deliverable D2.2. The deliverable documents the information that has been made available to the Beacon project by the project partners and associated organisations. The information related to experiments at a variety of scales and also modelling studies that have been undertaken. It was outside the scope of this deliverable to conduct a detailed comparison of modelling approaches. However, some brief discussions of modelling approaches were provided. This deliverable used information supplied by Beacon partners on experiments that have been carried out in previous projects to build a database of experiments which can be used during the Beacon project and beyond. The deliverable documented the available data but, as agreed with Beacon partners who attended the WP2 workshop held in London on 23rd and 24th October 2017, the deliverable did not attempt to propose any experiments for consideration within the Beacon project. This was left to the Work Package leaders to undertake, based on the information contained in the deliverable. This deliverable provided a summary information on a range of experiments, as well as clear referencing to the underlying reports which contain further information, to facilitate the process of selecting datasets for modelling within Beacon.

The purpose of deliverable D2.3 was to summarise the knowledge gained since the publication of Beacon Deliverable 2.2. Deliverable 2.2 presented a summary of the current conceptual understanding and available mathematical models of bentonite mechanics at the start of the Beacon project. It also provided a compilation of available information on bentonite mechanical evolution in the form of a database of known experiments. The experiments cover a range of scales from small-scale laboratory experiments, large-scale mockup laboratory experiments, and full-scale field experiments. The database contains information on the type of bentonite considered in the experiments, the boundary conditions and heterogeneities within the experiments and also the range of measurements taken in the experiment. Deliverable D2.3 provided an updated version of the database including experiments that have been undertaken during the Beacon project. Deliverable D2.3 supported Deliverable 1.3, the final assessment report, which aimed to address the extent to which evidence from the Beacon project can be used to support safety case claims and arguments about the contributions of bentonite components to providing safety. New experiments undertaken in Work Package 4 was summarised and added to the database that was initially developed for Deliverable 2.2. The updated database is captured in the deliverable and is available in a searchable webpage format, Database Bentonite Experiments – Beacon – Bentonite Mechanical Evolution (beacon-h2020.eu). The new experiments provide additional information on the mechanical evolution of bentonite with initial or introduced heterogeneity, including its gap filling capacity, the behaviour of dual-density systems such as bentonite blocks and pellets, and information about the bentonite micro and macrostructure. New experimental methods have been developed and employed to provide more detailed understanding of heterogeneity in bentonite samples.

## 3.3 WP3

Deliverable 3.3 contains the final account of the activities performed in Work Package 3 (WP3) during the project. It includes a summary description of the final state of the constitutive models developed in the project (conceptual bases, mathematical description and model capabilities) with particular attention to the improvements achieved during the project. The results of a verification exercise based on the modelling of a set of oedometer tests following two different stress paths are also presented. The deliverable shows that important and substantial advances have been achieved in the framework of BEACON's WP3 regarding the development and improvement of constitutive models and their implementation in computer codes. The models encompass a wide range of approaches and can deal with an extensive combination of simulation conditions. The models developed are able to reproduce what are considered to be key features of behaviour underlying homogenization processes such as stress path dependency, strain irreversibility, and others. As a result of this project, modelling capabilities in this area have been enhanced very significantly. The performance of the models when applied to the simulation of relevant problems is assessed in WP5.

In the context of these advances, several modelling teams have also identified areas of further constitutive model developments that are deemed necessary to improve simulation capabilities. In addition, outstanding uncertainties remain concerning the detailed knowledge of some of the individual phenomena: the underlying homogenization, the precise role of different components and parameters of specific models.

## 3.4 WP4

In the frame of WP4 of the Beacon project, eight experiment teams have performed laboratory tests involving different bentonite materials, different setups, and different hydraulic and mechanical boundary conditions. The results and conclusions of these experiments are presented in deliverable D4.3 of the project. It is the sequel and completion of deliverable D4.1 "Bentonite mechanical evolution – experimental work for the support of model development and validation" which documented the state of the experimental work after two years of Beacon. Deliverable D4.2 "Creep in bentonite – a natural analogue study" was issued in April 2020. It represents the final report on a self-contained part of WP4 that does not include new experimental work. Thus, D4.2 and D4.3 together represent the complete output of Beacon WP4.

The experiments performed in Beacon WP4 addressed:

- the influence of hydro-mechanical path and aggregate size distribution for several macroscopically homogeneous bentonite materials, such as MX-80 and BCV (Cerny vrch bentonite),
- the gap filling behaviour of swelling bentonite for numerous different configurations and conditions, involving MX-80, BaraKade bentonite, FEBEX bentonite, BCV, and Calcigel, with instant water contact or one-sided hydration, including hydration in the vapour phase,

- the hydration-induced homogenisation of different binary systems like block/pellet and pellet/powder as well as block/powder systems or systems of two blocks with different initial densities,
- and the shearing behaviour at a bentonite/steel interface.

With regard to bentonite homogenisation, the experimental results show that a completely homogeneous system will not be achieved in the short term after hydration, instead, it seems that once full saturation is reached the current status (in terms of dry density distribution) is kept. Although slow processes which are outside the laboratory observation scale may be possible, the results of the natural analogue study performed in the frame of Beacon give no hints in this direction. Consequently, the question of the persistence of inhomogeneities in the long term remains unresolved. In any case, bentonite barriers will have to be designed in a way that a sufficient degree of homogeneity will be achieved (or maintained) within the hydration phase, so that the bentonite barrier fulfils the assigned safety functions.

## 3.5 WP5

The work in Work Package 5 was divided into four tasks, each with a specific goal. The two first tasks were based on experimental information that was available prior to Beacon. Task 3 concerned an evaluation of prediction capacity of the models. This test case was built on experiments performed within Beacon and included a blind prediction of an experiment. The last task was dedicated to assessment cases. The test cases were proposed by waste management organizations (WMO) and were based on specific components taken from actual repository designs.

The first task was dedicated to calibration/validation of the models. For this purpose, three sets of laboratory tests were chosen. The choice was made based on the initial heterogeneity of the materials or the introduction of perturbations during the test to induce some heterogeneities. These tests were complementary and represent relevant situations encountered in a repository when installing an EBS. In this task the dispersion of results was rather large. This was especially true regarding the calculated stresses. For the final dry density in the test, the calculated values were in better agreement with the measured values. At this point, many teams were also rather inexperienced with this type of issues.

The second task dealt with large scale experiments. The objective of this task was to show the capacity of the models to reproduce in situ experiments. Three experiments were selected:

- EB - Engineered Barrier Emplacement Experiment (EB experiment),
- FEBEX - Full-scale Engineered Barrier Experiment in Crystalline Host Rock,
- CRT - Canister Retrieval Test (CRT)

Task 2 was much more difficult than the previous one due to complexity of the geometry, the uncertainties on the boundary and initial conditions and sometimes in the analysis of the information given by the sensors. Moreover, for two of the tests (CRT, FEBEX), it was necessary to consider the temperature and the couplings between the thermal part and the hydro-mechanical behaviour. Despite this, many teams managed to get a rather good estimate of the final state of the barrier in all three tests. One reason for this may be that the uncertainties in the initial conditions allow for more freedom in the setup of the models.

One of the main challenges in modelling swelling materials is the capacity of the models to perform predictive simulations. The presence of initial heterogeneities in these materials or heterogeneities due to external conditions increase the complexity of predicting the evolution of swelling clay materials. In the third task, tests performed within the Beacon project were simulated to evaluate the ability of the models to predict hydromechanical evolution of bentonite. Two tests were already finished at the beginning of the task. All the data available on these tests were given to the partners. The purpose was to have a first calibration step. For these tests, the bottom part of the cell was filled with bentonite pellets with an average dry density close to 1.30 g/cm³ and the top part with a bentonite block with a dry density of 1.60 g/cm³ (Figure 2). Hydration with deionized water took place through the bottom. In the first case, a constant pressure was imposed and in the second a constant flow was imposed. One test was selected for predictive modelling. The results of this test were not given to the participants. The conditions of the test were similar to the first test except that the pellets layer was located in the upper part of the cell and block in the lower part. Predictive simulations of water intake, dry densities, gravimetric water content and stresses were expected on this test case. The results from the predictions of dry densities as well as the experimental results can be found in Figure 3.

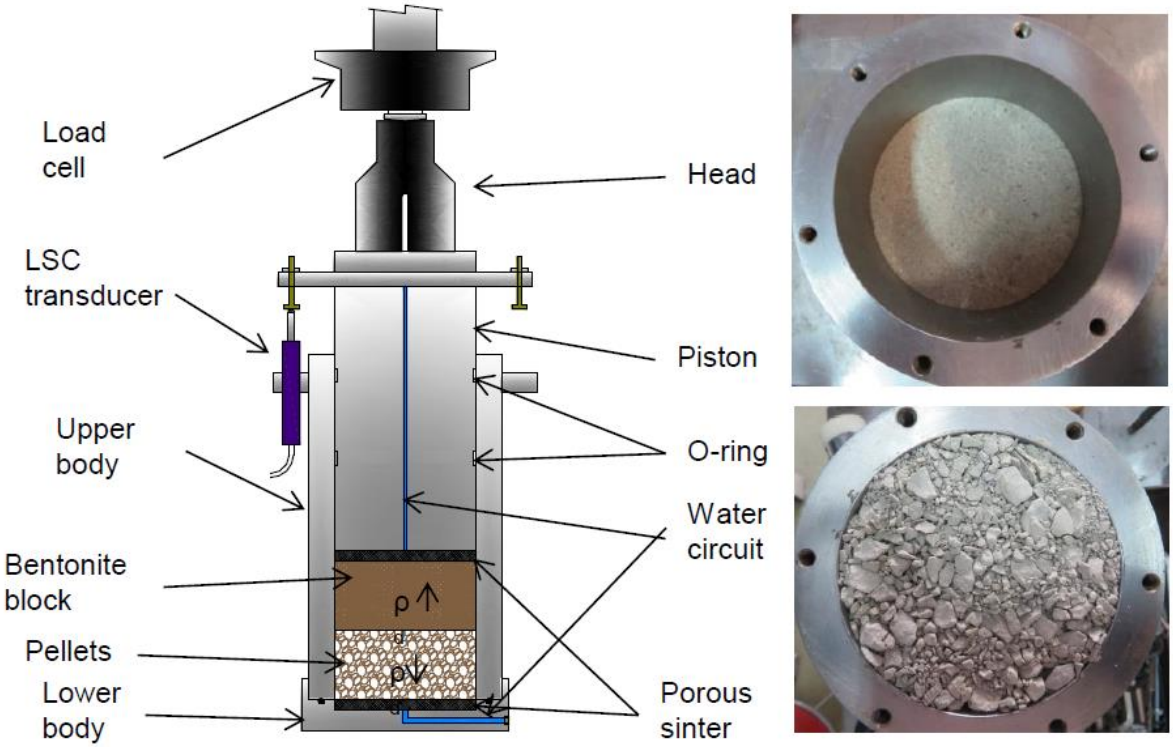


***Figure 2 Schematic representation of the test cell and images of the block (upper right) and pellets (lower right). In the predictive test the block was placed in the bottom of the cell (Villar et al 2021).***

The water intake with time seems well modelled by most teams. However, one may observe a number of variations or divergences. Moreover, prediction is less easy for early times of hydration. These globally good results may be surprising considering the very large range of permeability used in the simulations by the different teams. As seen in Figure 3, the final (at saturated state) dry densities are well reproduced. They do not depend significantly on the mechanical models (including law and friction aspects). It was very difficult to predict the stresses final value and time evolution. Stress evolution showed much variation between teams. Two teams modelled friction at the cell wall – bentonite interface. These teams managed to satisfactorily blind-predict the evolution of axial stress in the test.

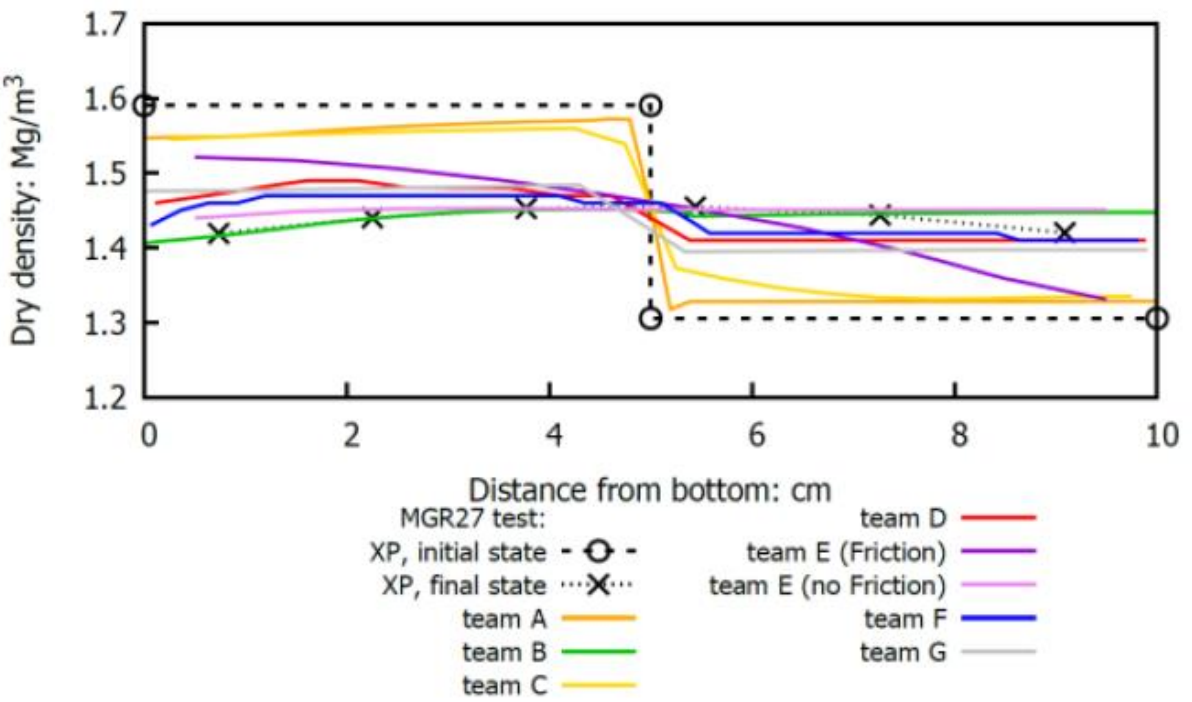


***Figure 3 Dry densities at saturation for the experiment used for predictive modelling.***

The last task of WP5 was focused on direct application of the models to real assessment cases in actual repository systems. A few cases from relevant repository systems were therefore selected as test examples. Three cases were proposed: 1) a tunnel plug based on the Andra design, 2) a disposal cell from the Nagra concept, 3) the KBS-3 deposition tunnel backfill. These are representative of the primary areas of uncertainty in density homogeneity. Here, the teams divided the cases and only 3-4 teams modelled each particular case. The results from the modelling showed a rather strong divergence in results for the final dry density distribution for all three cases. For the Andra and SKB cases, the calculated values were still within the range that would be acceptable for repository performance, but that was less true for the Nagra case. This shows that there are challenges to move from modelling of laboratory and field experiments, where results are available, to simulations of repository performance.

## 3.6 WP6

Deliverable D6.2 is a part of the WP6 effort for dissemination to civil society (CS) of the Beacon project. In the previous deliverable D6.1 "Scoping of the Beacon project, initial CS perspectives and enhanced work plan for years 2-4", an enhanced work plan for the work of WP 6 for the years 2-4 of the project was described. The work during the remainder of the project for the WP 6 CS experts in the project was to focus on the WP 5 subtasks and deliverables, and to provide a description of the work and results targeted at civil society. The other WP´s were also followed, but not in the same detail.

# 4 Training

Beneficiary no 9, UPC, organized a Training course (D7.5) in ·Hydromechanical behaviour of bentonite: constitutive and numerical modelling" early in the project (period 1). The course was held in Barcelona from 17 to 19 January 2018 and UPC contributed also to the lectures and organized the hands-on training session that ran over a full day. The rest of the lectures were given by personnel from SKB, EPFL, Université de Liège, Imperial College and Charles University. There was a total of 37 participants. The course was very successful; the venue had to be changed because of higher than expected demand from both within and outside the project.

# 5 Mobility of staff

Several exchanges between partners and incidents of mobility were foreseen in Beacon and some was possible to realise, but Covid-19 prevented some.

One exchange was planned and described in the proposal, between VTT and LEI, and it took place in March 2018. Asta Narkūnienė visited VTT during a week with an intensive schedule. The second visit of this exchange took place in August 12-16, 2019 in Lithuanian Energy Institute. 4 participants from LEI and one participant from VTT (Veli-Matti Pulkkanen) had a discussion on specialized topics. Two more staff exchanges were planned in 2020-2021 period, but the Covid -19 affected the possibilities of physical meetings. Considering the benefit of theses exchange, it was decided to proceed with remote mode. The third meeting was held in Teams platform in April 6, 8, 11, 13 2022. The fourth session is planned to be held in April 28-May 4, 2022 on Teams.

Jose Bosch Llufriu from EPFL also spent one week in the Université de Liège, from 19 to 23 of August 2019. Robert Charlier hosted him in their group to help with the implementation of EPFL´s model in their computer code Lagamine. Discussions took place between him and with Robert Charlier, Albert Argilaga (a post-doc in Liége) Liliana Gramegna and Prof. Frédéric Collin, which according to Jose Llufriu gave him very useful information about the code of Université de Liège. It was also a good opportunity to exchange views on the different approaches that these two Beacon partners use for modelling bentonite.

# 6 Project review

The Expert Advisory and Review Board (EARB) consisted of experts which were representatives of organisations from outside of the project, and is in charge to advise the Technical Coordinator, and the Executive Board and the commission with critical evaluation concerning research quality and significance of outputs.

The review documents were produced in conjunction with the initial workshop and all the annual project meetings. The documentation of the reviews can be found in deliverables D8-13 and Deliverables D8.8 – D8.11.

# 7 Summary

The Beacon project has made a significant contribution to improving knowledge on bentonite behaviour and the simulation of bentonite-based components for radioactive waste underground repository. While much of the project was devoted to modelling and model development, the implementation of experimental tests using novel techniques such as imaging provided important data to calibrate and feed the models specially to describe the coupling between micro and macro scales.

The development of a database integrating a description of experimental tests from the bibliography identified at the beginning of the project to establish the state of the art and information on the THM models used to represent the behaviour of bentonites has constituted one of the first tasks. The database is now available and updated with the results obtained during the project.

The modelling teams participating in Beacon have significantly improved the capabilities of their models through the test cases proposed and simulated along the project. As a result of these developments and improvements, 10 teams are now equipped with coupled THM models that reasonably represent the behavior of bentonite-based components in the context of an underground radioactive waste repository. Thanks to this, they were able to model test cases representative of the engineered barrier and sealing concepts proposed by SKB, Nagra and Andra in the final modelling stage. Teams are generally able to reproduce and predict the mechanical evolution of bentonite in small-scale and large in-situ experiments, particularly the final swelling pressures, dry densities and degrees of saturation of the bentonite. These are key safety indicators for bentonite used as a buffer or seal in geological disposal facilities for radioactive waste.
The progress made throughout the project are illustrated by the improved agreement between models and experiments. This is a consequence of model updates with the inclusion of friction, improved formulations of water retention curves, inclusion of thermal effects, and the development of numerical solvers. At the beginning of Beacon, there was very little experience on this type of issue, but thanks to the joint effort, there are now at least 10 teams in the European Community that can deal with the mechanical evolution of bentonite barriers.

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