D2.3 BEACON

Bentonite Mechanical Evolution

Identification of captured knowledge of bentonite mechanical evolution gained over the duration of the Beacon project

DELIVERABLE (D2.3)
Report

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Abstract

The Beacon (Bentonite mechanical evolution) project has studied the performance of inhomogeneous bentonite barriers in the context of disposal of high-level radioactive waste and spent fuel in geological repositories across Europe. A key aspect of the performance of bentonite barriers is how the bentonite evolves from its installed state to become a fully functioning long-term barrier. During the Beacon project, 15 new sets of experiments considering the mechanical behaviour of bentonite have been undertaken. In parallel with this work, 12 modelling teams have developed and tested different conceptual and numerical models of bentonite hydro-mechanical behaviour. The purpose of this report is to summarise the key learning from the experimental and modelling work undertaken during the Beacon project and how this work has contributed to reducing the uncertainties regarding bentonite mechanical behaviour.

This report summarises the knowledge gained since the publication of Beacon deliverable 2.2 (a review of the data and models on the mechanical properties of bentonite available at the start of Beacon) alongside an updated database of experimental data. The database has been designed and populated as a collaborative effort between the participants of the Beacon project and includes experiments undertaken during the project. 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. This will also be available in a webpage format to allow Beacon partners and the wider community to interrogate the database and find experiments of interest for furthering understanding of the mechanical behaviour of bentonite.

Content

1 Introduction

The Beacon (Bentonite mechanical evolution) project has studied the performance of inhomogeneous bentonite barriers in the context of disposal of high-level radioactive waste and spent fuel in geological repositories across Europe. A key aspect of the performance of bentonite barriers is how the bentonite evolves from its installed state to become a fully functioning long-term barrier.

In disposal concepts, there are likely to be initial inhomogeneities resulting from the bentonite form (e.g. use of bentonite pellets) and the presence of initial void spaces caused by the difficulty of precisely emplacing bentonite components, as well as heterogeneous boundary conditions. Heterogeneities may also arise in initially homogeneous systems due to the presence of heterogeneous boundary conditions, such as hydration. To have confidence in the ability of a bentonite buffer or seal to fulfil its intended safety functions, including acting as a barrier to advective transport and providing mechanical protection for other components, it is important to understand how the bentonite dry density distribution will evolve and whether any heterogeneity will affect performance. This includes understanding to what extent bentonite will be able to fill void spaces as it saturates and swells, and whether it will reach a sufficiently high density in those voids to avoid potential erosion in the presence of flowing features.

During the Beacon project, 15 sets of new experiments considering the mechanical behaviour of bentonite have been undertaken in Work Package (WP) 4. In parallel with this work, 12 modelling teams have developed (WP3) and tested (WP5) different conceptual and numerical models of bentonite hydro-mechanical behaviour. The purpose of this report is to summarise the key learning from the experimental and modelling work undertaken during the Beacon project and how this work has contributed to addressing some of the uncertainties regarding bentonite mechanical behaviour.

This report forms Deliverable 2.3 of WP2 of the Beacon project. The aim of WP2 is to collate and share knowledge on the available information about bentonite mechanical evolution. The purpose of this deliverable is to summarise the knowledge gained since the publication of Beacon Deliverable 2.2 (a review of the data and models on the mechanical properties of bentonite available at the start of Beacon). Deliverable 2.2 (Thatcher et al., 2017) 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. This report provides an updated version of the database including experiments that have been undertaken during the Beacon project.

The remainder of this report is structured as follows:

- Section 2 sets the context for the work by describing the safety-relevant functions commonly assigned to bentonite in a disposal system for high-level radioactive waste and spent fuel;
- Section 3 presents the captured knowledge from Work Packages 3, 4 and 5;
- Section 4 summarises the key learning points from the Beacon project and how the Beacon project has contributed to reducing uncertainties;
- Section 5 discusses knowledge gained from outside the Beacon project since 2017; and
- Section 6 presents some conclusions and suggestions for future work.

This report is based on contributions from all Beacon partners, who were asked to complete templates summarising their key findings from the Beacon project. Appendix A contains the completed templates from each Beacon partner.

Appendix B presents templates describing experiments relevant to understanding bentonite mechanical evolution, including new experiments that were not captured as part of Deliverable 2.2. Experiments undertaken during the Beacon project as part of WP4 are included in Appendix B.4. Appendix C presents the updated database of bentonite experiments, which has been populated with the experiments detailed in Appendix B. The database has been designed, populated and updated as a collaborative effort between the participants of the Beacon project. It will also be made available in a webpage format to allow Beacon partners and the wider community to interrogate the database and find experiments of interest for furthering understanding of bentonite mechanical behaviour.

This report will feed into Deliverable 1.3, the final assessment report, which aims 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.

2 Safety-relevant functions of bentonite

Bentonite is used as part of the Engineered Barrier System (EBS) in many geological disposal concepts for radioactive waste. However, the safety functions assigned to the bentonite may differ in different disposal concepts and will depend to some degree on the components in which bentonite is used. Examples considered in Beacon are a tunnel plug based on the Andra design, a disposal cell from the Nagra disposal concept and the KBS-3 deposition tunnel backfill.

A common feature of all of the proposed uses of bentonite is the assumption that bentonite swells, exerting a swelling pressure on the surrounding host rock and other components in contact with it. Depending on the disposal concept, this swelling pressure provides functions including mechanical stabilisation, prevention of significant extension of the Excavation Damaged Zone (EDZ), protection of the waste canister from displacements, and minimisation of microbial activity. The swelling pressure depends on factors including the dry density of the bentonite and the composition of both the bentonite and the groundwater. When the bentonite is installed in the repository, there are inevitably initial contrasts in dry density as a result of the practicalities of emplacement. Examples of initial dry density contrasts include the technological void surrounding the bentonite in Andra's tunnel plug, and the variations within the KBS-3 deposition tunnel backfill, which is composed of blocks surrounded by pellets. Dry density contrasts may also arise after emplacement, for example as a result of heterogeneous water inflow. One of the main objectives for the Beacon project was to build an understanding of how the dry density distribution might evolve during the post-closure phase, considering:

- Whether the bentonite will evolve towards a homogeneous distribution;
- Whether any remaining heterogeneity will affect performance; and
- Which factors affect the degree of homogenisation that is achieved.

Other safety-relevant properties of bentonite in different disposal concepts were considered in Work Package 1, Deliverable 1.1 (Wigger et al., 2017), and include:

- Low hydraulic conductivity for ensuring diffusive transport, limiting radionuclide release and also limiting transport of corroding substances;
- Permeability for gas transport without compromising the hydraulic barrier;
- Suitable heat conduction for transferring heat away from the wastes; and
- Stabilisation and mechanical protection of the waste container and other components.

Understanding the mechanical evolution of bentonite is therefore important for building confidence in safety cases. Uncertainty and variability in the thermo-hydro-mechanical properties of bentonite are only significant if they affect the safety functions of the bentonite. For example, it may be important to understand the expected timing and extent of self-sealing of voids for a bentonite barrier to provide a low-permeability diffusive barrier to transport and to avoid erosion of the bentonite. It is also important to understand the development of swelling pressures in the bentonite, within a given range; for example, the target swelling pressure in Posiva's bentonite backfill is greater than 1 MPa, whereas the swelling pressure for Andra's bentonite seals should be greater than 3-4 MPa (Wigger et al., 2017). If the bentonite is prepared and emplaced properly, it is not expected that heterogeneities will be problematic for safety cases.

To limit the scope of the Beacon project, not all potential safety functions of bentonite components are considered. The focus is on the mechanical evolution and coupled hydro-mechanical processes of bentonite components, rather than the interaction of bentonite with other components. Chemical processes are not considered, although the influence of chemistry (water salinity) on hydro-mechanical processes is considered to some extent. High temperatures (above 100°C), reactive transport and gas transport are also generally not considered within the project.

For safety cases, it is also important to build confidence in our understanding of bentonite behaviour and the capability of models to predict the mechanical evolution of bentonite. The rest of this report discusses knowledge gained during the Beacon project in respect to the safety-relevant mechanical properties of bentonite, and remaining uncertainties in the application of models to experiments.

3 Summary of captured knowledge from individual Work Packages

This Section summarises the key learning points from Beacon Work Packages 3 (Model Development), 4 (Experimental Work) and 5 (Testing, Verification and Validation of Models). Inputs have been provided by the Work Package leaders. Section 3.4 summarises and brings together the key learning points from all three work packages.

Throughout this report, the term 'granular bentonite' is used to refer to both bentonite pellets and granules, to differentiate them from compacted block bentonite.

3.1 WP3

3.1.1 Overview

The main goal of Work Package 3 was the development of improved constitutive models for the description of the mechanical, hydro-mechanical (HM) and, optionally, thermo-hydro-mechanical (THM) behaviour of bentonite-based materials with the aim of introducing them into numerical tools capable of analysing problems of engineering significance. In particular, the Beacon project was especially focused on the processes of homogenisation or, conversely, the development of heterogeneity throughout the initial transient hydration phase of engineered barriers and seals evolution. The proposed scope of potential developments is wide: saturated and unsaturated materials, isothermal and non-isothermal conditions and different types of bentonite components (e.g. compacted blocks, pellets-based granular bentonite). Nine research teams (specified in Section 3.1.2) have performed model development activities with support of four other organizations:

- Gesellschaft fuer Anlagen- und Reaktorsicherheit (GRS);
- Karlsruher Institut fuer Technologie (KIT INE);
- Posiva; and
- Teknologian tutkimuskeskus VTT (VTT).

The work in WP3 has included not only the development and improvement of constitutive models, but also tasks of model implementation into computer codes to be used in the solution of boundary value problems at different scales. Initially, a series of conceptual tests were proposed to identify the basic features of the constitutive models that were considered useful for the purpose of addressing homogenisation issues. Those capabilities were collected in an initial Table of Capabilities for each model (Gens, 2018). The same tables have been updated at the end of the project to provide a summary view of the developments (Gens, 2021).

In accordance with the project plan, a task was proposed (Task 3.3) for the verification of the basic features of the models against simple benchmarks. It involved a set of oedometric tests on compacted MX-80 bentonite performed and made available by Ecole Polytechnique Federale de Lausanne (EPFL). This task is discussed further in Section 3.1.3.

The state of the constitutive models at the start of the project has been reported in Deliverable 3.1 (Gens, 2018). Deliverable 3.2 (Gens, 2020) describes the developments carried out up to the half-point of the project (2 years). Deliverable 3.3 (Gens, 2021) contains the description of the final state of the constitutive models developed in the project (conceptual bases, mathematical description and model capabilities) as well as some assessment of their predictive power. The updated tables of model capabilities are included in Deliverable 3.2.

It is important to note that the development of the constitutive models for WP3 has been driven and influenced in large measure by their performance in the simulation of the benchmarks defined in WP5. Therefore, a proper understanding of the WP3 work can only be achieved by simultaneously considering the WP5 activities and results (Section 3.3).

3.1.2 Model developments

There has been a large number of constitutive model developments and improvements carried out by the different teams; they are not necessarily reflected in the updated Table of Capabilities where only large and substantial modifications are included. A brief summary of the main model developments and implementation work is as follows:

- Bundesanstalt fuer Geowissenschaften und Rohstoffe (BGR)
    - Development of a double structure model (hydraulic model);
    - Incorporation of the elasto-plastic Modified Cam-Clay model for mechanical behaviour allowing for irreversibility and stress path dependency; and
    - Incorporation of a newer simulation environment (OpenGeoSys6).
- Charles University – Czech Technical University (CU-CTU, CZ Consortium)
    - Calibration/verification/validation of a double structure hypoplastic model (hydraulic and mechanical);
    - Advanced water retention model with a smooth transition between saturated and unsaturated states;
    - Alternative formulation of the effective stress for the macrostructure and incorporation of suction dependence of the quasi-elastic stiffness; and
    - Development of finite element models using partially-coupled and fully-coupled algorithms.
- Clay Technology (ClayTech)
    - Development of the Hysteresis Based Material (HBM) model for general stress states and general degrees of saturation;
    - Incorporation of vapour transport;
    - Modification of the original version of HBM to represent granular bentonite; and
    - Implementation of HBM into COMSOL Multiphysics (ongoing).
- Ecole Polytechnique Federale de Lausanne (EPFL)
    - Development of a new constitutive model based on a hydro-mechanical coupling framework;
    - New water retention curve considering adsorbed and free water;

  - Modified loading collapse curve function of degree of saturation instead of suction; and
  - Implementation of the new model in the Lagamine computer code.
- Imperial College, London (ICL)
  - Double-porosity structure mechanical model (ICDSM);
  - Van Genuchten-type soil water retention (SWR) model;
  - Variable permeability model dependent on suction; and
  - Small numerical adjustments of the ICDSM model in the ICFEP computer code.
- Lithuanian Energy Institute (LEI)
  - Development of a hydro-mechanical model;
  - Coupling of the two-phase formulation with heat transfer;
  - Formulation of a nonlinear elastic hydro-mechanical model;
  - Van Genuchten water retention curve with void ratio-dependent air entry; and
  - Implementation of the models in COMSOL Multiphysics.
- Quintessa
  - Coupled hydro-mechanical Internal Limit Model (ILM);
  - Development of a friction boundary condition;
  - Inclusion of thermal dependency (vapour diffusion, thermal expansion, and temperature-dependent water retention); and
  - Implementation of the ILM in COMSOL Multiphysics (ongoing).
- Universitat Politècnica de Catalunya (UPC)
  - Hydraulic non-equilibrium between structural levels;
  - Separate micro and macro water retention curves as the microstructure may be unsaturated;
  - Incorporation of thermal effects, first stage (BExM-T); and
  - Implementation of the BExM-T in CODE_BRIGHT (ongoing).
- Université de Liège (ULg)
  - Development and calibration of an enhanced Barcelona Basic Model (BBM) (mechanical);
  - Examination of the dependence on degree of saturation and pressure of the elastic compressibility coefficient for suction changes;
  - Use of an interface element to simulate friction; and
  - Development of a new double structure hydromechanical model (Mohymar).

General comments on the developments reported are presented in a later section. It should be indicated that most modelling teams also propose additional improvements and developments for the immediate future, in the last 6 months of the Beacon project.

3.1.3 Task 3.3: verification

The verification of the basic features of the models has been based on a set of oedometric tests on compacted MX-80 bentonite performed and provided by EPFL (Appendix B4.7). The experiments followed two different stress paths (Figure 3-1): stress path 1 involved a saturation-induced swelling under a low applied stress followed by a load compression up to a large vertical stress (about 20 MPa); stress path 2 involved a swelling pressure test (saturation under isochoric conditions) followed by a load compression to the same large vertical stress. Mercury Intrusion Porosimetry (MIP) results have been supplied to provide information on the porosity structure of the bentonite at various stages of the tests.

Several significant features of behaviour could be noted that can be used as reference verification yardsticks:

a) Development of large swelling strains under low applied stresses;
b) Sharp yield point when loading after swelling;
c) Magnitude of swelling pressure;
d) Stress path dependency at the value of swelling pressure; and
e) Convergence of the compression lines at large applied vertical stresses.

These are illustrated in Figure 3-1. From the point of view of bentonite barriers and seals, features a), c) and d) are likely to be the most relevant.

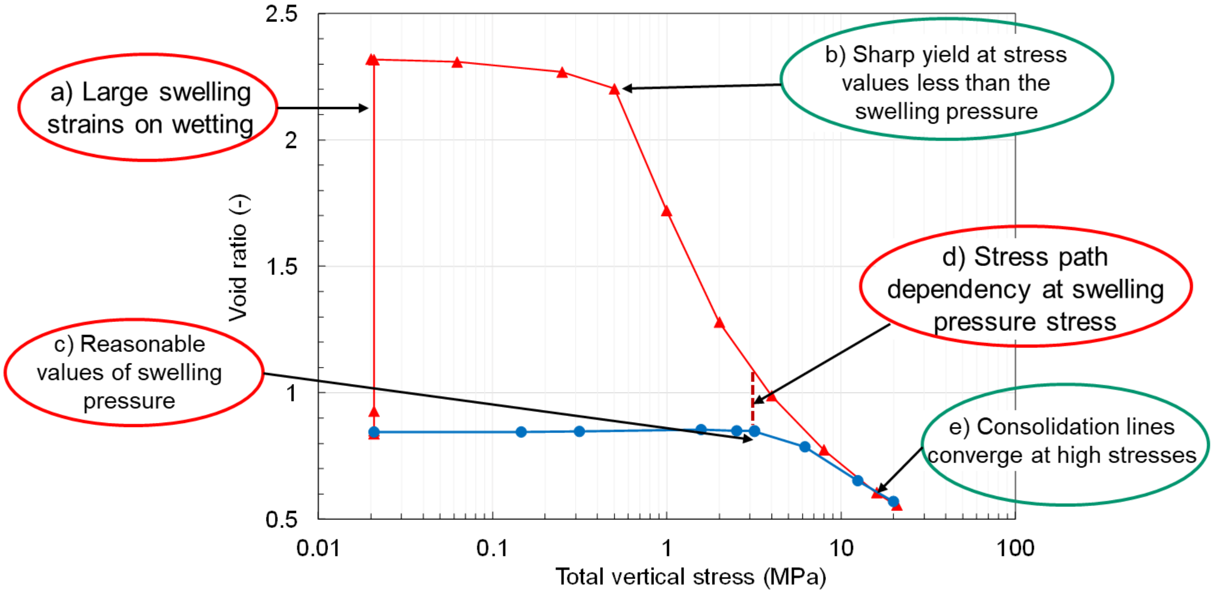


Figure 3-1: EPFL void ratio results for two different stress paths (stress path 1 in red, stress path 2 in blue), with features used to assess the models indicated.

All modelling teams have performed the analyses specified in this Task; some have considered the experiments as single-element tests and some have undertaken the analyses as boundary value problems. No apparent differences ensue from the two approaches.

In general, the modelling teams have achieved a quite satisfactory representation of the observed behaviour from a qualitative point of view. Quantitative comparisons are less pertinent as it was not a blind prediction exercise and there were no constraints in the selection of parameters. The rate of success in capturing the behaviour features listed above is generally high. Feature a): all 9 teams successful, feature b): 7 teams successful, feature c): all 9 teams successful, feature d): 7 teams successful, and feature e): 4 teams successful.

In spite of the fact that a number of double structure models have been used in the Task, only one team has endeavoured to compare model results with MIP observations. The results were consistent with observations.

3.1.4 General comments on model development, capabilities and performance

The developments and improvements to the models by the different modelling teams have been extensive and varied. There have been a variety of drivers, including widening the scope of applications, the desire to include fabric and microstructural considerations, the need to improve their performance when applied to the WP5 benchmarks and the requirement to move to non-isothermal problems. The extent of the modifications has depended strongly on the state of the model at the start of the projects; some teams have only needed to carry out minor modifications whereas other teams have had to develop a constitutive model starting from a very basic formulation. In spite of the wide range of model developments and improvements, specific to each modelling team, it is possible to derive some general observations.

As the updated Table of Capabilities illustrates (Deliverable 3.3), it can be stated that the models developed are able to reproduce behaviours such as stress path dependency and strain irreversibility that are considered to be the key features of behaviour underlying the homogenisation processes. This is confirmed by the mostly satisfactory performance of all of the models in the conceptual stress path modelling and in the reproduction of the Task 3.3 experiments.

Most models are developed within an elastoplastic framework. One model adopts a hypoplastic formulation and another one uses a swelling nonlinear elastic model. Two models (HBM and ILM) are based on a fundamental curve, experimentally determined.

Double structure models have become dominant in WP3 developments. Sometimes both hydraulic and mechanical models are based on a double structure formulation (4 teams) and, in other cases, only one of the components includes a double structure approach (4 teams). Those double structure developments try to incorporate in the model information on the fabric and microstructure of the material. However, it has not been demonstrated that the improved model results (if identified) compensate for the added complexity and the need to determine values for a larger number of parameters and initial conditions.

Most water retention curves are based on the Van Genuchten original expression or on a slightly modified form. Water retention hysteresis is largely ignored (only three teams incorporate it) whereas most teams (7) consider the dependence on void ratio.

Only three teams have developed a thermo-mechanical model that includes explicitly the effects of temperature on mechanical behaviour. It appears however that the simple inclusion of an overall thermal expansion of the material is sufficient to achieve satisfactory modelling results in non-isothermal problems at least up to the temperatures contemplated in the Beacon project. It is unknown whether the same conclusion applies to higher temperatures.

In spite of the prevalence of the double structure models, only one team has reported the predicted evolution of micro and macro void ratios and has compared it to experimental MIP results. Predictions appear to be rather consistent with observations. The criterion to distinguish between the two porosity levels remains an issue, though.

Although it has been proved that lateral friction has an important influence on some laboratory results, only three teams report explicitly the development of appropriate formulations for inclusion in the analyses.

The proper evaluation of the performance of the constitutive models developed in WP3 must be based on their applications to the proposed WP5 benchmarks. Those benchmarks also provide the information required to identify the learning points acquired from the modelling of experiments involving mechanical evolution and homogenisation of the bentonite.

3.1.5 Outstanding uncertainties and predictive power of the models

A source of uncertainty identified by practically all models is the scarcity of experimental data to determine all the parameters required by the constitutive models. This is especially apparent concerning the modelling of the pellets (granular bentonite); the situation for compacted bentonite is somewhat better. Against that observation, it must be admitted that the number of parameters in many of the models used in the project is very large. Another common remark is the lack of information on the repeatability and reliability of the experimental results in the proposed benchmarks that may underlie some of the modelling difficulties encountered by various teams.

A general observation is that the final state of the bentonite (in terms of swelling pressure and/or dry density distribution) is more robustly predicted than the transient behaviour; the comparison of the time variation of the various relevant parameters with experimental results is sometimes rather poor. This may be due to the inherent sensitivity of the transient phenomena to small changes in parameters and initial and boundary conditions but the difficulty in determining precisely the required parameters with available information may also play a role.

There is general agreement that there are still limitations in the fundamental knowledge of the basic processes underlying homogenisation and other related mechanical phenomena. In this respect, the performance of simple well-designed small-scale laboratory tests addressing individual relevant phenomena is likely to be the most efficient way to advance knowledge. Large field-scale tests, though useful to bring all the relevant phenomena together in a realistic setting, are less convenient for enhancing fundamental knowledge. Naturally, the relevant phenomena have to be selected based on the requirements of end-users.

The corresponding activity in terms of constitutive model development would be the performance of sensitivity analyses to establish unambiguously the role and effects of each parameter or group of parameters in relation to different basic behaviour features and phenomena. Because of the large number of cases that had to be modelled in the project (in order to increase the scope of the work), the sensitivity analyses performed have been very limited.

Another uncertainty involves the way of incorporating microstructural information in modelling and deciding in which circumstances it is advisable to resort to the unavoidable higher complexity of double structure models. In any case, experimental fabric determination should become a standard feature of laboratory testing. It is unclear at present whether the same model can be used for compacted bentonite and granular bentonite by simply changing the parameters. It is likely, however, that the variation of hydraulic parameters is quite sensitive to the evolution of fabric that is bound to be quite different in the two types of materials.

The consideration in the models of thermal effects on the mechanical behaviour of compacted and granular bentonite is also limited at present, beyond the consideration of a simple thermal expansion coefficient. It appears that this has been sufficient for successful modelling of non-isothermal problems so far but may not be sufficient when moving to higher temperatures. Finally, it is imperative that friction is introduced in the simulation and interpretation of at least some laboratory experiments.

There have been no predictive exercises performed within WP3; the results of Task 3.3 were known to the modelling teams. Therefore, there are no objective bases to evaluate the predictive power of the different models within the WP. In WP5, however, there has been a prediction exercise in Step 3 involving calibration tests quite similar to the experiment selected for blind prediction. Some teams have also reported good quantitative predictions of large-scale tests where many of the parameters have been determined independently from laboratory tests. Although they are not strictly predictive tasks, they provide further confidence in the potential of the models. Overall, it is undoubted that the predictive power of the models developed has increased significantly as a result of the project. However, more efforts are still required to achieve a wider evidence-based assessment of the predictive capabilities of the models and their range of applicability.

3.1.6 Concluding remarks

Important and substantial advances have been performed 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 the key features of behaviour underlying the homogenisation processes such as stress path dependency, strain irreversibility, and others. 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 constitutive model development that are deemed necessary to improve simulation capabilities. In addition, outstanding uncertainties remain concerning the detailed knowledge of some of the individual phenomena underlying homogenisation, the precise role of the different components and parameters of specific models and the actual predictive power of the formulations developed in the project.

3.2 WP4

3.2.1 Overview

The objectives of the experimental work performed in Beacon Work Package 4 were to provide input data and parameters for development and validation of models describing bentonite hydro-mechanical behaviour and to reduce uncertainties about conditions and phenomena influencing bentonite homogenisation. The Beacon partners devised and carried out a wide range of experiments to provide the data needed. The partners involved were:

- British Geological Survey (BGS);
- Commisariat a l'Énergie Atomique et aux Energies alternatives (CEA);
- CIEMAT;
- Ceske Vysoke Uceni Technicke v Praze (CTU);
- Univerzita Karlova v Praze (CU);
- EPFL;
- Jyväskylän Yliopisto (JYU);
- KIT; and
- GRS.

The experiments addressed:

- The influence of hydro-mechanical path and aggregate size distribution for several macroscopically homogeneous bentonite materials,
- The gap filling behaviour of swelling bentonite for numerous different configurations and conditions,
- The hydration-induced homogenisation of different binary systems like block/pellet and block/powder systems, or systems of two blocks with different initial densities; and
- The shearing behaviour at a bentonite/steel interface.

The detailed results and conclusions are given in the respective sections of Deliverable D4.3 (Bernachy-Barbe et al., 2021).

The purpose of this Section is to sum up overall conclusions from the combined results and to identify open questions or issues that need additional in-depth consideration.

3.2.2 Macroscopically homogeneous bentonite

The influence of aggregate size distribution on swelling behaviour was explored by EPFL. At free swelling, EPFL found a higher volume increase for unifractional samples (MX-80 of 1-2 mm aggregate size) than for bi-fractional samples (where 20% aggregates of 0.08-1.25 mm were added) which started with a higher dry density. The resulting porosity difference was mainly attributed to macroporosity (see Section 3.2.5). The result is in line with gap filling phenomena observed (see Section 3.2.3). The effect was not observed for confined samples.

EPFL also tested hydro-mechanical path dependence (see Section 3.1.3). EPFL used granular MX-80 bentonite with a Fuller-type aggregate size distribution[1] to (a) hydrate under constant low stress (nearly free swelling) with subsequent stress increase, or (b) hydrate under constant volume conditions with subsequent stress increase to the same value as in (a). Despite having the same degree of saturation afterwards and being subjected to the same final value of

[1] $U_i = 100 \times (i/D_{max})^n$ where i is the diameter of aggregate in each size group, U_i is the cumulative percentage of aggregate smaller than i, D_{max} is the maximum diameter of aggregate, n is the Fuller exponential (0.33-0.5).

vertical stress, a difference in void ratio of 0.13 (15% of initial void ratio) between the two samples was obtained. This path dependence was also confirmed by CTU using pellet and powder materials (Cerny vrch bentonite). While having comparable microporosities, the difference is in the macroporosity of the samples undergoing different paths (see Section 3.2.5).

Samples of different initial void ratios saturated under different stress tend, however, to arrive at similar states after cycles involving high compressive load, as shown by CU for compacted bentonite and by CTU for pellets and powder (both using Cerny vrch bentonite).

Constant load swelling tests of CU with variable dry density (Cerny vrch bentonite, homogeneous material of 1.27, 1.6 and 1.9 g/cm^3), hydraulic path and confining conditions showed that the water retention behaviour was not significantly influenced by the initial dry density for bentonite blocks of different densities (Figure 3-2). The final void ratio of saturated samples under the same load was independent of the initial compaction.

Stress evolution in an instantaneously flooded unifractional pellet cluster (pillow-shaped MX-80 pellets of 16-17 by 8 mm) of GRS was rather complicated and not monotonic (compare Section 3.2.4). Both GRS and CTU observed that the initial stress in pellet clusters at low density may collapse when water is introduced.

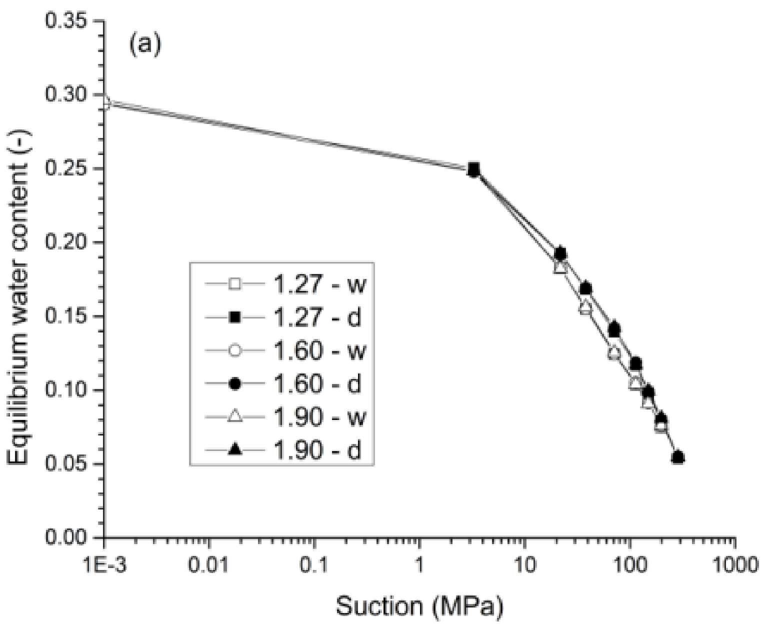


Figure 3-2: Water content with respect to suction along the wetting and drying path at dry densities of 1.27, 1.60 and 1.90 g/cm^3 in CU constant load tests. Reproduced from Baryla et al (2019).

3.2.3 Gap filling

A very clear result of the experiments is the high gap filling capacity of the bentonite. In CIEMAT's tests (FEBEX bentonite), voids of 17% - 24% of the sample size were filled; BGS found that even void spaces of 45% of the test cells were filled completely (MX-80). The gap filling capacity will of course depend on the dry density and the type of bentonite.

A sample swelling into a gap does not have a homogeneous density distribution afterwards. In those experiments that involved a progressive water supply (JYU, CIEMAT) it was found that density gradients reduced with time and increasing saturation (Figure 3-8). Once full saturation was reached, no further homogenisation could be observed. A decrease of gradients was also observed in BGS' gap filling tests where water was supplied at once. These tests had a duration of 100 days, and in all of them density gradients remained. Lower gradients were obtained with lower overall dry density (due to higher saturated permeability and possibly also due to the lower swelling capacity of low-density materials, which results in less steep gradients in the beginning) and when a greater degree of swelling was allowed to occur (due to the reduction in dry density). Some evidence indicated elevated temperatures may influence the degree of residual density gradients, but more data are required to understand this. Higher fluid salinity was observed to lead to higher gradients, however.

A spatially inhomogeneous swelling pressure distribution tends to homogenise with progressing swelling, as shown in BGS' and KIT's experiments (both using MX-80), but there is only a partial homogenisation. Remaining stress gradients in the gap filling tests can be widely explained by the varying local swelling pressure caused by density gradients. Friction may also play a role.

A very prominent result is the dependence of density homogenisation on the hydration velocity – for both gap filling setups and binary systems (see Section 3.2.4). A lower hydration velocity (e.g. due to a lower suction) results in a more homogeneous end product (Figure 3-3). In the gap filling case, CIEMAT states that hydration via the gap allows the samples to saturate faster because they swell into the open void and take up water very quickly, developing higher internal gradients than when they are saturated from the bentonite side, where no free space is available and a low permeability is maintained (see Sections 3.2.4 and 3.2.5). If hydration is performed via a vapour phase, higher relative humidities (faster vapour supply) likewise result in faster hydration and larger gradients.

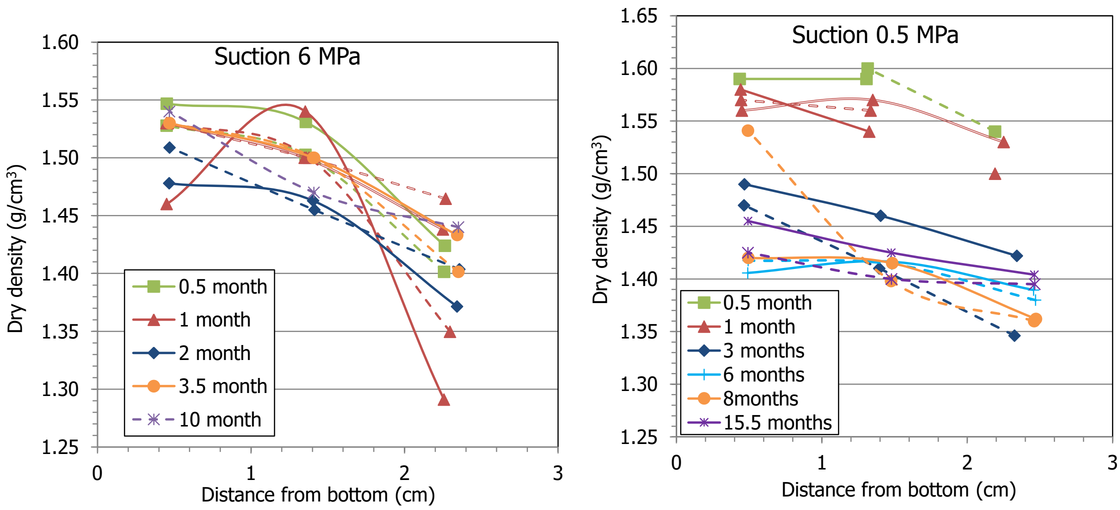


Figure 3-3: Final dry density profiles of subsamples of the gap-filling tests performed under 6 MPa suction (left) and 0.5 MPa suction (right) in CIEMAT axial swelling tests. Reproduced from Appendix B4.8. Continuous lines: hydration through gap. Dotted lines: hydration opposite gap.

3.2.4 Binary systems

In analogy to the gap filling tests, homogenisation of a granular material/block system used by CIEMAT depended on the hydration direction and kinetics (see Section 3.2.3, Figure 3-3). CIEMAT used systems of FEBEX bentonite (block and Fuller-type granular material) and MX-80 (block and pellet/powder mixture) (Figure 3-4). A (faster) hydration (via the granular material or because of higher water availability) resulted in larger final density gradients than an intrinsically slower hydration via the block or under restricted water flow. Similar results were obtained by CEA using block/block systems of different block densities. CU also investigated a block/block system and observed the same effect, although the difference due to the hydration direction was rather small. This may be due to the fact that both blocks had a rather high dry density to start with, so that the hydration was slow even when performed via the less dense block.

Swelling pressure evolution in binary systems is complicated and not necessarily monotonic, especially in systems with granular material or powder (CIEMAT, CEA).

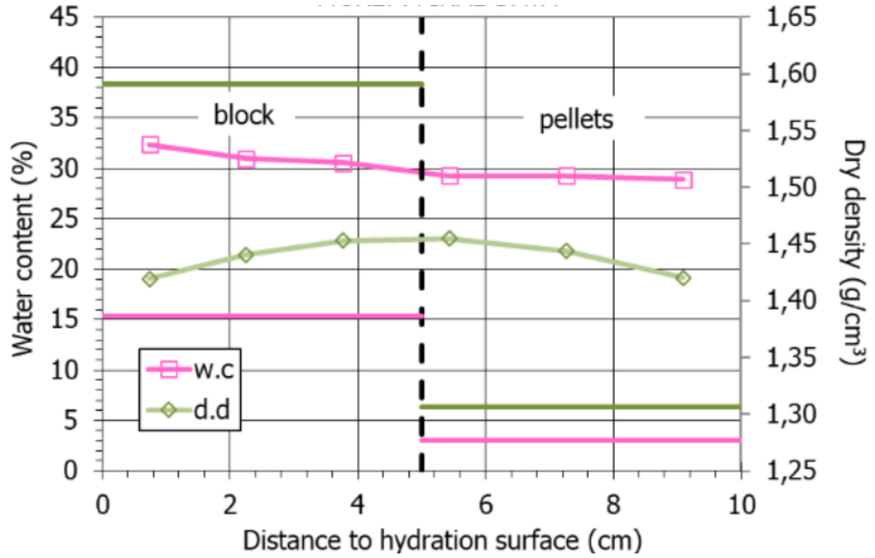


Figure 3-4: Final water content and dry density profiles of dual-density pellet-block system for CIEMAT test MGR27, compared with initial state (thick horizontal lines). Reproduced from Charlier et al (2021).

3.2.5 Porosimetry

Many of the experiments performed involved porosimetric characterisation before and after testing, and thus enabled a view on pore size evolution (e.g. Figure 3-5). The results all suggest that an initial saturation at low confining stress, possibly with a high hydration velocity, leads to irreversible strains that affect the macrostructure. The subsequent evolution of the system is conditioned by this early evolution. This interpretation is supported by the fact that it is the macropore volume that gets mostly modified as a result of the initial hydration and swelling. Since this effect seems to be persistent, it may need to be considered when modelling system evolution. Current dual-porosity models should be suited for this.

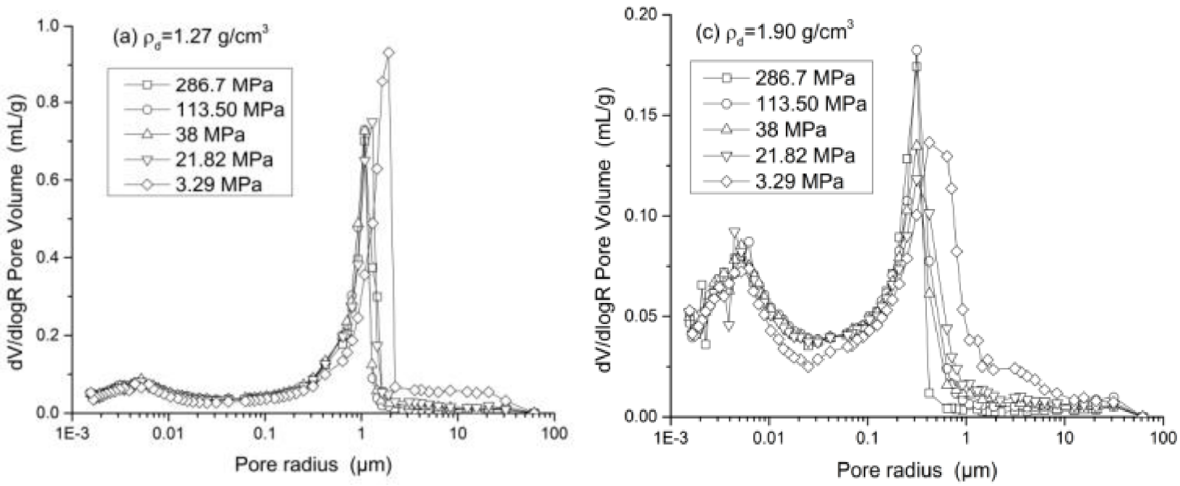


Figure 3-5: Pore size distribution curves of samples with different suctions at different initial dry densities from CU constant load tests at 1.27 g/cm³ dry density (left) and 1.90 g/cm³ dry density (right). Reproduced from Baryla et al (2019).

3.2.6 Influence of the degree of saturation on the shearing behaviour at a bentonite–steel interface

EPFL investigated the internal shearing of granular MX80 bentonite as well as the shearing at a steel-bentonite interface (Figure 3-6), for a Fuller-type (D_{50}=0.8 mm) and a unifractional aggregate size (1.5 mm) distribution. For both tested granulations, the interface shearing strength of the material at hygroscopic state was lower than the internal shearing. Unifractional samples showed lower values of shear strength parameters in comparison to those prepared with a Fuller-type granulation. Samples characterized by a higher water content showed a higher peak of shearing strength when compared with samples of lower water content. The increase of strength appears to be governed by the increase of adhesion between steel-bentonite upon hydration.

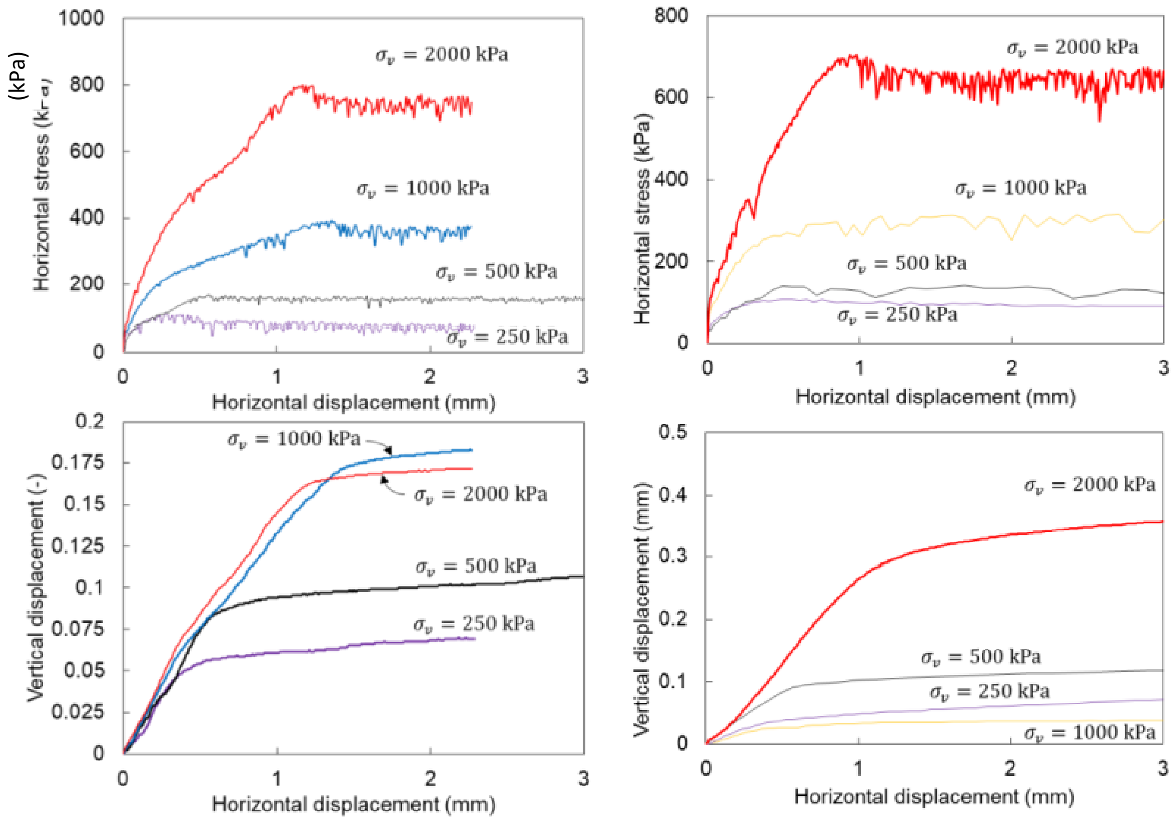


Figure 3-6: Results of bentonite-steel interface shearing, for granular bentonite with a Fuller-type granulation (left) and unifractional granulations (right) at hygroscopic conditions. Reproduced from Baryla et al (2019).

3.2.7 New experimental methods

In the Beacon project, new experimental methods were developed and tested, such as particle tracking in combination with X-ray imaging. CEA used X-ray tomography (Figure 3-7) and JYU used X-ray radiography. Another new method is small-scale spatially resolved stress measurement developed by KIT. These methods proved successful and can be used in future investigations. Especially with regard to stress measurement, the inhomogeneous stress distributions found in all test setups with spatially resolved measurement indicate that interpretation of conventional oedometer tests with just one axial pressure measurement needs care. A more detailed stress measurement and/or control may be advisable for future experiments.

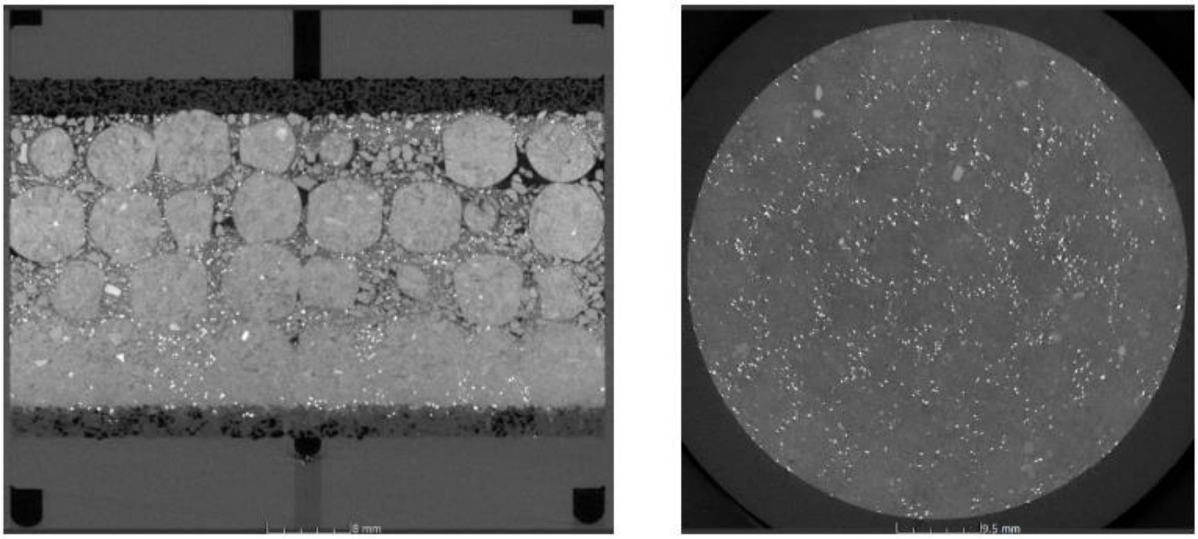


Figure 3-7: Vertical (left) and horizontal (right) slice at the midplane of a pellet layer at 1-day hydration. Reproduced from Baryla et al (2019).

3.2.8 Remaining questions

While a comparatively high total number of experiments was performed, these could of course not cover all relevant combinations of conditions: the effect of different bentonites (sodium versus bivalent), solutions, textures (blocks, pellets, powder and their combinations) and granulations as well as hydration and stress paths could be investigated in more detail to achieve a more complete database. Observed phenomena, like the apparent influence of hydration velocity on density distribution, should be further investigated. The effect of temperature is not established yet, there were only a few first tests performed. A question that has not been addressed in the experiments is the fate of the air initially contained in the bentonite.

All experiments presented here are small-scale laboratory tests. It would be advisable to compare the results to existing large-scale experiments in order to get an idea about scale effects. Also, not all the experiments performed were used for model simulation. Experiments provide input to model calibration or validation, but on the other hand, modelling an experiment can also help in its interpretation, thus reducing uncertainty about the results and increasing confidence.

3.3 WP5

3.3.1 Overview

The main goal of Work Package 5 was to propose relevant test cases to calibrate and validate constitutive models used by the partners involved in the project. The main idea is that the numerical results obtained on these test cases help to identify the weaknesses and the strengths of the models in order to allow the partners to improve these models in the framework of WP3, which was dedicated to development activities. Throughout the project a strong link has been created between WP3 and WP5. Feedback from WP5 is one of the main inputs to orientate the development of hydromechanical models in WP3.

WP5 has been divided into four tasks, each with a specific goal. For the first two tasks, test cases were built around experimental work identified in the framework of WP2. All the test cases have been taken from Deliverable 2.2 (Thatcher et al, 2018), produced at the beginning of the project. Task 3 concerned an evaluation of prediction capacity of the models. The test case was built on experiments performed during the Beacon project in WP4.

The last task was dedicated to assessment cases. The test cases were proposed by waste management organisations (WMO) and are based on specific components taken from repository designs.

3.3.2 Verification/validation test cases

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. The tests must have been finished, well documented, and provide enough relevant data. The choices of the tests were discussed and validated during a WP3/WP5 meeting held in January 2018.

The three tests picked up from the WP2 database and proposed for the first task were (Talandier, 2018a):

- 1a - swelling pressure tests for compacted plugs with free volume available (Test B1.7) from Clay Technology AB, SKB;
- 1b - swelling pressure tests for pellets mixture (Test B1.16) from CEA, Andra; and
- 1c - swelling pressure tests with two layouts for the swelling material: block and pellets (Test B1.6) from Posiva.

These tests are complementary and represent relevant situations encountered in a repository when installing an EBS. Technological voids are unavoidable when filling a tunnel with bentonite type materials. Pellets are used as a constitutive material in some repository designs (for example, seals for Andra or EBS for Nagra). Block and pellet mixtures are used at the same time to build the EBS (for example, pellets around compacted block in the KBS-3 design, pellets/blocks for Nagra's EBS). In the three situations, the role of heterogeneities has to be evaluated with regard to the expected properties attributed to the component.

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. The main criteria for the experiments were:

- The experiments have to be well described and dismantled;
- The experiments have to be relevant to disposal concepts used by project partners; and
- The experiments should highlight the role of heterogeneities in the bentonite components.

Based on these criteria and after discussions during the annual meeting in May 2018, 3 experiments were selected (Talandier, 2018b):

- EB - Engineered Barrier Emplacement Experiment (EB experiment), dismantled after almost eleven years of operation, has been a long, well monitored, and full-scale demonstration of the use of granular bentonite material as a clay barrier. The experiment was carried out in a gallery excavated in the Opalinus clay of the Mont Terri Underground Research Laboratory. The EB experiment was designed in order to demonstrate a new emplacement technique of the bentonite barrier according to the Swiss concept and to represent the saturation phase with artificial hydration of the barrier and under isothermal conditions.
- FEBEX - Full-scale Engineered Barrier Experiment in Crystalline Host Rock, is a research and demonstration project that was initiated by ENRESA (Spain). The aim of the project is to study the behaviour of near-field components in a repository for high-level radioactive waste in granite formations. The main objectives of the project can be grouped in two areas:
    - Demonstration of the feasibility of constructing the engineered barrier system in a horizontal configuration according to the Spanish concept for deep

geological storage, and analysis of the technical problems to be solved for this type of disposal method.
    - Better understanding of the THM and thermo-hydro-geochemical processes in the near field, and development and validation of the modelling tools required for interpretation and prediction of the evolution of such processes.

  The last section of FEBEX was dismantled after 18 years of heating and natural hydration.
- CRT - Canister Retrieval Test (CRT) is a project that was initiated by SKB at Äspö Hard Rock Laboratory. The Canister Retrieval Test was a full-scale field experiment simulating a deposition hole in a high level radioactive waste KBS-3V repository. It was designed to demonstrate the ability to retrieve a deposited canister at full buffer saturation. This in-situ experiment was carried out from 1999 to 2006. The experiment consisted of a cylindrical deposition hole hosting a canister encapsulated in a clay buffer. Cables attached between the host rock and a plug on top of the buffer retained the buffer vertically and simulated the reaction force of a tunnel backfill. The canister was equipped with heaters to simulate the thermal activity of nuclear waste and strips of plastic filter were installed at the deposition hole provide a controllable simulated groundwater inflow. CRT was dismantled after 5 years of heating and artificial hydration.

3.3.3 Predictive test case

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 increases the complexity of predicting the evolution of swelling clay materials. The idea was to select some tests performed in WP4 from Beacon project and to perform a simulation of a specific test to evaluate the ability of the models to predict hydromechanical evolution of bentonite.

CIEMAT performed a series of tests in isochoric cells with two layers: one made with pellets mixture, the other one made with a compacted block (Appendix B4.4,4.5). This situation implies an initial heterogeneity in the material and the evolution of this heterogeneity is followed during the test. The selection of those tests for this task (5.3) was approved during the WP3/WP5 meeting in February 2020. The selection of these laboratory tests was based on:

- Initial heterogeneity due to the presence of one block and pellets mixture;
- The FEBEX bentonite type used. It is the same material as for two of the tests performed under Task 5.2. The basic properties are then available; and
- The similarity of the test to Test 1c (Task 5.1) performed by Posiva where two layers with a high contrast of density are introduced in an isochoric cell.

Two steps were proposed for this task (Talandier, 2020a):

- Calibration of models to available results (tests MGR22 and MGR23); and
- Predictive simulations for ongoing test (MGR27).

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 is filled with bentonite pellets with an average dry density close to 1.30 g/cm^3 and the top part with a bentonite block with a dry density of 1.60 g/cm^3. Hydration with deionised water takes place through the bottom. Among a set of seven experiments, two of them were selected to compare the experimental results with the models (MGR22 and MGR23). The main interest is that the tests are performed under the same conditions except the boundary conditions concerning the water supply. In one case, a constant pressure is imposed (MGR23) and in the other a constant flow is imposed (MGR22).

One test was selected for predictive modelling (MGR27). The results of this test were not given to the participants. The conditions of the test are similar to test MGR23 except that the pellets layer is located in the upper part of the cell and block in the lower part. Predictive simulations were expected on this test case.

3.3.4 Assessment cases

The last task of WP5 was focused on direct application 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. These examples cover a broad range of issues, and the results should also be applicable to other concepts and systems. At this stage, the idea was to capitalize on the developments performed under WP3 activities and use the experience gained in the previous tasks to deal with complex cases representative of a real structure.

- Nagra case – high level waste (HLW) drift. HLW canisters are introduced to a tunnel of about 3 meters diameter. They are emplaced on a pedestal made of compacted bentonite blocks. The tunnel is backfilled with granular bentonite material (pellets). Initial heterogeneities are due to the presence in the cavity of blocks and pellets. Possibly, segregation in the pellets mixture could lead to dry density variations.
- SKB case - backfill in the KBS-3 repository. The backfill is the material installed in deposition tunnels to fill them. It consists of compacted bentonite blocks stacked on a compacted block, and the gap between the blocks and the rock surface will be filled with bentonite pellets. The heterogeneity is due to the simultaneous presence in the tunnel of pellets and blocks of bentonite. It is due also to the possible irregularity of the gap to be filled by the pellets along the tunnel walls.
- Andra Case – Gallery Seal. Seals are built at different locations in repository tunnels (about 10 meters diameter). The tunnel at this location is filled with a bentonite pellets mixture on a length of about 20 meters. Emplacement of this mixture leads to variation of dry density with height, and presence of apical technological voids can't be excluded. This leads to initial heterogeneous distribution of dry density.

For this task, no data were provided and this exercise constituted a real predictive test.

3.3.5 Models and partners involved in tasks from WP5

A large number of partners have been involved in the tasks of WP5 and performed some or all simulations of the proposed test cases: Quintessa, Clay Technology, UPC, ULG, SKB, Andra, EPFL, VTT/UCLM (University of Castilla-La Mancha), CU/CTU, ICL, LEI and BGR. Some of the partners performed only one or two tests (Andra, SKB) but most of them participated in all the tasks proposed.

The starting point of the partners was not the same. Some models and numerical tools were already very advanced at the start of the project. For other partners, a huge investment has been necessary in terms of developments and acquisition of the skills to manipulate the complex models needed to represent the hydromechanical evolution of the bentonite. At the end, 10 teams were able to produce results for the assessment cases which could be considered as the most complex tests proposed during the project. This also illustrates a real success of the project that was able to bring several teams to a sufficient degree of maturity to handle safety assessment cases.

A detailed description of the models used and developed during the project has been provided in the deliverables from WP3. It is important to notice that a large variety of models and tools have been used. In several models, a double structure approach has been used for the mechanical coupling, hydraulic coupling or both of them. Some teams introduced a double structure approach into their models during the project. This dual structure description (micro/macro) has been identified as important to well reproduce the processes or at least measurements obtained from small scale tests. On the other hand, the introduction of such complexity in the model is associated with several parameters that help in any case to fit the experimental results.

The numerical tools used during the project include CODE_BRIGHT, Lagamine, OpenGeoSys, ICFEP and Sifel (Section 3.1.2). Several partners introduced their own models in COMSOL Multiphysics.

The strength of the project was certainly the broad range of approaches chosen by the partners for the THM models. Nevertheless, it added difficulty to clearly identifying the origins of the differences obtained in the numerical results.

3.3.6 Lessons from the test cases

During the project, about 15 test cases have been modelled within WP5. For each test, several partners provided results. Comparisons between the results and, when available, with measurements have been done. Table 3-1 summarises the partners involved in each test case.

Table 3-1 Partners involved in each of the WP5 tasks

	Task 5.1				Task 5.2			Task 5.3*			Task 5.4		
	1a01	1a02	1b	1c	EB	FEBEX	CRT	MGR22	MGR23	MGR27	Nagra	SKB	Andra
ICL	X	X	X	X		X	X	X	X	X		X	
BGR	X		X	X		X		X	x	X	X		
Claytech	X	X	X	X		X	X	X	X	X		X	
EPFL	X	X	X	X		X		X	X	X	X		
LEI	X		X	X		X		X	x	X		X	
Quintessa	X	X	X	X		X		X	X	X			X
SKB		X											
ULG	X	X	X	X	X			X	X	X			X
CU-CTU	X	X	X	X			X	X	X	X		X	
VTT/UCLM		X	X	X			X					X	
UPC	X	X	X	X	X			X	X	X	X		
Andra													X

* MGR21 and MGR24 were also simulated by some teams.

The comparison and elements of analysis were compiled in four reports produced during the project.

- D5.2 - Synthesis of the results obtained of verification/calibration tests (Talandier, 2019);
- D5.4 – Synthesis of the results obtained of large-scale tests (Talandier, 2020b);
- D5.6 – Synthesis of results obtained of predictive test cases (Charlier et al, 2021); and
- D5.7 – Synthesis of results obtained of assessment test cases (Talandier, 2021).

The first tests (tests 1a01/1a02) showed a large dispersion of the results. One of the difficulties was representing the initial gap evolution. This difficulty was accentuated by the fact that the materials in contact were close to total saturation, at which point some models encounter problems in calculating the developed swelling pressure. An example of comparison between the axial pressure measured (test 1a02) and the numerical predictions illustrates the difficulties of modelling this case. Most of the simulations failed to obtain the estimation of the final axial pressure or the pressure evolution in time or both of them (see Figure 3-8a). These initial tests can be seen as representative of the state of the models at the start of the Beacon project.

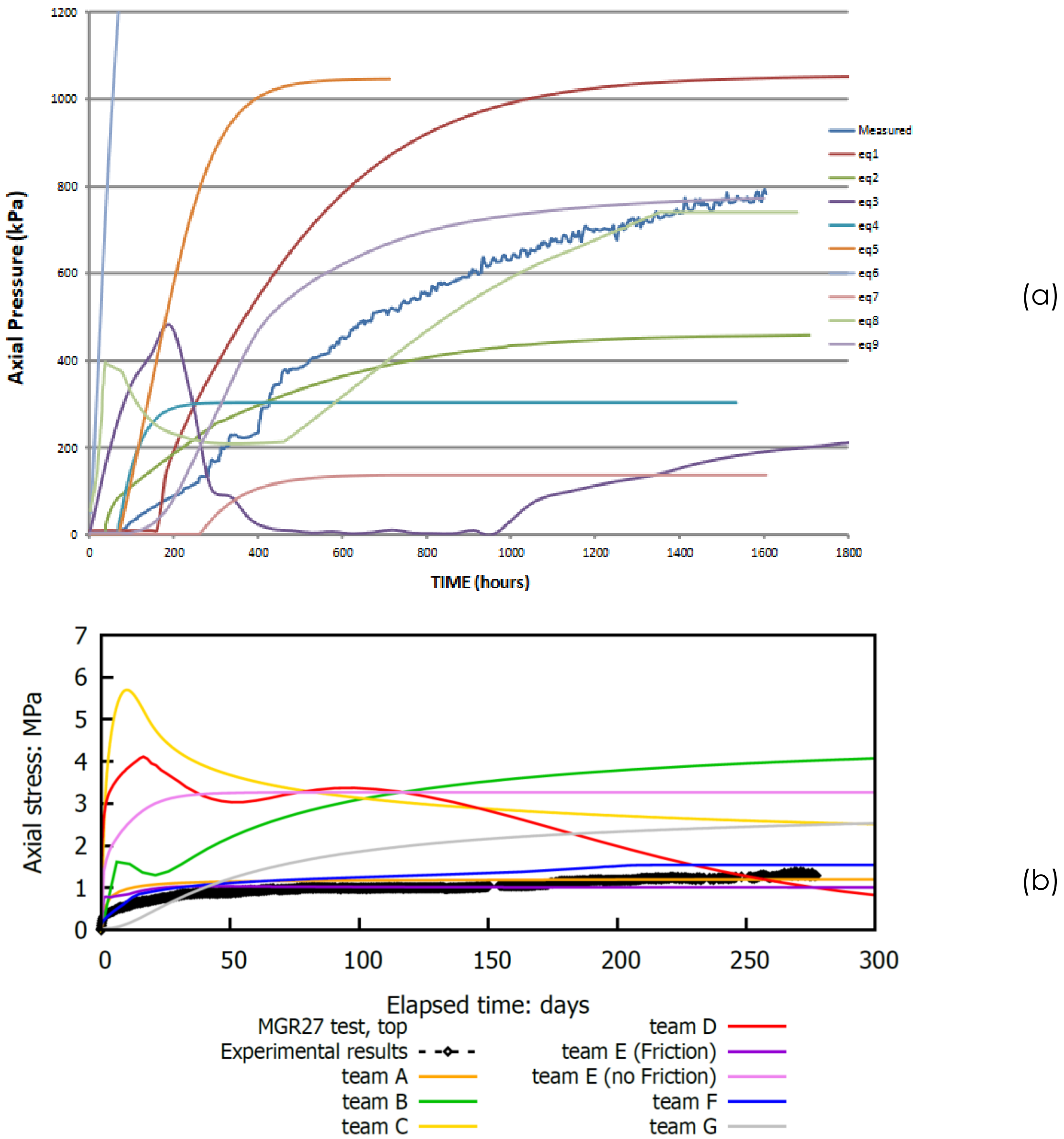
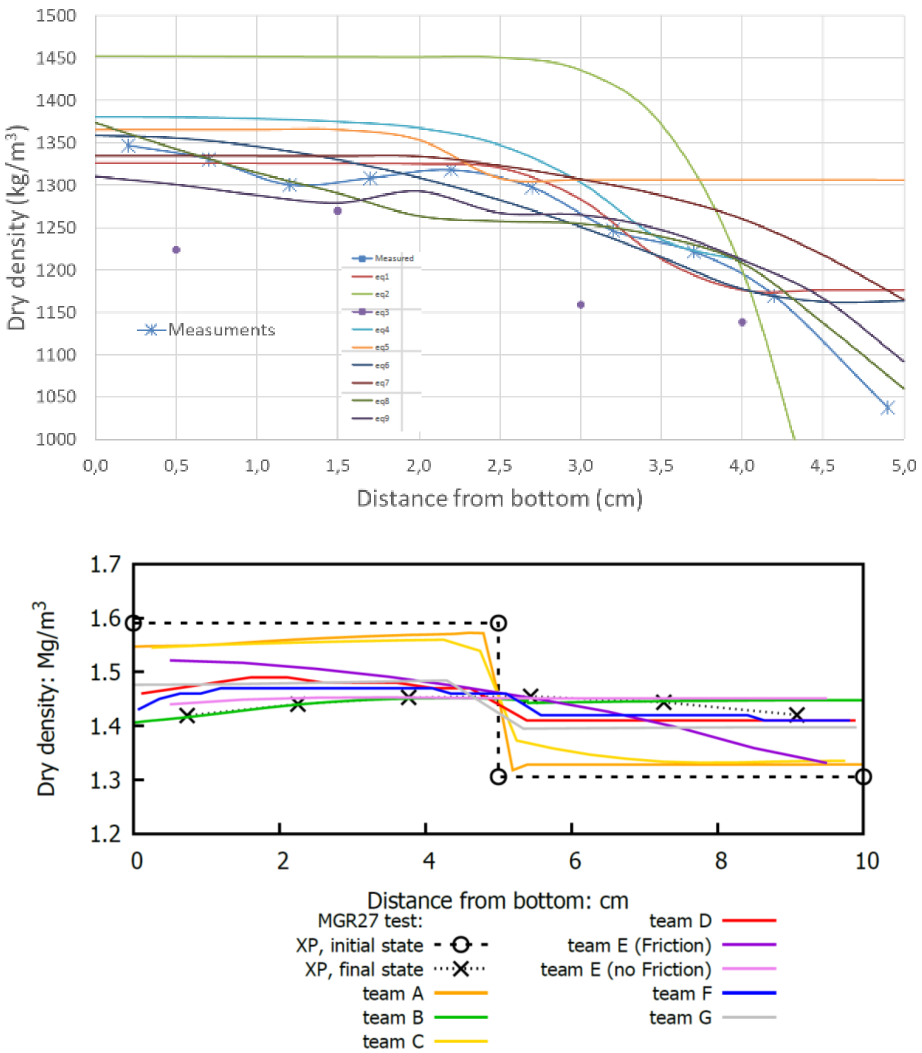


Figure 3-8 Comparison between axial pressure evolution measured on the top of the cell and the predictions for test 1a02 (a) and MGR27 (b). Each equation (eq) in (a) corresponds to a different modelling team.

The feedback from the overall project is that the stress field was globally not well reproduced by the models at least during the transient phase. It was difficult to fit both the axial pressure and the radial pressure (when it was measured). Nevertheless, an improvement of the models has been observed all along the project and leads to a better agreement between the measurements and the results obtained by simulation. This could be illustrated on the predictive test MGR27 performed under Task 5.3. In this particular case (MGR27), the experimental results were not given to the partners before the benchmark (Figure 3-8b).

The influence of friction is suggested as a possible origin of the difficulties in reproducing the stress field. In particular, it was not possible to obtain two different pressures at the top and bottom of the samples (as shown in test 1c) without introducing friction between the material and the cell wall. In several modelling runs of laboratory tests, the introduction of friction has greatly improved the results obtained in both amplitude and time evolution. This can be seen on Figure 3-8b where two teams (E and F) have modelled friction at the cell wall – bentonite interface. These teams satisfactorily blind-predicted the evolution of axial stress. Team A also performed well against the measured axial stress but underestimated the degree of homogenisation in the final dry density distribution (Figure 3-9b).

The dry density distribution, which is one of the important bentonite properties that the Beacon project is aiming to understand, can be known at the end of the experimental tests by post-mortem analysis. This is also one of the outputs provided by the modellers for each test case. For most of the test cases, the final dry density distribution measured is comparable with the predicted one even if the numerical results were improved during the project. The results shown on Figure 3-9 illustrate this for test 1a01(Figure 3-9a) and MGR27 (Figure 3-9b).



(a)

(b)

Figure 3-9 ***Comparison between vertical profiles of bentonite dry density after dismantling and the numerical results obtained in the project for test 1a02 (a) and test MGR27 (b). Each equation (eq) in (a) corresponds to a different modelling team.***

Models confirmed what was observed in experimental work performed in WP4, in large scale experiments or from the tests collated in WP2. The final state is not completely homogeneous and variations in dry densities persist even once a stabilised hydromechanical state is reached. This heterogeneity is due to the initial state (for example contrast of dry density at the beginning - pellets/block) but it can also be induced by the flow (flow rate, local water supplied…) or the stress field.

The main difficulties in modelling were observed when large differences of initial dry density have been introduced in the domain (for example - test 1c). Considering an initial gap also seems to be a challenge for most of the models.

Nevertheless, it was encouraging to see that the in-situ test modelling carried out in Task 5.3 gave results close to the measurements. The final states of all the test cases proposed in this task (EB, FEBEX, CRT) were well approximated by most of the models, despite the complexity of the studied systems. These observations concern especially both dry density distribution and the final distribution of water in bentonite materials.

By the end of the project, most of the partners used a double porosity constitutive model to represent the mechanical or hydraulic behaviour of bentonite materials. They clearly showed the interest of this type of approach to simulate the bentonite component evolution during hydration and the contribution of such models to predict the final state. The main difficulty is to calibrate the function/parameters to manage the interactions between micro and macro porosity. It has been shown that the representation and the choice of the interaction functions in the model plays a significant role in the quality of the results. Experimental determination of the precise shape and magnitude of the interaction functions is therefore an essential issue in order to improve the representativeness of the models.

Sensitivity analyses have been performed on some test cases. They highlighted the real usefulness of these approaches in identifying the most important parameters in the simulations of such cases. Interestingly, in an analysis performed on the buffer for HLW from Posiva's design, one of the more influential parameters is the function that describes the micro/macro interaction (Gharbieh, 2021). In this study, the final degree of homogenisation of the bentonite is the main indicator.

Finally, the implementation of the models used in the project on the assessment cases showed interesting results and went in the direction of capturing the main trends driving the evolution of the disposal structures. However, in detail, differences are highlighted between the models in terms of the time taken to reach equilibrium and for several indicators (including dry density, swelling pressure, and water content). This illustrates the need to continue efforts to develop models for swelling clays that are able to describe all the complexity of such materials, particularly in the presence of initial heterogeneities.

3.4 Summary

There is a significant degree of connection between the three work packages. The model developments undertaken in WP3 have resulted in improved model results in WP5, and the modelling difficulties experienced in WP5 have highlighted areas for techncial development in WP3. The experimental results from WP4 have been used to inform parameterisation and model processes, and the modellers have informed the requirements for the experimental work. This section summarises and brings together the key knowledge from the work packages. Section 4 discusses the importance of this captured knowledge in the context of the safety case.

The key aim of the work packages was to develop understanding of bentonite mechanical evolution, in particular, the extent of homogenisation of bentonite. Experiments undertaken in WP4 have considered different origins for bentonite inhomogeneity, including dual-density systems (Section 3.2.4) and the presence of initial gaps (Section 3.2.3). They then explored inhomogeneous wetting, and how the process of homogenisation is affected by factors such as the rate of hydration and the initial dry density distribution of the bentonite. These experiments have demonstrated that there is a significant degree of homogenisation as the bentonite saturates and swells, but some heterogeneity (in dry density and swelling pressure gradients) persists over time. The degree of homogenisation is significantly affected by the rate of hydration.

In WP5, modelling teams have generally been successful at predicting the degree of homogenisation in terms of final dry density and water content distributions of bentonite in the tests – for both laboratory experiments and large-scale in situ experiments (Section 3.3.6). Test cases have included those with initial heterogeneities (dual density or voids) and those that are observed to become heterogeneous from a mainly-homogeneous initial state (such as the FEBEX experiment). Modelling results improved throughout the Beacon project as a result of the developments in WP3. For example, teams found that the inclusion of friction was necessary to reproduce the observations of different axial stress throughout the sample in the Posiva swelling pressure tests (Task 5.1c). Several teams developed their models to include a capability for modelling friction, and improved their results for that test. In Task 5.3, most teams were able to successfully predict the higher degree of homogenisation in the test with slower water uptake. Predictions of final swelling pressure have shown significant improvement throughout the project but there is still significant dispersion in the results between the different modelling teams. Most of the tests have focused on prediction of axial stress and have not considered radial stresses, so there is scope for further modelling of deviatoric or shear behaviour.

Experiments in WP4 have also demonstrated the high gap-filling capacity of bentonite (and the effect of hydration velocity, bentonite type, temperature and salinity on this behaviour – Section 3.2.3). The presence of initial voids is still significant because the bentonite is not homogenous when the system reaches steady state after filling the gaps. However, many modelling teams have struggled to represent systems with initial voids (Section 3.3.6). Further model development work is needed in this area; in some cases related to code development, and in other cases related to the representation of the processes by which bentonite expands into a water or vapour-filled void. The work package summaries do not generally mention the water chemistry used in experiments, which was in some cases deionized (Task 3.3, 5.1a, 5.3) and in some cases synthetic or reference groundwater (Task 5.1b, 5.1c); in the modelling, this was assumed not to affect the swelling behaviour since chemical coupling is outside the scope of Beacon.

Another area of difficulty for the modelling teams in WP3/WP5 has been the representation of pellets. The models were developed primarily for compacted block bentonite, so had to be adapted to model pellets and pellets/powder mixtures for tests including Task 5.1b (Section 3.3.2). Modelling approaches have ranged from a simplified representation of pellets as a low-density bulk material, to development of models to account for the void space between pellets (Section 3.1.2). In general, modelling results for experiments involving pellets have agreed less well with data than equivalent experiments with block bentonite (Section 3.3.6), although it is not certain that this is because the experiments used pellets – it may be because of the dual-density materials or the boundary conditions used. Experiments in WP4 that have used pellets have noted the complexity of pellet saturation and saturation of dual-density systems (Section 3.2.4).

It is noted in Section 3.1.2 that several of the teams in WP3 have developed their models to include a double structure formulation in the hydraulic and/or mechanical models. The motivation for these developments is the clear evidence of a dual-peak 'micro' and 'macro' structure in pore size distributions of bentonite samples, as shown for example in Figure 3-5. These teams have shown corresponding improvements in their modelling results for the various WP5 tests, as noted in Section 3.3.6. However, it is unclear whether these improvements result directly from the inclusion of micro and macro porosity or from the increased number of parameters which can be calibrated to fit results. Sensitivity analyses conducted in WP5 demonstrated that models are sensitive to parameters defining the distribution between micro and macro porosity. There was limited porosimetry data for the experiments featured in WP5, which adds additional uncertainty to double structure models, but the modelling team who did compare predictions to MIP results found good agreement. Many of the experiments conducted in WP4 included measurements of pore size distribution and showed the importance of accounting for double structure effects; for example, stress path dependence of macroporosity (Section 3.2.2).

Finally, a key outcome of the Beacon project is the increased capabilities of individual partners. For the modelling teams, there have been significant developments in WP3 (listed in Section 3.1.2) including development of improved numerical solvers; use of additional codes; and new capabilities of some teams to model unsaturated conditions, plastic deformation, thermal effects and processes, pellets, and new types of geometries and boundary conditions including voids and friction. As noted in WP5 (Section 3.3.5), 10 modelling teams were able to produce results for the modelled assessment cases. Although the focus of Beacon was on modelling a wide range of test cases, rather than concentrating in detail on a particular test case, some modelling teams were able to undertake sensitivity analyses to develop a better understanding of the model sensitivity to various parameters. The large number of modelling teams involved in modelling the same experiments has also provided insight on the sensitivity of results to the modelling approach. For the experimental teams, WP4 (Section 3.2.7) notes the development of new experimental methods, including x-ray tomography and x-ray radiography, as well as small-scale spatially resolved stress measurements. These techniques are able to provide more detailed information in the future about the mechanical evolution of bentonite, to inform our understanding of the homogenisation process.

In general, application of models to simple experiments has built confidence in the ability of the models to represent and, in some cases, to predict the mechanical evolution of bentonite. The application to larger scale experiments has demonstrated that the models can be upscaled to represent real engineered structures. Indeed, many modelling teams were able to produce better results for the large scale test cases than for the laboratory tests. This may be because small uncertainities in the initial conditions and bentonite properties are less significant on large spatial and timescales and tend to average out. The full scale experiments may also be less affected by the boundary conditions, such as friction and voids, which are difficult to model. This may suggest that there does not need to be a focus on difficulties experienced in modelling small-scale laboratory tests, if they are not relevant to assessment cases. However, it should also be acknowledged that the large scale tests are often less well-characterized than lab tests, allowing modellers an increased degree of freedom to calibrate their model parameters which may not reflect the predictive capabilities of the models.

4 Key learning points and outstanding uncertainties from the Beacon project

In this section, the captured knowledge of bentonite mechanical evolution and the outstanding uncertainties from the Beacon project are considered in the context of safety cases for geological disposal for radioactive waste (based on the context provided in Section 2). These are summarised from inputs provided directly by the Beacon partners, listed in full in Appendix A.

Some uncertainties address processes and interactions that were out of scope for the Beacon project, but have been addressed in other projects. Some of these external projects are briefly discussed in Section 5.

4.1 Updated understanding of bentonite mechanical evolution

Through the Beacon project, many teams have made significant advances in modelling and experimental capabilities, as described in Section 3.1.2 and Section 3.2.7. This section focuses on developments in the conceptual understanding of bentonite gained through experimental work and applications of models in the Beacon project.

4.1.1 Initial heterogeneity – gap filling capacity of bentonite

A key focus of the Beacon project has been on the evolution of initially heterogeneous bentonite systems, including the presence of initial void spaces. In disposal concepts, there are likely to be technological voids due to the difficulty of precisely emplacing bentonite components – including voids between bentonite blocks, and between bentonite and adjacent components (e.g. rock, steel canisters). To have confidence in the ability of a bentonite buffer or seal to act as a barrier to advective transport, it is important to understand to what extent bentonite will be able to self-seal and fill the void spaces as it saturates and swells. In some geological settings, there may also be a possibility for a void at the point where a flowing feature intersects the rock wall. In this case, it is important for the bentonite to fill the void with a sufficiently high density, to avoid erosion and damage of the bentonite component.

Experiments in WP4 have shown the high gap filling capacity of bentonite, with small samples able to swell to fill up to 180% of their initial volume (Section 3.2.3). The swelling capacity has been shown to depend on the type of bentonite and its initial dry density, which supports previous findings in this area, and may help to inform specifications of required bentonite properties for EBS components. Heterogeneous dry density gradients remain after the void space is filled, but these are extreme tests; in an EBS, voids are likely to be small in comparison to the overall volume of bentonite. However, modelling teams in Beacon have shown the sensitivity of models to the bentonite dry density. It has been established that there is an exponential dependence between dry density and swelling pressure of bentonite, so even small changes in the average bentonite density due to expansion into a void space can have a significant impact on the achieved swelling pressure in the bentonite close to the initial void.

Some of the assessment cases considered in WP5 Task 4 (e.g. the Andra gallery seal) considered the impact of an initial void; modelling results suggested that the void would be fast to reseal, and reasonable magnitudes of dry density, swelling pressure and permeability were achieved in the bentonite close to the void. However, the time taken for bentonite to fill any gaps will be affected by the availability of water, likely to be particularly limited in clay host rock repository concepts. In the lab tests performed by CIEMAT, the gap in the tests saturated under 6 MPa suction was never filled (Appendix B4.8).

4.1.2 Initial heterogeneity - behaviour of granular bentonite and binary systems

Initial heterogeneity has also been considered in the form of bentonite pellets and granules. Several repository concepts propose to construct barriers from high density compacted blocks with pellets used to fill gaps around the blocks (e.g. KBS-3). It is therefore useful to understand the degree of homogenisation of these dual systems.

Some experiments in WP4 have studied the hydration of pellets (e.g. Appendix B4.2, B4.4, B4.5). These experiments demonstrated that hydration of dual-density systems with blocks and pellets is more complex than hydration of compacted bentonite blocks, and the evolution of swelling pressure in pellets also appears to behave differently to the evolution in compacted bentonite. In general, a good degree of water content and dry density homogenisation has been observed across block-pellet boundaries in most experiments (e.g. Appendix B4.1), although persisting differences in microstructure have been observed. The rate of swelling pressure development in both pellets and bentonite blocks has been observed to be non-monotonic with phases of stabilisation, increase, and decrease.

Modelling studies in Beacon have considered several tests involving bentonite pellets (e.g. Task 5.1b, Task 5.3 – see Section 3.3). Many teams have been able to successfully predict the degree of homogenisation in experiments with blocks and pellets, in terms of the final dry density and water content profiles. Outstanding uncertainties related to the behaviour of bentonite pellets are discussed in Section 4.2.2.

4.1.3 Sensitivity of homogenisation to boundary conditions

The degree of homogenisation obtained in samples of bentonite (both free-swelling compacted bentonite, and dual-density systems) has been observed to be dependent on factors including type of bentonite, initial dry density, water salinity and temperature. Boundary conditions can also introduce further heterogeneity to a bentonite component. Here, we discuss two factors that have been found to have a significant impact on the degree of homogenisation: rate of water uptake, and friction.

Rate of hydration

Experiments undertaken in WP4 have shown that a greater degree of homogenisation is observed in tests with a slower rate of hydration. This behaviour can be reproduced by the modelling teams, as seen in Task 5.3 (Section 3.3.3). Therefore, to understand the degree of homogenisation expected in bentonite components, it will be important to understand the expected rate of saturation. It is likely that rates of natural resaturation of an in-situ bentonite component will be much slower than the artificial hydration applied in tests, which implies that the degree of homogenisation should be good but may take a very long time (see Section 4.2.1).

Throughout the Beacon project, several modelling teams have made progress towards greater understanding of bentonite hydration and have implemented new water retention curves (Appendix A.5, A.9). Other teams have demonstrated the sensitivity of their models to parameters such as permeability, suggesting that rates of hydration are particularly sensitive to values of initial permeability. This is discussed further in Section 4.2.1.

Friction

One finding from the test cases considered has been that friction appears to play a significant role in some of the studied systems (e.g. WP5 Task 1c). Friction can reduce the degree of homogenisation expected in the bentonite, leading to increased heterogeneity of stresses throughout the sample. In response to these observations, several modelling teams have developed capabilities to model friction and have been able to successfully reproduce the observed behaviour. It is uncertain to what extent this is applicable to full-scale bentonite components (see Section 4.2.3).

4.1.4 Behaviour of micro/macrostructure

In both experimental and modelling work during Beacon, there has been significant progress in understanding and representing the double porosity structure of bentonite. Many of the experiments conducted in WP4 used porosimetry to measure the evolution of micro- and macro-porosity (Section 3.2.5). In parallel, many of the modelling teams in WP3 have developed double structure formulations of hydraulic and/or mechanical models (Section 3.1.2). Models which include this double structure formulation have been shown to be sensitive to parameters that describe the interactions between micro and macro porosity, so the porosimetric characterisation in WP4 is useful in providing greater understanding of these interactions. However, it is unclear whether detailed understanding and representation of the micro and macro structure is necessary to understand the bulk behaviour of bentonite in the context of the safety case, or whether it simply introduces additional parameter uncertainty.

4.2 Experimental and Modelling Uncertainties

4.2.1 Transient behaviour

As noted in Section 3.1.5, final values of dry density, swelling pressure and water content have proven to be less variable and easier to predict than transient behaviour. This may be partially explained by the sensitivity of the hydration process to parameters such as hydraulic permeability. The permeability of a bentonite sample is not constant, but varies with its dry density/porosity and with its water content, since this changes the pore size distribution.

Various different relationships have been proposed to relate bentonite permeability to dry density, but there remains uncertainty in the value of permeability for any particular bentonite sample.

The ability to understand and predict the transient development of swelling pressures in bentonite is further complicated by the non-monotonic evolution of stresses, as observed in experiments by CIEMAT (Appendix B4.8) and GRS (Appendix B4.2); swelling pressures do not always monotonically increase with saturation, but are sometimes seen to plateau or oscillate. This is particularly the case with granular bentonite, as noted in Sections 3.2.2 and 3.2.4. It is not always clear to what extent the details of transient behaviour are reproducible between experiments.

In the safety case, the short-term transient behaviour of a bentonite component may not be as important as its final state, depending on the safety functions of the component. For example, bentonite may only need to provide a diffusive barrier to radionuclide transport once a canister has failed. However, it may also need to provide a barrier for corrodents reaching the container from the time of emplacement.

The rate of hydration has also been observed to affect the degree of homogeneity (dry density and stress gradients), as discussed in Section 3.2.3; slower hydration results in increased homogenisation. However, some experiments (Appendix B4.8) demonstrated that similar swelling pressures were obtained in tests hydrated at different rates. Fundamentally, experiments are fixed in duration and the 'final' measured state of the bentonite only reflects a snapshot of its behaviour, generally once full saturation is reached. The bentonite may continue to gradually homogenise over a longer time period; models are therefore important for predicting longer-term bentonite evolution.

The majority of the experiments modelled in Beacon have considered small laboratory samples which saturate over a timescale of days or months. In repository concepts, bentonite buffers and backfills are expected to saturate over an estimated period ranging from hundreds to thousands of years (e.g. Nagra, 100 years; GRS, 5,000 years). Assessment timeframes are generally in the region of 100,000 years with the transient phase of bentonite evolution expected to last up to 10,000 years (e.g. Posiva, SÚRAO). The relation of temporal scales between small bentonite samples and large in-situ experiments remains a further uncertainty, particularly due to the difficulty in obtaining experimental data over long timescales. One solution is the use of natural analogues; Deliverable 4.2 (Sellin and Villar, 2020) studied a natural analogue consisting of a vertical drill core from a bentonite deposit, to determine the effect of long-term creep. This suggested that inhomogeneities could persist over geological timescales.

On these very long assessment timescales, other processes may place a significant role. For example, evolution of the bentonite as a result of cation exchange with the surrounding porewater, and long-term alteration/transformation of the bentonite in high pH environments. These processes have generally been outside the scope of the Beacon project; the focus has been on the initial phase of resaturation and homogenisation of the bentonite, rather than long-term chemical interactions. It should be noted, however, that there is some evidence from Äspö (Muurinen, 2011) that mineralogical changes can occur over shorter timescales of a few years at higher temperatures.

4.2.2 Behaviour of granular bentonite

Significant progress has been made in the Beacon project in developing model representations of, and collating experimental evidence on, the behaviour of granular bentonite (i.e. pellets); see Sections 3.2.4 and 3.3.2. The behaviour of dual density systems containing pellets and blocks is more complex than that of compacted bentonite blocks, and remains more difficult to model.

Different modelling teams used different approaches for representation of granular bentonite; from single-porosity and double-porosity models, which represent the pellets as an average bulk material, to triple-porosity models, which explicitly represent the voids between pellets as well as the double-structure macro- and micro-porosity within pellets. Each approach has advantages; triple-porosity models are capable of representing the complex water uptake behaviour seen with hydration through pellets, but require additional parameterisation to represent the evolution of different porosities and the interactions between them, which introduces additional uncertainty and requires a large number of model parameters to be determined.

The simplified approach of representing granular bentonite as a bulk material with averaged properties (lower average dry density) appears to be sufficient to estimate the final dry density and swelling pressure of the fully-saturated pellets, in pellet cluster and binary systems. This addresses one of the key safety functions of a bentonite buffer. However, the permeability of granular bentonite requires a more sophisticated representation; experiments have shown that water uptake is initially rapid as the pore space between the pellets is flooded (e.g. Appendix B4.4, CIEMAT). Therefore the complexity of the model required to model granular bentonite will depend on the importance of the transient resaturation phase to the safety case, as discussed in Section 4.2.1. If it will not be possible to parameterise triple-porosity (or even double-porosity) models with empirical data to a sufficient degree of confidence, then they may not provide any advantage for safety cases. Further work may be needed to test the robustness of these models.

Experiments have shown persisting microstructure differences between blocks and pellets even after full saturation (Appendix B4.5, CIEMAT), but in general a good degree of homogenisation in dry density is observed which is likely to satisfy most safety functions. Development of new experimental techniques has enabled the homogenisation of pellet clusters to be observed in greater detail, which should inform understanding of their behaviour.

4.2.3 Applicability of results to repository concepts and in-situ conditions

The experimental work undertaken in Beacon WP4 has focused on small, well-controlled laboratory experiments. These have been used to inform model development (including measurements of material properties) and develop understanding of bentonite mechanical evolution over practical timescales. However, there is a question over how the behaviour observed will scale up to the large bentonite buffers and seals that will be installed in repositories: are processes that are important at the laboratory scale still important for larger bentonite components? Do interactions with other repository features (e.g. saline groundwaters, high-temperature wastes, cementitious components) significantly change the behaviour of the bentonite? Are models robust enough to predict the behaviour of bentonite with more heterogeneous and less well-characterised initial and boundary conditions?

For example, friction between the bentonite and container walls was noted by many teams to have a significant effect on measured stresses in some lab tests (notably WP5 Task 1c). It is not clear to what extent friction between bentonite with a larger volume-surface area ratio and neighbouring components will affect its mechanical evolution, or how friction may evolve over longer timescales.

Some of these questions were tested in WP5 Task 5.2, in which teams modelled the evolution of in-situ experiments: the Full-Scale Engineered Barrier Experiment (FEBEX; Enresa, 2006), Engineered Barrier Experiment (EB; Mayor et al., 2005; García-Siñeriz et al., 2015) and Canister Retrieval Test (CRT; Kristensson and Börgesson, 2015). As described in Section 3.3.6, the models performed well in terms of predicting the final states of these experiments, particularly the final dry density and water content distributions. This is particularly of note, since one of the drivers of the Beacon project was to understand the final state of the EB experiment, which showed a significant degree of homogenisation. The models were able to achieve reasonable results, despite the fact that large-scale components are likely to have a higher degree of uncharacterised initial heterogeneity than laboratory experiments. This may indicate that this level of initial heterogeneity is not significant for predicting the behaviour of the components over timescales of a few years, since there is a larger amount of 'averaging' over these spatial and temporal scales. It may also indicate that boundary conditions such as friction are less important.

The models used for the in-situ experiments were generally calibrated to data from laboratory experiments on the same types of bentonite, indicating that the material properties and processes which are suitable for modelling small-scale experiments are also appropriate for large in-situ experiments and disposal concepts. However, it should be noted that these were not blind predictive models so there may have been some scope for calibration of parameters or boundary conditions which are not well-constrained by experiments.

Many of the modelling teams in Beacon reported that focusing on small, well-controlled experiments is more useful for model development because the models are better-constrained. This provides more focus on fundamental behaviour rather than 'feature-fitting'. Some modelling teams undertook sensitivity analyses to understand the impact of parameter uncertainties on their results, which highlighted that some parameters with a significant degree of uncertainty can have a large impact on the results. Further sensitivity analyses of this type would be useful to direct future efforts. Several partners also suggested that it would be useful for experimentalists to undertake repeated tests, to better quantify the uncertainty in various parameters and processes.

The focus of the Beacon project has been on the coupled hydro-mechanical behaviour of bentonite. Consideration of chemical processes (including the effect of water salinity and bentonite alteration), high temperatures, and gas transport has been beyond the scope of the project. The experiments used as the basis of modelling studies in WP3 and WP5 have used MX-80 or FEBEX bentonites, and have mostly used deionized water (Task 3.3, 5.1a, 5.3) or mildly saline groundwaters (Task 5.1b, 5.1c, and the in-situ tests in Task 5.2). These conditions are not representative of all disposal concepts considered; for example, SÚRAO plans to use other types of bentonite and RWM is considering a range of geological settings and generic disposal concepts which may include highly saline groundwaters and temperatures above 100°C. It is therefore important to know to what extent the learning points from the Beacon project are applicable to other concepts and sites. For example, it is noted in Section 3.1.6 that consideration of thermal expansion is sufficient for most modelling teams to reproduce temperature-dependent effects of tests such as the FEBEX experiment, but at higher temperatures a fully-coupled thermo-mechanical model and consideration of chemical effects may be required. These factors have been considered in some projects outside of Beacon (Section 5).

5 Research outside the Beacon project

Appendix C includes a collation of experiments undertaken prior to the Beacon project (2017) and Deliverable 2.2 (Thatcher et al, 2017) contained a summary of data and models available at the start of Beacon. Alongside the experimental and modelling work undertaken in the Beacon project, research tasks in other programmes have also focused on mechanical evolution of bentonite; including overlapping and complimentary areas. This section gives a brief summary of some notable external work involving partners from the Beacon project.

Work Package 7 (HITEC[2]) of the European Joint Programme on Radioactive Waste Management (EURAD) project concerns the THM behaviour of clay based materials at elevated temperatures. The aim of HITEC is to develop improved THM understanding of clay

[2] https://www.ejp-eurad.eu/implementation/influence-temperature-clay-based-material-behaviour-hitec

based materials (including bentonite buffers) exposed to temperatures above 100°C for extended durations, and to determine whether temperature influences the buffer safety functions (including swelling pressure, hydraulic conductivity, erosion and transport properties). This work is currently in progress and involves some of the Beacon partners, but an initial deliverable providing the state-of-the-art understanding of THM behaviour of buffer clay materials is available (Villar et al., 2020). This identified that the effect of temperature on hydro-mechanical properties of bentonite is quite well established with respect to safety functions for temperatures up to 100°C and for compacted bentonite; temperature modifies some properties (including hydraulic conductivity and swelling capacity) but they remain within ranges acceptable for complying with safety functions. Less is known with respect to HM properties for temperatures above 100°C.

Several other programmes are considering bentonite at high temperatures, with recent work in this area including reviews undertaken by RWM (Börgesson et al, 2020b; Hoch et al, 2020), an ongoing Czech in-situ experiment at the Josef Underground Research Loboratory (URL)[3], and an ongoing experiment (HotBENT) at the Grimsel Test Site[4]. These conditions are potentially relevant for bentonite in the presence of high heat generating waste. Börgesson et al. (2020b) considers mechanical and chemical erosion of bentonite, and Hoch et al. (2020) considers the effects of steam on bentonite; none of these processes were explicitly considered in the Beacon project. The reviews identified knowledge gaps in the understanding and modelling capability of these processes, including the evolution of swelling pressure in steam-treated bentonites and the ability of bentonite to self-seal piping channels. HotBENT aims to address some of these questions with planned experimental and modelling activities, including an in-situ test with MX-80 and Czech BCV bentonites heated to 175-200 °C.

THM studies of bentonite are also being undertaken within the SKB EBS Task Force (e.g. Åkesson, 2021a,b; Börgesson et al., 2020a; Birgersson, 2019). The aim of the Task Force (TF) is to develop tools for coupled thermo-hydro-mechanical-chemical (THMC) analysis of bentonite clay backfills and buffers, by modelling experiments undertaken at the Äspö Hard Rock Laboratory (HRL). Some of the THM tasks have significant similarities with modelling studies conducted in Beacon; for example, the modelling task reported in Åkesson (2021a) concerning water transport in pellet-filled slots. One task focused explicitly on bentonite homogenisation (Börgesson et al., 2020). The key conclusions of that task were that models were able to reproduce the main features (evolution of stresses and final dry density distribution) of the homogenisation tests; consistent with the findings of Beacon. Unlike Beacon, the EBS TF also considers chemical processes (e.g. Birgesson, 2019), including ion exchange, and anion and salt diffusion. Work is still undergoing on several of these tasks. One ongoing experiment considers the behaviour of bentonite in long tubes, which will be useful for quantifying the effect of friction.

The Finnish Research Programme on Nuclear Waste Management (KYT) has also funded a programme of studies on bentonite buffers within project THEBES[5] (e.g. Abed and Sołowski, 2020; Abed and Sołowski, 2021). These have some similarity to modelling studies undertaken within Beacon, but further consider chemical aspects including salt transport.

The international DECOVALEX[6] (Development of Coupled Models and their Validation against Experiments) project has also included some tasks which focus on the behaviour of bentonite buffers, in both the current phase (DECOVALEX-2023) and previous phase (DECOVALEX-2019) which have run during the Beacon project. This includes Task A from DECOVALEX-2019 and

[3] https://ceg.fsv.cvut.cz/en/annual-report-2020
[4] https://www.grimsel.com/gts-projects/hotbent-high-temperature-effects-on-bentonite-buffers/hotbent-introduction
[5] https://www.aalto.fi/en/department-of-civil-engineering/thebes
[6] https://decovalex.org/

the follow-on Task B in DECOVALEX-2023 which aim to model the advective movement of gas in bentonite (Tamayo-Mas and Harrington, 2020). Task D from DECOVALEX-2019 looked at the THM behaviour of the EB and FEBEX experiments (Gens et al, 2020), with similar findings to Task 2 of Beacon WP5.

6 Conclusions

Throughout the Beacon project, there has been significant progress made by experimental and modelling teams in advancing the understanding of bentonite mechanical evolution.

New experiments undertaken in Work Package 4 have been summarised and added to the database that was initially developed for Deliverable 2.2. The updated database is captured as Appendix C of this report and will be available in a searchable webpage format. 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.

The modelling teams participating in Work Packages 3 and 5 have shown significant developments in their capabilities, with 10 teams able to develop coupled THM models of bentonite components from one of Andra, Nagra and SKB's repository concepts. Teams are generally able to reproduce and predict the mechanical evolution of bentonite in small-scale and large in-situ experiments, particularly the final 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. Progress has been made throughout the project, with improvement seen in the agreement between models and experiments, although there remains a significant level of dispersion in predictions of transient behaviour and swelling pressures. The improvement in the modelling results is a consequence of updates to the models such as calibration to new datasets, inclusion of friction, improved formulations of water retention curves, inclusion of thermal effects, and developments to numerical solvers.

Suggested future work should focus on reducing uncertainties in the mechanical evolution of bentonite which may affect confidence in its safety-relevant properties. Modelling tasks in Beacon have shown the sensitivity of models to parameters such as permeability and assumptions relating the microstructure and macrostructure. Further sensitivity analyses could be useful to direct future efforts. Further experimental work could focus on reducing the uncertainty in key material properties and demonstrating the reproducibility of results (including for different types of bentonites). There is also uncertainty related to the effect that in-situ conditions (temperature, porewater chemistry, interactions with other components) may have on the conclusions drawn from laboratory experiments, which could be addressed in future work.

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Appendix A: Inputs from Beacon Partners

23 organisations have participated in WP2 of Beacon[7]. Partners have contributed towards this deliverable through a workshop held in May 2020 and via the WP3, 4 and 5 summaries. In addition, partners involved in the experimental and modelling work were asked to complete a template answering the following questions:

- What have been the main learning points from the work your organisation has undertaken during the Beacon project? (What have you learned from experiments or from modelling of experiments about the mechanical evolution and homogenisation of bentonite?)
- What are the main outstanding uncertainties regarding mechanical evolution and homogenization of bentonite? Do you have any recommendations for how these could be investigated in future work?
- Are you aware of any external work since the start of the Beacon project which could feed into the Beacon project?

The completed templates have been used to inform discussions in Sections 4 and 5 of this report. They are also included in this Appendix in full.

Appendix Reference Number	**Organisation**
A.1	BGR (Bundesanstalt fuer Geowissenschaften und Rohstoffe)
A.2	CIEMAT (Centre for Energy, Environmental and Technological Research)
A.3	Clay Technology AB
A.4	CZ Consortium (CU - Charles University, CTU - Czech Technical University, SÚRAO – Czech Radioactive Waste Repository Authority)
A.5	EPFL (Ecole Polytechnique Federale de Lausanne)
A.6	GRS (Gesellschaft fuer Anlagen- und Reaktorsicherheit)
A.7	ICL (Imperial College London)
A.8	JYU (Jyväskylän Yliopisto)
A.9	LEI (Lithuanian Energy Institute)
A.10	Quintessa Ltd
A.11	University of Liège
A.12	UPC (Universitat Politècnica de Catalunya)
A.13	VTT (Teknologian tutkimuskeskus VTT)

[7] SKB (as project coordinator), SURAO, Posiva, Andra (as WP5 leader), Nagra (as WP1 leader), RWM (as WP2 leader), UPC, GRS, CTU, CU, CEA, VTT, University of Liège, BGR, KIT INE, CIEMAT, CT, EPFL, ICL, Quintessa, BGS, JYU.

A.1 BGR

Description of the work your organisation has undertaken during the Beacon project (in Work Packages 3, 4 and/or 5) The BGR has participated in the modelling tasks of WP3 and WP5. In WP3, the BGR documented the state of the isothermal, coupled hydro-mechanical model available at the start of the project (OpenGeoSys5) using a set of simple boundary value problems. The aim of the exercise was to document model functionality in the focus regions of WP3, which applied to the persisting model at the time viz., stress path dependency, irreversibility in strains under isothermal conditions. During the course of the project, model development progressed in parallel and an improved model in a newer simulation environment (OpenGeoSys6) could be tested in Task 3.3 and compared to the measurements provided. The model demonstrated its mechanical behavior for swelling under a confined and an unconfined saturation process followed by a mechanical compaction. With the developed double structure model, a physical meaningful evolution of the porosity on the macro and micro scales could be predicted. Furthermore, it is highlighted that the model is now capable of reproducing stress-path dependency comparable to experimental observations. A non-isothermal model formulation is prospective. In WP5, the BGR participated in model verification with small and large-scale test cases using the existing isothermal and non-isothermal linear-elastic sequentially coupled hydro-mechanical models present in OpenGeoSys5. For the simulation of the blind-prediction tests (Task 5.3) the BGR switched to the more recent simulation environment OpenGeoSys6. Task 5.3 was solved in a monolithically coupled way with a new, hydro-mechanical elastoplastic model as constitutive framework for the balance of linear momentum and a single structure hydraulic model with swelling and an explicit treatment of porosity evolution. The simulations of the assessment cases were performed with a non-isothermal version of the model. The models used in WP5 differ from the model used in Task 3.3 of WP3. The different models used in the WPs reflect the different states of model development and applicability within the project.
What have been the main learning points from the work described above? (What have you learned from experiments or from modelling of experiments about the mechanical evolution and homogenization of bentonite?) WP3: The non-monotonous evolution of the swelling pressure under saturation in bentonite is the most significant hydraulic phenomenological observation that currently drives model development. This is accounted to the bimodal, hierarchical porosity structure observed in bentonite. Another aspect, which is under investigation, is the interpretation of suction value in bentonite and the Bishop's function, which controls the HM coupling. High suction initial states such as the ones commonly encountered in bentonite experiments lead to unrealistic stress evolution when used directly in determination of effective stresses using models that presume capillarity as the dominant water retention mechanism. Therefore, the initial suction has to be reinterpreted and only the mechanically effective part should be used in the determination of effective stresses. From Task 3.3 is also observed that the water uptake in bentonite is heavily influenced by its confinement state. WP5: The experiment 1a02 demonstrates that a saturation dependence of the swelling law may not be always adequate to describe the swelling behavior. It suggests that water uptake in bentonite is driven by a potential which continues to exist even after the available pore space is fully filled and causes large strains when unconfined. The experiment 1c suggests that wall-friction might be significant, especially at higher radial stresses. The modelling of the FEBEX experiment as a test case was highly simplified, both in the technical aspects such as excavation and ventilation and in the geological/geotechnical aspects such as assuming uniform radial saturation from the host rock, neglecting water conducting geological features, constant temperature boundary at the heater, neglecting technical voids etc. The bentonite

was also modelled with the available non-isothermal linear-elastic HM model using the Richards' approximation, which is able to capture the trends in all measured quantities very well. This test case can potentially be used to test and validate the improved model and allows for improvement in the level of detail in the model.

In Task 5.3 the homogenization of the dry density for an initially highly heterogeneous specimen is studied. The experiments show a high degree of homogenization, which cannot be reproduced by the numerical model. Since the trend of the results is correctly predicted and the model was enhanced since the report of task 5.3, this issue can probably be solved by a more accurate model calibration.

In the last task of WP5 the NAGRA assessment Case was studied. The ability of the simulation environment to compute the multi-physical boundary value problem in a moderately large-scale numerical experiment is tested. It shows that the used environment and the underlying mathematical models are stable and fast even in a pure sequential computation. By analyzing the model there are two main lessons learned during the assessment case. The interpretation of the suction of a material entirely by capillary pressure has a huge impact on the mechanical work done in the model. Here the above-mentioned reinterpretation of the suction would improve the behavior. Furthermore, the assessment case was the first experiment in which an inhomogeneous distribution of the dry density within a material was studied. The observed evolution of swelling stress did not reflect this inhomogeneity (dry density dependency of the swelling pressure) and therefore the underlying model needs to be revised.

What are the main outstanding uncertainties regarding mechanical evolution and homogenization of bentonite? Do you have any recommendations for how these could be investigated in future work?

The most persistent uncertainty across test cases is the lack of mechanical characterization data of the used materials, in the sense of mechanical parameters needed as input for classical elastoplastic HM models. This uncertainty is compounded by the nature of the experiment such as in-situ compaction in experimental ring vs. bored specimen placed in experimental ring; hygroscopic water content as initial condition vs. a specified saturation as initial condition. For test case 1b, it is not clear whether the nature of packing influenced the heterogeneous stress evolution that was observed. For test case 1c and in the MGR tests, it is not clear how to consider the (non-)equilibrium conditions at the interface in the homogenized models used in simulations and the (potential) role of friction. With these considerations, repeatability of experiments (e.g. 1b) and subjecting similar probes to a battery of tests (hydraulic, mechanical, at selected saturations etc.) would help shed some more light on material behaviour and would help in parametrization of models.

For the models developed in BEACON a full sensitivity analysis should be performed before applying them on further large scale experiments. If the influence of geometry, boundary condition and material parameter to the results is clear, the ability of transferring parameters from one experiment to the other can be estimated more accurately.

Are you aware of any external work since the start of the Beacon project which could feed into the Beacon project?

A.2 CIEMAT

Description of the work your organisation has undertaken during the Beacon project (in Work Packages 3, 4 and/or 5)

WP4: CIEMAT's work has focused on the conceptual understanding of the evolution of bentonite fabric and microstructure upon hydration and the factors affecting them. The laboratory tests carried out are described below. The results coming from the tests in the first two bullets have been published and discussed in a paper (https://doi.org/10.1016/j.enggeo.2021.106272).

1. Tests in isochoric cells to analyse the fabric and microstructure evolution of initially inhomogeneous bentonite (binary mixtures). Seven tests in a large-scale oedometer (10x10 cm) were performed and dismantled and another one is currently running. In these tests half of the sample is composed by a low-density mixture of bentonite pellets and the other half by a higher density bentonite block. During saturation the water intake and the axial pressure on the sample surface opposite to hydration were measured. The aim of these tests was to check the effect of saturation rate (constant water flow or constant water pressure) and boundary conditions (saturation through pellets or block) on pressure development and bentonite homogenisation. FEBEX bentonite has been used in all the tests.

2. Tests in transparent cells (12x12x2 cm) to obtain qualitative information about the texture evolution of initially inhomogeneous bentonite upon hydration, complementing those described above. A test has been performed with saturation through the pellets and another one with saturation through the block part. FEBEX bentonite has been used in both tests.

3. Gap filling test: a compacted bentonite sample was allowed to swell into a void for different periods of time and using different saturation mechanisms: water vapour (with suction control) or liquid water. In all the tests the initial dry density of the FEBEX bentonite was 1.7 g/cm^3 and the gap thickness was initially of 0.5 cm (for a sample height of 2-2.5 cm). In the tests performed in perforated cells the samples were subjected to total suctions of 6 and 0.5 MPa and the gap closing and changes in bentonite water content, dry density and pore size distribution were followed over time. Tests were performed in a different kind of cells using liquid water injected at a very low flow rate either through the gap or through the opposite side of the sample. A report dedicated to these tests was prepared and is being updated.

4. A new large-scale cell was set up in 2019 to perform hydration tests in binary mixtures as those described in the first bullet. This new cell allows to follow relative humidity and pressure evolution at different levels along the sample height as well as pore pressure on top. The test has been running for two years using an MX80 pellets/powder mixture and a compacted MX-80 block of the same dry density.

WP5: three of the tests described in the first bullet were selected as Task 5.3 of WP5, and a report and corresponding spreadsheets were prepared for their use in WP5.

What have been the main learning points from the work described above? (What have you learned from experiments or from modelling of experiments about the mechanical evolution and homogenization of bentonite?)

Concerning the hydro-mechanical evolution of a two-component bentonite buffer material –low density pellets mixtures and higher density compacted blocks– upon saturation under isochoric conditions (bullets 1, 2 and 4 above), the following conclusions can be drawn:

- Because of their low density and large macroporosity, hydration through the pellets was initially quick, even though the water injection pressure was very low.
- The way of hydration conditioned the water intake and the pressure development kinetics. Slow hydration (e.g. under a controlled low flow of through the high-density block) delayed the start of pressure development, but allowed higher pressures to be reached for lower overall degrees of

saturation. The reason could be the longer time available for water redistribution from the macropores to the microstructure (particularly the montmorillonite interlayer), which would be the responsible for swelling. The interplay between the different strengths of the two components may also be a relevant factor on the axial load measured at the first stages of saturation.

- Irrespective of the way of saturation (constant flow or pressure), the pressure development away from the hydration surface (both axial and radial) was not continuous. After a first sharp increase (which was quicker when hydration took place under constant water injection pressure), there was an intermediate period of pressure stabilisation. Only when the overall degree of saturation was very high, the pressure increased again until its final equilibrium value. This pressure development pattern had been previously observed also in samples of compacted bentonite and of pellets.
- The stress measuring devices reflect local stresses which are conditioned by the local dry density. Hence, when the block part was on top, the final pressure value of the saturated sample was higher than the value expected for smaller samples of bentonite compacted at the same average dry density. When the pellet part was on top, the contrary happened. Friction between the bentonite and the cell steel wall could also contribute to these differences. This research has put forward the necessity of using testing devices in which pressure can be measured at different locations to correctly assess the stress state of inhomogeneous samples.
- Bentonite water content and dry density gradients were observed at the end of the tests. For a given hydration rate they were dependent on the hydration time and, although they attenuated over time, they persisted even after full saturation was reached. Saturation under very low water inflow rate (either imposed or resulting from the low permeability of the block part when saturation took place through it) resulted in more uniform water contents and smoother gradients, also in terms of pore sizes.
- In contrast, the microstructure of the bentonite in the two components was very different even after full saturation. Despite of the drastic reduction in the volume and size of macropores in the pellets part, they continued to be higher than in the block part and consequently the e_m/e_M was lower in the pellets part. The basal spacing of the smectite, which is an indication of the number of water layers in the interlayer, was higher in pellets samples than in block samples. However, an overall trend to pore size homogenisation towards smaller sizes over time was observed.
- The water content and dry density gradients were not affected by the pellets/block interface. After full saturation the pellets/block interface was impervious to gas.

The evidence provided by these experimental results along with the outcomes of the large-scale EB test, in which a similar two-component barrier was tested for 10.5 years, suggests that, although the initial heterogeneity of the barrier system and the deformations induced in the first stages of saturation tend to attenuate over time, residual inhomogeneities will persist and remain even after full saturation. The kind and extent of these heterogeneities will depend on the initial and boundary conditions of the barrier.

Concerning the tests on gap filling performed by CIEMAT (bullet 2 above), the evaluation of the results obtained in the two kinds of cells indicates that the persistence of water content and dry density gradients was linked to the velocity of saturation: the quicker the hydration took place, the steeper and more persistent the gradients were. Hence the gradients were more remarkable and persistent when hydration took place in the water phase, then under “high” suction and finally under low suction. The samples under suction 6 MPa hydrated faster than those under suction 0.5 MPa, and the strains that occurred under quick hydration were larger and irreversible. There was also a difference related to the velocity of saturation in the two kinds of tests performed with liquid water, even though the flow rate prescribed was the same in the two sets of tests. When water was supplied through the gap, the samples saturated more quickly because they were able to swell into the open void and take water very quickly, developing higher internal gradients than when they were saturated from the opposite side to the gap, where no free swelling was readily allowed.

Hydration brought about an overall increase in the void ratio corresponding to all pore sizes (because of the swelling into the gap). Although the volume of pores smaller than 200 nm was initially higher, over time the volume of macropores increased more. The average size of the macropores also tended to increase. In agreement with the different hydration kinetics of the different kinds of tests, the overall void ratio increase took place very quickly in the samples tested with liquid water and under suction 6 MPa but took longer in the samples tested under suction 0.5 MPa. Initially, the increase in macropore void ratio took place mainly in the more hydrated samples, but over time this increase was also notable in the samples farther away from the hydration surfaces.

What are the main outstanding uncertainties regarding mechanical evolution and homogenization of bentonite? Do you have any recommendations for how these could be investigated in future work?

The behaviour of a two-component barrier can be affected by the particular dry density and water content of each barrier component as well as their size and geometry, and by the boundary conditions, such as the existence of gaps, temperature and water salinity and availability. So far, just the effects of geometry and water availability have been analysed. The analysis of the remaining aspects should be considered in future research. The results available from very long large-scale tests should be considered to complement the laboratory tests and assess aspects of the long-term evolution of the system.

All the tests on gap filling were performed with the same initial dry density, but since the initial swelling seems to considerably affect the "long-term" evolution, samples with different initial dry density, and consequently, swelling potential, may behave differently. Also the size of the gap, and consequently the minimum density that the samples may reach, is a factor that may affect the irreversibility of the strains and gradients observed. For the samples saturated in the water phase, the effect of water injection pressure should also be checked.

Most of the tests by CIEMAT were performed with FEBEX bentonite, which contains mainly divalent cations in the interlayer. It is known that the kind of exchangeable cations affects the swelling potential, water adsorption and potential for colloid formation. Hence, the homogenisation process and the gap filling ability may differ between bentonites. Comparison of the results obtained by CIEMAT with FEBEX bentonite and similar ones obtained with a sodic bentonite (e.g. BGS results on gap filling with MX-80) may help assess this impact.

What is the effect of a not complete homogenization? Is it relevant for the safety functions? For example, the barrier of the FEBEX in situ test was still inhomogeneous after 18 years, but it had fulfilled its sealing function. Furthermore, models were able to reproduce the hydro-mechanical evolution of the barrier.

Another uncertainty could be the effect of temperature on the processes studied in BEACON. It has been checked that at large scale a block/pellets barrier can become quite homogeneous if hydration is quick and temperature homogeneous (EB test in Mont Terri). But this would have to be confirmed for slower hydration and under thermal gradient.

Scaling is also a critical point.

Are you aware of any external work since the start of the Beacon project which could feed into the Beacon project?

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A.3 Clay Technology AB

Description of the work your organisation has undertaken during the Beacon project (in Work Packages 3, 4 and/or 5)

Clay Technology has participated in the modelling tasks of WP3 and WP5.

In WP3 the Hysteresis Based Material (HBM) model has been developed from a version which was only valid for isotropic fully water saturated conditions to the present version valid for general stress states, general degrees of saturation, and where vapor transport is included. Much work has gone into development/generalization of the formulation, then recasting the formulation into a format suitable for implementation in COMSOL Multiphysics and finally carrying out the implementation. Within WP3, simulations of one-element tests, where different aspects of the model come into play, have been performed. These shows that the model is very promising in that it is capable to give realistic responses using a single set of parameter values for very different scenarios.

In WP5 the capabilities of HBM were tested by performing simulations of different experiments. The first task, where different small-scale homogenization tests were simulated, gave a lot of information on where to improve the model. When undertaking the second task, simulating the Febex test, vapor flow and thermal physics were introduced to the HBM-formulation. More knowledge was gained regarding how to properly setup the clay potential. The third task gave insight about the limitations of the original version of HBM when representing a granular filling material. The model had to be changed in order to get reasonable solutions. The modelling of a two-component system also led us to implement an "interface" representation to circumvent problems with large differences in neighboring materials. In the final task within WP5, we have chosen to model the SKB assessment case where the homogenization of tunnel back filling is studied.

For one element tests it was often possible to perform calculations using mathematical software such as Mathcad. For more complex tasks, however, a more complete and competent numerical software was needed and for this purpose HBM was implemented into COMSOL Multiphysics. The implementation strategy has changed during the project. First, the possibility to write and link a C-subroutine with a predefined interface in COMSOL was tested. When unsaturated conditions were introduced into the formulation this method was found too limited. The strategy then shifted into introducing the material relations as individual distributed differential equations so that a mixed formulation was obtained. The implementation into COMSOL is still under development.

What have been the main learning points from the work described above? (What have you learned from experiments or from modelling of experiments about the mechanical evolution and homogenization of bentonite?)

Some tasks have given further indications that friction may have a potential to significantly contribute to the behavior of some of the studied systems. We have, however, experienced difficulties (due to the nonlinearity) when trying to incorporate a proper representation of friction in our simulations.

The modelling work has shown that it is essential to properly parametrize and fit the clay potential in the HBM model in order to arrive at proper solutions. Due to the model's strong coupling between mechanics and hydraulics it is important to consider both types of experimental data (hydraulic and mechanical) in order to achieve representative solutions for both physical processes.

When the granular filling was considered in WP5.3, we realized that one must be careful when using the HBM model for representing a material where the assumed material structure is violated. The original model was developed for compacted bentonite blocks, and when considering pellets or granular (crushed pellets) fillings the assumed material structure is no longer suitable. In WP5.3 this was treated in a pragmatic way by changing the mechanical and hydraulic properties without reconsidering the material structure. In other cases, the material model might have to be reformulated by altering the assumed material structure and re-formulate the material model with this in mind.

We have also experienced difficulties with simulating two-component systems where two materials have significant differences in initial conditions. Due to the strong imbalance in the system from start it becomes numerically difficult to properly solve the equations and find a convergent solution.

During the entire project we have gained much knowledge regarding how to implement nonlinear and highly coupled systems of equations in COMSOL Multiphysics. There is probably a lot more to know about this in order to obtain a sturdy and efficient implementation. How to solve the system of equations is also an area where knowledge has been gained, but even more is needed.

Both “virtual” experiments as well as real ones has merits when testing and developing material models. With the flexibility of virtual experiments, several well-defined scenarios can be tested which may point at limitations in the formulation. Real experiments with accurate data sets, on the other hand, give connections to the real world which can point out issues with parameter selection and sensitivity of the model.

Smaller scale experiments are often better for evaluating material models as compared to large in-situ experiments due to the inherit uncertainty in for example initial and boundary conditions in the latter one’s. Simulations of large in-situ experiments often turn into chasing “artefacts”, things which significantly affect the experimental behavior, but is not what is interesting when evaluating material models.

What are the main outstanding uncertainties regarding mechanical evolution and homogenization of bentonite? Do you have any recommendations for how these could be investigated in future work?

Influence from wall friction may be considered an uncertainty. This could for instance be the case when determining material model parameters. The calibration/fitting of material models should preferably rely on experimental setups where the effect from wall friction is negligible in order to only account for the actual behavior of the bulk material.

Wall friction should thus be avoided when determining material model parameters, but it is nevertheless important to be able to include it in simulations. Knowledge about the characteristics of wall friction could be of importance when considering the ability of the bentonite to homogenise in tunnels, deposition holes or boreholes. Knowledge could also be used to further understand the limitations of the homogenisation process. Density gradients remaining after long time and at stress equilibrium could be studied from results of tests designed such that wall friction has a very large effect on the results, for example swelling in long tubes.

Uncertainties could also be linked to the path dependence of bentonite. In the HBM model the ability of the bentonite to sustain anisotropic stress states is governed by the path dependence and this is coupled to the strength (deviatoric stress at failure) and hysteresis of the retention behaviour. Further studies of the path dependence and hysteresis effect could therefore give valuable information about bentonite’s behaviour and homogenisation process.

Another source of uncertainty when calibrating/fitting the HBM material model parameters is the experimental data sets. To get accurate predictions from the model, consistent experimental data sets (swelling pressure, deviator stress at failure, and retention data) with high accuracy are needed when determining the clay potential parameters. When it comes to permeability, it seems to be difficult to determine a precise value for a given dry density. This has a significant influence on the simulated evolution rate of variables.

New forms of bentonite buffer such as pellets/granular seem to have significantly different behavior both mechanically and hydraulically (perhaps also thermally) as compared to compacted blocks due to large differences (increased complexity) in the material structure. It is unclear how the homogenisation evolves at the relatively low densities of these forms, e.g. can larger channels seal and homogenise? Well defined and dedicated experiments could be beneficial for gaining knowledge about how other forms of buffers behave.

An important issue for making accurate predictions over large time scales and which could be considered a significant uncertainty is the unknown long-term behavior of the bentonite buffers. Will

the final equilibrium state of our current simulations be representative? Or could there be time dependent properties, properties that change significantly if the material undergoes alterations? For example, what happens if the wall friction has a time dependency or undergoes changes when the material is altered?
Are you aware of any external work since the start of the Beacon project which could feed into the Beacon project? **Homogenisation in long steel tubes.** SKB is running a project where the homogenisation properties of bentonite are studied. One important part of the study is the long-time homogenisation tests in steel tubes. The purpose of these tests is to study the effect of wall friction on limiting the degree of homogenisation and also to study the influence of time on the remaining density gradients after completed swelling and compression. Different test durations are used to study the influence of time and creep on the distribution of density. Three tests have been finished (after 2, 4 and 6 years) while seven tests are still ongoing. A comprehensive description of the tests and the results can be found in Dueck et al. (2018, 2021). **Influence of water uptake rate.** In this SKB project, tests have been run to study influence from rapid or slow water uptake on the density gradients in a profile. A test series at medium scale has been completed (Dueck et al. 2021) and a tests series at a smaller scale is ongoing. **References** Dueck A., Goudarzi R., Börgesson L., 2018. Buffer homogenisation Status Report 4. SKB Technical Report TR-17-04. Dueck A., Goudarzi R., Jensen V., Börgesson L., 2021. Buffer homogenisation Status Report 5. SKB Report in preparation.

A.4 CZ Consortium

Description of the work your organisation has undertaken during the Beacon project (in Work Packages 3, 4 and/or 5)

Czech consortium (SÚRAO, Czech technical University and Charles University) participated in:

WP3: Charles University, Czech Technical University

WP4: SÚRAO, Charles University, Czech Technical University

WP5: Charles University, Czech Technical University

The Czech consortium continues the study of Czech BCV bentonite aimed at characterising the basic hydro-mechanical properties (such as swelling pressure, swelling strain, compressibility, water retention properties, hydraulic conductivity) focusing particularly on homogenisation processes (2 blocks with differing dry densities). The THM hypoplastic model was calibrated/verified/validated and further developed based both on the experimental results obtained and the benchmarking tests performed as part of WP3 and WP5 of the BEACON project.

WP3: As part of WP3, a series of benchmark tests was performed aimed both at demonstrating the capabilities of the developed hydro-mechanical (HM) and thermo-hydro-mechanical (THM) models and at comparing their predictive capabilities with the results of other models based on different theories and developed by other research teams. The benchmarking was simulated employing a THM double-structure hypoplastic model compiled in the Triax single element code of the Charles University and the SIFEL finite element code of the Czech Technical University.

The finite element models were developed using both partially-coupled and fully-coupled algorithms employing two finite element modules, both of which were developed at the Czech Technical University. The first module allowed for the conducting of coupled heat and moisture transfer analyses based on the micromechanical approach, while the second served for the description of the suction- and temperature-dependent mechanical behaviour using the Charles University double-structure hypoplastic model developed for the description of the THM behaviour of the bentonite.

Several improvements have been made to the model during the course of the BEACON project aimed at enhancing its predictive ability. In particular, the relatively simple bi-linear water retention model was replaced by a more advanced model for the prediction of the smooth transition between the saturated and unsaturated states, which not only improved the experimental fit, but also acted to stabilise the convergence problems encountered in the finite element simulations. Further, aimed at improving the predictions of swelling capacity, the effective stress of the macrostructural part of the model has been replaced by an alternative formulation, and the concept of the suction-dependency of the quasi-elastic stiffness has been introduced so as to allow for the prediction of the higher swelling capacity of the saturated samples.

WP4: As part of WP4, a (hydro)mechanical investigation of Czech B75 and BCV bentonite has been conducted on powder/compacted samples and the pelletised material. The following (T)HM tests have been performed: a total/swelling pressure and permeability test (constant volume tests), oedometric tests with various wetting/loading/unloading stress path combinations, and swelling into a void space (small scale experiments). The density distribution changes and homogenisation were investigated employing dual density samples at both the Czech Technical University and the Charles University.

The constant volume tests focused on the investigation of the development of total pressure during saturation. Moreover, these tests helped to fill in some of the gaps in the research of the swelling pressure and permeability versus dry density relationship, the investigation of water front movement during saturation (saturation development over the sample height over time) and the investigation of the porosity distribution with samples maintained at a constant (overall) volume. These tests were also performed using dual density samples in order to investigate the density changes (homogenisation).

The oedometric tests focused on the investigation of stress paths. The tests were configured so as to allow for free swelling/compaction under load. Various load scenarios were investigated including the introduction of saturation to the samples at various stages. Tests were conducted on both powder/compacted and pelletised BCV.

Water retention tests have been performed aimed at the characterisation of the water retention properties of the bentonite at various dry densities in both the block and powder states along wetting and drying paths under both unconfined and constant volume conditions.

Small-scale experiments have been designed for the investigation of the progress of saturation and density changes at the larger scale (compared to the permeameter constant volume cells). Several configurations have been applied according to which the cells were either fully or partially filled, and the progress has been monitored over time. The cells have provided valuable information on both density distribution changes and the development of saturation over time. Both the block and pelletised materials have been subjected to investigation.

The results of WP4 were used as a tool for the calibration of the WP3/5 mathematical models.

WP5: The first task of WP5 involved the creation of the numerical models required for the 1a, 1b, and 1c swelling pressure tests. The finite element analysis input files were set up according to the testing specifications for bentonite blocks and pellets (Czech Technical University). The model parameters were calibrated and validated against experimental measurements (Charles University), accompanied by the introduction of further modifications to the model aimed at improving the experimental fit.

The extended THM model was employed for the second WP5 assignment, i.e. the benchmark simulation of large-scale experiments. The Czech consortium selected the CRT test as the most appropriate approach to investigating the predictive capabilities of the models. The finite element mesh of the model was generated considering both the forms of the bentonite researched, i.e. blocks and pellets, and taking into account various defined boundary conditions (Czech Technical University). The calibration of the parameters was undertaken by the Charles University and subsequently applied to the simulations of the experiment.

The third part of WP5 involved the creation of numerical models for the MGR tests. Particular attention was devoted to the saturation dependency of the material parameters in the transport part, mainly with respect to the relative permeability. One of the most important considerations concerned the accurate setting up of the boundary conditions, which were designed to be time-dependent. The material parameters were validated in the same way as for the previous research assignments. The model correctly predicted the combined hydro-mechanical path-dependent behaviour of the soil.

What have been the main learning points from the work described above? (What have you learned from experiments or from modelling of experiments about the mechanical evolution and homogenization of bentonite?)

During the course of the BEACON project, the experimental results of the study of the behaviour of the bentonite were compared to the results obtained by other laboratories employing different experimental devices. The results were validated based on the comparison process, and the range of measured values indicated that the results were not dependent on the research approach. From the simulation perspective, the simulation abilities of the hypoplastic double-structure model developed in the SIFEL finite element code were compared with the predictive capabilities of the modelling approaches applied by the other BEACON partners; the results confirmed the good performance of the models employed by the Czech consortium.

The results of the laboratory research provided valuable data on homogenisation (dual density and laboratory tests), water front movement, stress path dependency and other phenomena. The results served for the quantification of the difference between the behaviour of the pelletised material and the compacted blocks, as well as the strong stress path dependence. The ability of the models to predict the mechanical evolution and homogenisation of the bentonite was successfully demonstrated, although the level of homogenisation determined by the experiment was higher than the level determined by the numerical simulation.

What are the main outstanding uncertainties regarding mechanical evolution and homogenization of bentonite? Do you have any recommendations for how these could be investigated in future work? The most important uncertainties concerning the numerical modelling of the mechanical behaviour of the bentonite are connected with the definition of the boundary conditions for the large in-situ tests. Although the laboratory tests have been well defined and satisfactory results have been obtained, a number of uncertainties regarding the various properties remain (for example, the variability of the measured swelling pressure for particular dry density values). The variability of the bentonite blocks and the pellets also resulted in numerical difficulties. In particular, the triple structure involved in the behaviour of the pelletised material is beyond the predictive capability of the THM hypoplastic models, thus resulting in the need for the determination of approximate solutions employing the double-structure approach. The same applied concerning some of the construction-based inhomogeneities of the larger experiments. This needs further investigation on both – laboratory and model development level. Finally, the numerical difficulties observed in the finite element model (solution oscillation and mis-convergence) persist, although they have, to a great extent, been reduced during the course of the BEACON project. Further work is required aimed at enhancing the robustness of the simulations.
Are you aware of any external work since the start of the Beacon project which could feed into the Beacon project? - The EURAD project (the GAS, DONUT, HITEC WPs in particular) are also investigating the behaviour of bentonite. While the scope of the EURAD project differs from that of BEACON, some of the results are of interest. - The Czech IB200C project is investigating bentonite heated up to 200°C. The project includes the conducting of an in-situ experiment that is potentially of interest to the BEACON partners.

A.5 EPFL

Description of the work your organisation has undertaken during the Beacon project (in Work Packages 3, 4 and/or 5) EPFL has been involved in WP3, WP4 and WP5. In WP4 small scale laboratory experiments have been performed focused on studying the mechanical response under well-defined stress and hydration paths. Based on the experimental results and previous experience from modelling bentonite, in WP3 a new constitutive model has been developed, based on a hydro-mechanical coupling framework, that has been also implemented in a finite element code (Lagamine). In WP5 the new model has been applied to the simulation of boundary value problems in all tasks. The model has shown good performance for bentonite compacted (or assembled in the case of pellets) at initial dry densities higher than 1.4 Mg/m^3. This has been demonstrated from the simulation of laboratory tests to the large scale test FEBEX.
What have been the main learning points from the work described above? (What have you learned from experiments or from modelling of experiments about the mechanical evolution and homogenization of bentonite?) From an experimental perspective, the results have shown that significant shear strength might develop at the interface steel-bentonite. The oedometric tests, combined with microstructural observations have resulted in a comprehensive overview of the stress-path dependent behaviour of MX80 granular bentonite. It is interesting to note that although the final state is stress-path dependent, the same virgin compression line is recovered irrespectively of the stress path followed to re-saturate the material. From a modelling perspective, a new water retention model and a modified loading collapse formulation are the most significant modifications to the original model. The new water retention model accounts for the different behaviour of adsorbed water and free water while the loading collapse curve is a function of the degree of saturation instead of suction. These two modifications have resulted in a significant improvement of the model. The model has been used in several application cases within the WP5. Among them, the FEBEX test has been simulated, which was a field scale that reproduced a repository under realistic conditions of operation. In order to test the predictive capability of the constitutive model, the input parameters were calibrated using laboratory tests. This aspect is also an advantage of the model, as it requires relatively few parameters, most of which have a clear physical meaning. The results have been overall satisfactory, giving confidence to the predictive capability of the model. It has been shown that good predictive capabilities of the model are achieved when the normal compression line at saturated states is well calibrated. This also requires to properly calibrate the water retention model as it defines the suction and void ratio at which saturation is reached. Finally, as of now, the loading collapse curve parameters need to be calibrated for each initial compacted state. Future developments could include the incorporation of hysteresis in the new water retention model and to enhance its performance with bentonites emplaced at relatively low density.
What are the main outstanding uncertainties regarding mechanical evolution and homogenization of bentonite? Do you have any recommendations for how these could be investigated in future work? Further experimental evidence is required to understand the stress path dependent behavior of bentonite. In particular, few data are available on the radial stress developed under oedometric conditions upon hydration. For the planning of future experiments, it would be also of interest to monitor the relative humidity (or total suction) in order to verify and derive new constitutive relationships.

Are you aware of any external work since the start of the Beacon project which could feed into the Beacon project?

A.6 GRS

Description of the work your organisation has undertaken during the Beacon project (in Work Packages 3, 4 and/or 5) Single pellet tests (performed at KIT) and pellet cluster tests (performed at GRS) were planned. Both test types use MX-80 pellets in constant volume cells: One pellet plus fragments representing neighbouring pellets in the single pellet cells, a volume of 50 mm diameter by 50 mm height in the pellet cluster test (PCT). Dry density in both test types was 1000 kg/m³. The PCT was preceded by pre-tests in acrylic glass tubes for visualisation. In the PCT, water flow and axial stress were measured over more than 7 months (continuing). Results were compared to KIT's single pellet tests with spatially resolved swelling pressure.
What have been the main learning points from the work described above? (What have you learned from experiments or from modelling of experiments about the mechanical evolution and homogenization of bentonite?) Wetting-induced swelling of a confined pellet(-cluster) is much more complex than the wetting processes applying to compacted and confined bentonite. The PCT shows that the pellet cluster has still not been at steady-state after 220 days despite being nearly instantaneously immersed in the solution. Had the individual pellets been confined, they would have shown the wetting characteristics of a compacted bentonite body and been fully saturated in a matter of days. The evolution of the swelling pressure follows a series of consecutive phases of increase and decrease. It increases in oscillation period but decreases in amplitude. At the end of the observation, changes in swelling pressure have come down to the range of the measurement accuracy. It is nevertheless quite possible that the end of this evolution has not been reached yet. Entirely unexpected is the significant continuous flow of solution out of the test cell beginning at about 130 days. The reason for this phenomenon is still unclear but it appears to be related to gas release which is indicated by measurements performed in the framework of the ongoing Sandwich project.
What are the main outstanding uncertainties regarding mechanical evolution and homogenization of bentonite? Do you have any recommendations for how these could be investigated in future work? From the GRS tests alone it is of course not possible to answer this question. Please refer to the WP4 overall conclusions.
Are you aware of any external work since the start of the Beacon project which could feed into the Beacon project? Laboratory work performed in the frame of the Sandwich-VP and Sandwich-HP projects (ongoing).

A.7 ICL

Description of the work your organisation has undertaken during the Beacon project (in Work Packages 3, 4 and/or 5)

Imperial College London (ICL) team participated in the modelling tasks associated with work packages (WPs) 3 and 5. All modelling tasks were performed with the finite element software ICFEP (Potts & Zdravkovic, 1999), employing a double-porosity structure mechanical model (ICDSM, Ghiadistri et al., 2018), a Van Genuchten-type soil water retention (SWR) model and a variable permeability model which allowed variation of bentonite permeability / hydraulic conductivity in terms of suction (Potts & Zdravkovic, 1999). All hydro-mechanical models were developed before the start of Beacon. While small numerical adjustments were made to the mechanical ICDSM model, its formulation remained the same throughout the project, as well as the formulations of SWR and permeability models.

The modelling activities for WP3 involved simulations of EPFL laboratory experiments which were performed during the Beacon project. This set of experiments comprised specimens of granular MX-80 bentonite. One was subjected to free swelling hydration in an oedometer under constant vertical stress until the swelling strains stabilized with time, followed by increase in vertical stress, while the other was subjected to constant-volume hydration under increasing vertical stress until swelling pressure stabilized with time, followed by further increase in vertical stress.

Input to WP5 started with simulations of oedometric swelling tests involving specimens made of compacted MX-80 bentonite blocks, pellet mixes and block-pellet arrangements, subjected to combinations of constrained and free hydration. A set of oedometer tests performed by CIEMAT during Beacon was also simulated, involving FEBEX bentonite specimens which combined block and pellet halves of a specimen in the vertical direction. Within the task of modelling large scale experiments ICL contributed with simulations of the FEBEX and CRT experiments, the latter involving MX-80 bentonite buffer. Both experiments involved thermo-hydro-mechanical (THM) coupling. The final modelling contribution has been the simulation of assessment cases for the evaluation of degree of heterogeneity, of which the ICL team simulated the SKB's KBS-3 backfill homogenization case, which involved only hydro-mechanical coupling.

Ghiadistri G.M., Potts D.M., Zdravkovic L., Tsiampousi A. (2018). A new double structure model for expansive clays. 7th Int. Conf. on Unsaturated Soils, E-UNSAT 2018, 3-5 August, 2018, Hong Kong.

Potts D.M. & Zdravkovic L. (1999). Finite element analysis in geotechnical engineering: theory. Thomas Telford Publishing, London, UK.

What have been the main learning points from the work described above? (What have you learned from experiments or from modelling of experiments about the mechanical evolution and homogenization of bentonite?)

Simulations of laboratory tests

With respect to simulated laboratory tests, which involved only hydro-mechanical (HM) coupling and either confined or free swelling, the constitutive model was shown capable of reproducing reasonably well the maximum values of swelling pressures (Tests 1a, 1b; Task 3.3). The model is isotropic in its formulation, hence predicting similar magnitudes of axial and radial swelling pressures measured in constant volume experiments, while the measurements showed these values to be different. It was difficult to assess whether measured data were a result of some inherent anisotropy in specimens of compacted bentonite (which is reasonable to expect to exist), as there also existed some uncertainty of the initial stresses in specimens before the start of their hydration. The simulations also under-estimated the initial rate of the swelling pressure rise (both axial and radial), which could be attributed to possible inadequate variation of permeability at the start of the experiment.

The post-mortem analyses of bentonite states at the end of laboratory tests showed that the model was capable of reproducing the correct trends and close magnitudes of the evolved void ratio / water content / dry density profiles interpreted experimentally.

Laboratory hydration tests under constant volume with mixed bentonite samples (half compacted block, half pellets, Test 1c, Task 5.3) showed fairly homogenised profiles of the evolved void ratio / water content / dry density at the end of experiments. The model was able to simulate the correct magnitudes of changes in these parameters (between the initial values and those at the end of the test) in both parts of the specimen (block and pellets), but still showing a distinction (jump-change) between the two parts. This was again attributed to inadequate permeability modelling especially at the start of the experiment.

Large scale in-situ tests

The large scale in-situ tests simulated as part of Task 5.2 (FEBEX and CRT) involved thermal coupling in addition to hydro-mechanical coupling. The constitutive model is not formulated in terms of temperature, but appropriate parameters for thermal conductivity and coefficients of thermal expansion were applied to bentonite buffer and the surrounding host rock, as well as appropriate temperature / thermal flux boundary conditions at the canister / buffer interface. In both cases the buffer was constructed from compacted bentonite blocks involving Febex bentonite in the Febex experiment and MX80 bentonite in the CRT experiment. The model parameters in both cases were the same as calibrated for the simulations of laboratory tests, the objective being to examine whether such model calibration can be extended for application to a large scale boundary value problem.

The numerical model was shown to reproduce very well the evolution of the temperature field in the buffer. The field tests involved essentially confined hydration (as buffer is entrapped between the canister and the host rock). The model reproduced very well the mobilised maximum swelling pressures measured at different cross-sections and in different rings of the buffer. The important part of comparison was also the interpretation of field measurements with respect to their operational time of the experiment, in particular in the case of the Febex test which spanned 18 years.

What was not well reproduced in simulations was the rate of wetting in the buffer rings interfacing the host rock, as near 100% relative humidity (RH) in those was measured within the first three years of the Febex experiment, whereas this was around nine years in the simulation. The agreement between the numerical results and measurements of RH evolution was improving for inner rings, given the scatter in measurements. Similar to laboratory experiments discussed above, this shortcoming of the simulation was attributed to inadequate permeability modelling at the start of the experiment.

The post-mortem examination of void ratio / water content / dry density radially across the buffer, after the Febex experiment was dismantled, showed very satisfactory agreement with measurements taken in different cross-sections of the buffer.

What are the main outstanding uncertainties regarding mechanical evolution and homogenization of bentonite? Do you have any recommendations for how these could be investigated in future work?

Analysing the ICL results from simulations at all scales (laboratory and field) it may be concluded that the applied modelling approach has shown to be broadly capable of reproducing the observed patterns of bentonite's HM and THM response and reasonable agreements between simulations and measurements. The principal uncertainties identified from all simulations were related to the characterisation of micro-structure in the double-porosity ICDSM model, as this strongly affects the evolution of swelling pressures. Equally uncertain was the characterisation of permeability / hydraulic conductivity in particular at early stages of hydration.

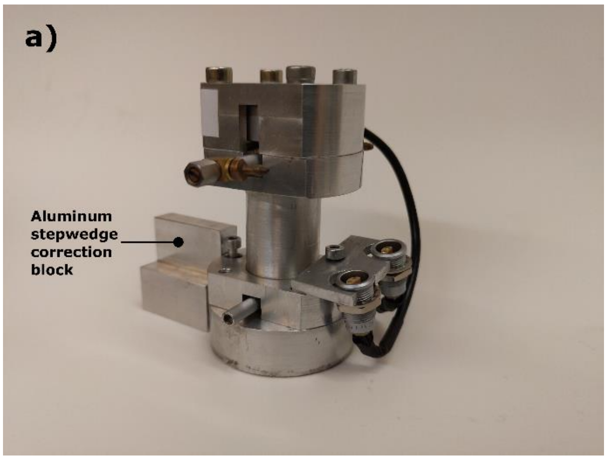
Are you aware of any external work since the start of the Beacon project which could feed into the Beacon project?

A.8 JYU

Description of the work your organisation has undertaken during the Beacon project (in Work Packages 3, 4 and/or 5)

JYU has taken part in the lab testing of WP4. In the experiments, method based on X-ray imaging and numerical image analysis was used to simultaneously measure water content and deformation of various swelling clay materials without disturbing or damaging the material samples.

Aim of the measuring setup was to simulate a situation where buffer material swells into bedrock cracks. For this purpose, custom build sample chambers were constructed (Fig 1). In the cylindrical chambers limited void expansion, saturation process and axial swelling pressures of compacted bentonite samples can be easily monitored by X-ray imaging and force sensors.



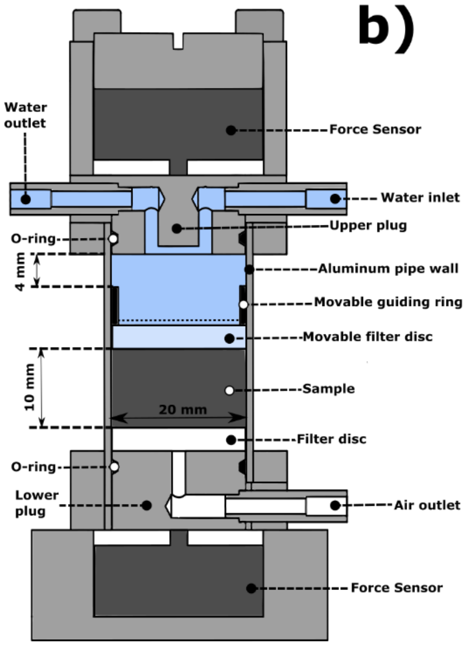


Figure 1: a) Sample chamber and its b) more detailed crosssection.

In the numerical image analysis part of the method, X-ray images of sample reference state is compared to the X-ray images of wet and deformed state. Samples are doped with ZrO_2 spheres which move when sample swells. This marker particle movement is tracked with block matching algorithm to determine the displacement field of the sample. Furthermore, change in the intensity values of the image pixels i.e., local linear attenuation coefficients (LAC) are analyzed in course of the saturation process. Displacements and LAC data is then used to compute time development of bentonite and water content in the samples. Example results of void expansion and sample saturation process with gravimetrical validation data is presented in Fig. 2. Furthermore, collection of sample swelling data is shown in Fig. 3.

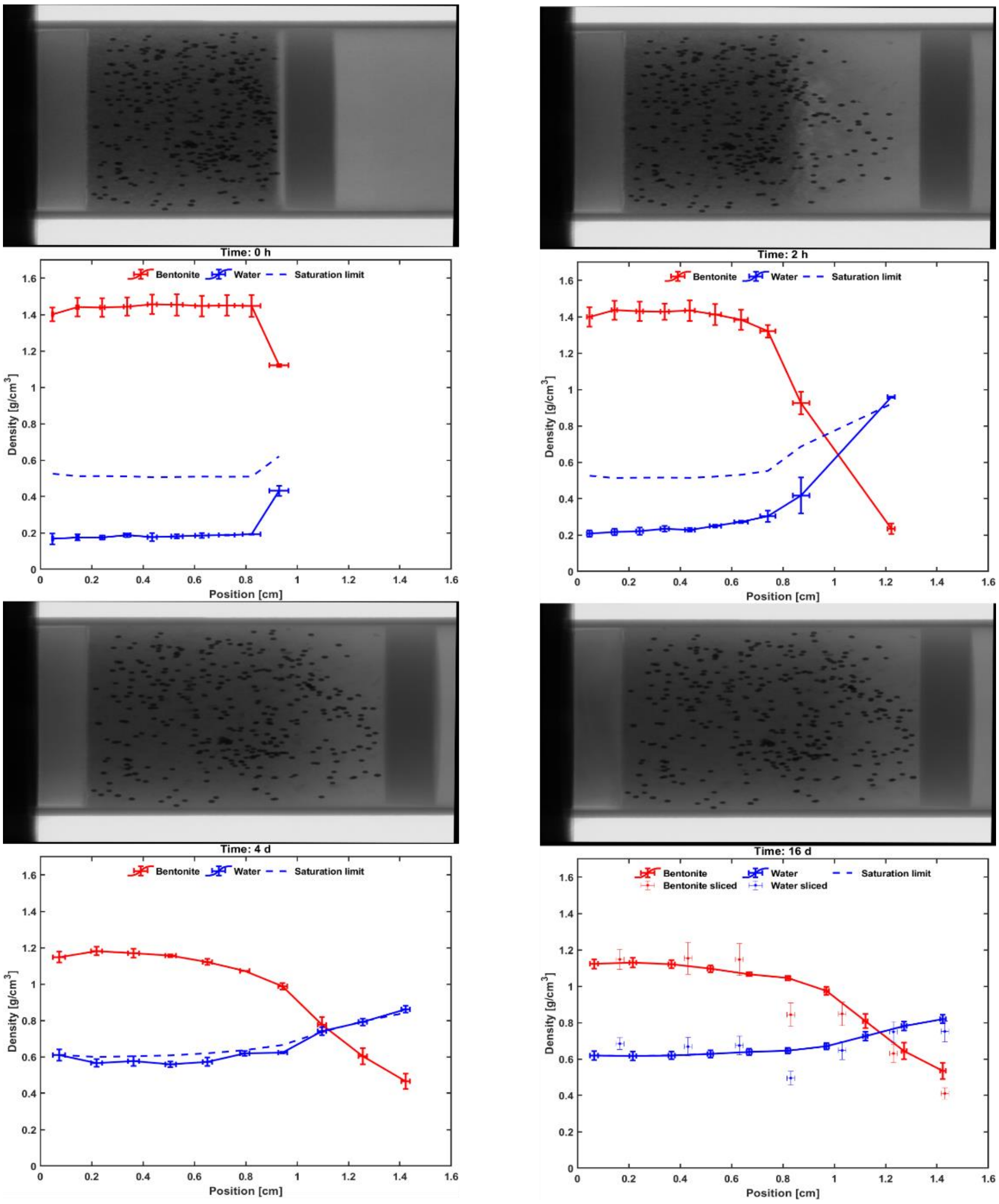


Figure 2: Bentonite (red curve) and water (blue curve) content profile development through duration of the 16-day saturation and swelling process. Saturation limit is shown in blue dashed curve. Gravimetrical validation analysis was performed at the end of the experiment by weighing and oven drying thin cut slices of the sample. Resulting local bentonite and water contents are plotted in red and blue dots respectively. X-ray images corresponding to the saturation process step are appended above the graphs.

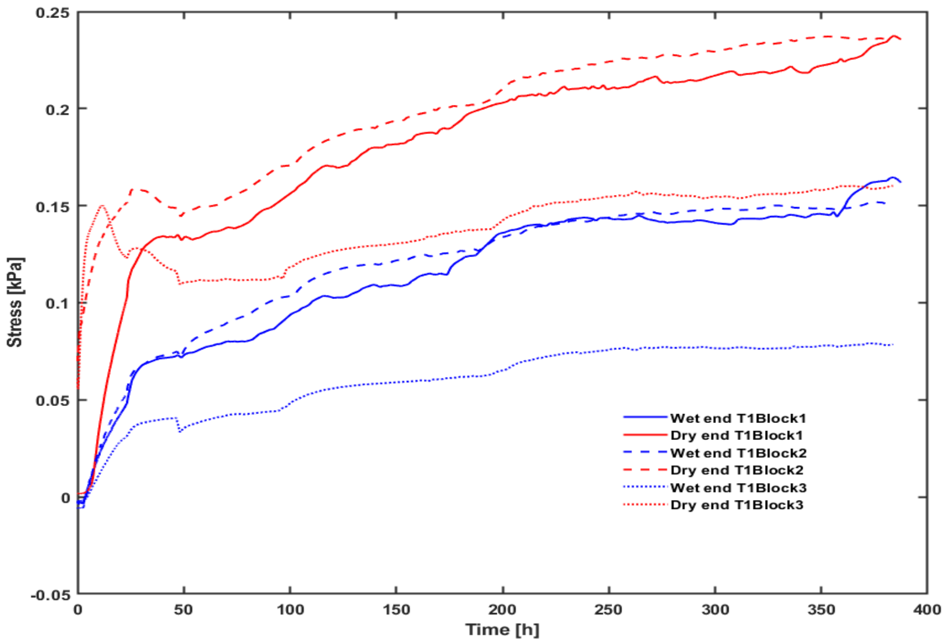


Figure 3: Axial swelling pressures of all the repeat measurements of sample with initial dry density of 1.4 g/cm3. Wetting solution (NaCl + $CaCl_2$) ionic strength in these experiments was 3.5 mmol/l.

Samples consisted broad set of experiments. Altogether 30 experiments were caried out with varying clay material, initial dry density and wetting solution composition and salinity. Saturation process for

individual sample test was monitored for 16 days. All the analyzed data has been made available in temporary data bank (http://users.jyu.fi/~joautant/BeaconDataBank.php).
What have been the main learning points from the work described above? (What have you learned from experiments or from modelling of experiments about the mechanical evolution and homogenization of bentonite?) The main learning point has been the strong influence the chemical salinity of the wetting water has on the swelling and saturation rates. Salinity also affects the swelling pressure values. Experiments with low salinity wetting water exhibit higher swelling pressures than high salinity. In fact, almost in all high salinity experiments pressure values seem negligible. This is partly due to the semi-free swelling of bentonite where energy is lost in initial void expansion. Chemical properties of bentonite seem to be crucial part of the experimental study of buffer material especially in future studies where thermomechanical properties are investigated.
What are the main outstanding uncertainties regarding mechanical evolution and homogenization of bentonite? Do you have any recommendations for how these could be investigated in future work? The experimental input should be increased even further to cover thermodynamical, hydromechanical and chemical coupling of clay material behavior. Experiments should also include more tests involving mechanical interaction in buffer-bedrock interface.
Are you aware of any external work since the start of the Beacon project which could feed into the Beacon project?

A.9 LEI

Description of the work your organisation has undertaken during the Beacon project (in Work Packages 3, 4 and/or 5)

Lithuanian Energy Institute (LEI) have participated in the modelling tasks of WP3 and WP5.

At the start of the project, model capabilities were limited only to the evaluation of transient water flow (Richard's approach). LEI developed hydro-mechanical model in WP3 and tested it against experiments of bentonite behaviour from WP5. Modelling tool COMSOL Multiphysics was used for the model implementation.
In parallel, two-phase flow formulation has been coupled with heat transfer and implemented in COMSOL Multiphysics in close cooperation with project partner VTT (Finland). Several staff exchange meetings were organized to share the knowledge and expertise in numerical model implementation aspects between modelling teams. Currently the work is ongoing to couple it with mechanical model.

In WP5 number of experiments of various forms and sizes of bentonite were modelled:

- Task 5.1 – three different laboratory scale tests were modelled using first formulation of mechanical part (linear swelling) in COMSOL Multiphysics. Limited agreement with experimental data were obtained. In parallel, two experiments were modelled using CODE_BRIGHT code (Richard's equation + BBM approach) to be confident on modelling assumptions and implemented mechanical model in COMSOL. By the end of the project, Test1a01 was re-run with the final model formulation in COMSOL Multiphysics which led to better agreement with experimental results.

- Task 5.2 – large scale FEBEX experiment was modelled using CODE_BRIGHT (THM processes coupling was not implemented in COMSOL Multiphysics at that time). In general, there was good agreement between LEI modelling results and measured data despite some discrepancies.

- Task 5.3 – five hydration experiments in an oedometer with two layers of FEBEX bentonite (pellets and block) were modelled using non-linear elastic swelling model implemented in COMSOL Multiphysics. Rather good agreement with experimental data was obtained. Due to limitation of the model (friction was not took into account), the same axial pressure profiles were obtained in the bottom and the top of the sample, which is not representative of such type of experiments. However, the peak pressure in the whole sample was predicted well that is crucial for repository safety.

- Task 5.4 – KBS-3 backfill homogenization assessment case was modelled using final formulation of non-linear elastic swelling model in COMSOL Multiphysics. Based on model output the backfill material would not be completely homogenized after fully saturated condition will be reached. The remaining heterogeneity is of such an extent that the difference between the block and the pellets varies between 10 % and 50 % in analysed sections in terms of void ratio. However, significant extent of homogenization was obtained compared to initial distribution of void ratios in both materials, where initial difference was about 200 %.

What have been the main learning points from the work described above? (What have you learned from experiments or from modelling of experiments about the mechanical evolution and homogenization of bentonite?)

The preliminary linear elastic hydro-mechanical model was applied for the task 5.1 tests in WP5 at the beginning of BEACON project. Limited agreement with experimental data was obtained with the first model formulation. During the project the model was developed further and finally evolves to non-linear elastic hydro-mechanical model. The final model formulation was used to re-run Test1a01 from task 5.1. The results were compared and better agreement with experimental data (compared to preliminary results) were obtained. Final formulation was also applied to test EPFL test case in WP3 and SKB assessment case in task 5.4.

The main improvement in the hydraulic part of the model was related to description of water retention curve. Water retention curve based on van Genuchten formulation with void ratio dependent air entry pressure was applied for particular tests. The tests where sample undergoes large deformations (free swelling) the need of suitable WRC was indicated and implementation of other forms than van Genuchten model was necessary.

The main improvement in the mechanical part of the model was related to definition of Young's modulus and swelling coefficient and their evolution. The comparison of modelling results and experimentally measured data indicated the trend that values of these parameters should be related to changes of saturation or/and porosity/void ratio changes instead of constant values.

The obtained results within WP3 and WP5 showed that model's predictive capabilities are limited for some analysed cases. The model output could be treated more as indicatory of trends (e. g., full saturation time under same hydration conditions, tendency of occurrence/absent of homogenization) but not the absolute values. In order to increase the predictive capacity of the model, the hydromechanical behaviour of bentonite under different material layouts, hydration conditions should be explored further experimentally and numerically. Further model developments are needed with the main focus of the consideration of friction (for laboratory scale experiments), the representation of irreversible strains.

What are the main outstanding uncertainties regarding mechanical evolution and homogenization of bentonite? Do you have any recommendations for how these could be investigated in future work?

During the mechanical model development there is a demand of various parameters characterising behaviour under external stress of the material of different type, density, form, different saturation, i.e. parameters from basic mechanical tests (oedometric tests, triaxial tests, etc.), measured water retention data. Some of those data could be found in published papers and separate reports over decades, potentially are compiled internally by different teams. However, the list of aspects playing an important role in overall bentonite behaviour is quite large, thus it was difficult to assess the scope, comprehensiveness and representativeness of available data. The sustainable database of bentonite material mechanical characterisation data in well-defined structure would be very beneficial for further model development and for assessment of needs for further experimental measurements (type, form, solution composition, boundary conditions, etc.).

The variability of modelling results of transitional phase during resaturation could be explored further by performing more experiments with the same set-up and identical samples. Within WP3 EPFL test was performed with 3 identical samples and transient swelling pressure evolution differed among the samples to some extent. Thus, it would be reasonable goal for numerical model to provide output within the range of experimental data. Nevertheless, the experimental procedure of sample preparation and test running have to be thoroughly followed and reported, measurement uncertainty should be reported too.

Are you aware of any external work since the start of the Beacon project which could feed into the Beacon project?

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A.10 Quintessa

Description of the work your organisation has undertaken during the Beacon project (in Work Packages 3, 4 and/or 5)

Quintessa have participated in the modelling tasks of WP3 and WP5.

In the first task of WP3, Quintessa participated in a series of benchmarking experiments to demonstrate fundamental capabilities of our model: irreversibility of strain, swelling pressure dependence on dry density, stress path dependence, temperature dependence. The stress path dependence was then quantitatively tested by modelling a set of EPFL oedometric tests.

In the first task of WP5, we built a series of 1D and 2D HM models of laboratory swelling experiments. This required modelling of both bentonite blocks and pellets (MX-80). Pellets were represented as a bulk medium with a low average dry density. A few different techniques for modelling the behaviour of pellets were tested (e.g. introducing a delay term in the swelling equation to represent water filling the voids between pellets). A simple specified-stress boundary condition was used to represent bentonite swelling into a fixed-volume void, but this was found not to be a good representation of swelling into a water-filled void (since it does not allow for immediate stress buildup). Further work is being done to improve our model of swelling into voids by looking at a series of BGS experiments. A friction boundary condition was developed to explain observations in one of the experiments. The third task of WP5 involved modelling of similar block-pellet laboratory experiments, in which blind predictions were made for one of the experiments.

In the second task of WP5, we built a THM model of the in-situ FEBEX experiment. Model parameters were updated to represent FEBEX bentonite and include thermal dependency (vapour diffusion, thermal expansion, and temperature-dependent water retention). 2D R-Z and R-theta models were built to investigate profiles of dry density in different directions. In the final task of WP5, we are building a model of Andra's assessment concept.

These models have all been built in QPAC, Quintessa's in-house code, using the same fundamental Internal Limit Model.

In WP3, work has been ongoing to implement bentonite models in COMSOL. This will enable comparison with the QPAC models and improve our 3D THM capabilities. We have independently implemented Richards Equation in COMSOL and are progressing by coupling this to the BBM.

What have been the main learning points from the work described above? (What have you learned from experiments or from modelling of experiments about the mechanical evolution and homogenization of bentonite?)

Friction appears to be a key process in some experiments. To model the Posiva laboratory swelling test (Task 1c, WP5) successfully, a friction boundary condition needed to be added to the model. This explained behaviour like different axial stresses at different heights in the sample. In other laboratory experiments where the surfaces were lubricated, friction did not seem to be as important. It is not clear whether friction will also be significant for large-scale systems.

Final states (stresses, dry densities, water contents) appear to be easier to predict than transients, which show more variation. In the FEBEX in-situ test, the rate of saturation varied significantly between sensors at the same radial and axial positions (by 1000s of days), suggesting heterogeneity in the sample. The models presented by teams often showed a lot of variation in the predicted stress transients, with more agreement on equilibrium values. There also appears to be variation between different experiments, suggesting transient behaviour may be sensitive to initial conditions and heterogeneities in the bentonite.

Bentonite does not appear to swell freely into water-filled voids. Experiments with such voids (e.g. SKB's experiment in Task 1a01, WP5) show an immediate buildup of axial stress, with no period of delay before the bentonite reaches the container lid. This suggests that model boundary conditions need to consider the interaction between the bentonite and water phases. There is some observational

evidence that highly-saturated bentonite at these type of boundaries behaves more like a 'gel' than a porous solid, which may require a different modelling approach.
What are the main outstanding uncertainties regarding mechanical evolution and homogenization of bentonite? Do you have any recommendations for how these could be investigated in future work? It is not always clear to what extent experimental behaviour is repeatable or how much it depends on very specific conditions under which the bentonite sample is prepared and saturated. The main uncertainties appear to be in the transient behaviour of swelling/stress evolution, which is difficult to compare quantitatively between experiments. It could be useful to run a series of identical experiments in which different laboratory teams follow the same set of procedures, and compare the range of behaviour in the results. There is also some uncertainty in scaling up experiments – how confident can we be that behaviour observed in the laboratory will be important in full-scale bentonite buffers?
Are you aware of any external work since the start of the Beacon project which could feed into the Beacon project?

A.11 University of Liège

Description of the work your organisation has undertaken during the Beacon project (in Work Packages 3, 4 and/or 5) WP3: • improvement of BBM, parameters evolution with stress and suction state. • BBM Parameters calibration as a function of density • Advanced use of friction interface model • Development of a new mechanical constitutive model, with double structure (Mohymar) • Validation of the 2 models, advanced BBM and Mohymar, on the benchmark based on EPFL tests. WP5: Most benchmarks have been done. When multiple options were possible, we have modelled the EB in situ test and the Andra assessment case.
What have been the main learning points from the work described above? (What have you learned from experiments or from modelling of experiments about the mechanical evolution and homogenization of bentonite?) BBM model performed well, surprisingly well compared to more complex models. However, some limitations invited us to build a new constitutive model (that still need to be used and valorized!). Double porosity models help understanding bentonite transient behavior. However, models with 2 porosity scale and experimental PSD curves are not easy to compare. Double porosity, mechanical aspects and water transfer aspects need to be considered. But how to demonstrate their added value? Friction on interfaces has been modelled in some benchmark, and has proved to give improvement of results. In the French concept, seal friction on liner or on clay host rock is an important aspect of the mechanical answer. Swelling at low level of suction / of stress: the BBM is not well designed for such state. Granular bentonite (incl pellets) was modelled successfully with BBM, as well as bentonite block. Existing constitutive models may be used for such “new” material. Transient behavior is less accurately modeled than final state. We pointed that the MGR tests by Ciemat are of great interest as they provide intermediate results at early time, with a lot of details (experiments stopped at an early time, and post-mortem data available at theses early times). Numerical simulations are expensive: the need a lot of modeler / engineer time, they are complex, strongly nonlinear and coupled. So not easy to manage! This don’t help to do variation, sensitivity analysis, etc., while it would be really interesting.
What are the main outstanding uncertainties regarding mechanical evolution and homogenization of bentonite? Do you have any recommendations for how these could be investigated in future work? Small heterogeneities, density varying of 0.05 to 0.10: how do the model parameters vary for such small density changes? Not clear presently! Constitutive models parameters: not easy to have data sets for various densities, including the initial density heterogeneity (in place before hydration). Need to improve this information, to elaborate.

Deviatoric stress paths are not enough explored experimentally: friction angle of bentonite? Depending on the saturation / suction or constant? Value? Also important for the experimental results analysis: deviatoric behavior will drive the radial stress development, which is a significant part of the friction mobilization. But what is the constitutive behavior or friction with variable suction? We lack experimental data. There is a lack of experimental data about swelling at low level of suction / of stress, which don't help to elaborate an improved model. Permeability is not enough documented. Especially permeability of granular bentonite in the dry state (before wetting) is probably very high, while decreasing quickly at the wetting beginning. But this was difficult to quantify. Efforts should be paid on transient behavior during a next research program. Test like the MGR one which are stopped at early times of evolution are very interesting for these early post mortem data.
Are you aware of any external work since the start of the Beacon project which could feed into the Beacon project? No

A.12 UPC

Description of the work your organisation has undertaken during the Beacon project (in Work Packages 3, 4 and/or 5)

In the BEACON project, UPC has contributed to the activities of WP3 and WP5.

The work concerning the development of the formulation and its implementation in a computer code have been performed within WP3. Given the main objective of the project, preferential attention has been given to the mechanical constitutive model, a double structure (or double porosity) model that distinguishes two structural levels: macro and micro. The basic physicochemical phenomena that underlie the swelling properties of the bentonite correspond to the microstructure leading to a behaviour that is assumed reversible but nonlinear. The macrostructural level corresponds to the overall arrangement of the larger components of the medium such as aggregates. The macro level is influenced by the microstructural strains, often in an irreversible manner. The relationship between the two structural levels is defined by two interaction functions, one for wetting paths and another one for drying paths, A feature of the model is the possibility of tracking the evolution of macro and micro porosities throughout the analysis yielding results that can be related to microstructural experimental observations.

In the initial stages of the project, a number of significant modifications were introduced to the existing constitutive model formulation. The most salient ones are: a more consistent definition of porosity and volume fractions, the fact that the microstructure may be unsaturated, and it is not assumed that there is hydraulic equilibrium between microstructure and macrostructure. The micro-macro transfer of liquid (or, sometimes, gas) is governed by a linear law between flow and micro-macro potential difference at a rate controlled by a newly introduced leakage parameter. Subsequent developments have included the clarification of the physical meaning of the interaction functions via DEM simulations and the examination of the relationship between the micro and macro elastic components that lead to a direct relationship between the two sets of elastic parameters.

In the latter part of the project, the main activity has been related to the incorporation of thermal effects into the double structure constitutive law in a rigorous manner. This has required the modification of a large proportion of the model formulation. The work is still ongoing but a first version incorporating the thermal expansion of constituents and of the overall medium is available and has been used to perform the analysis of a non-isothermal assessment case.

Model developments have also involved the hydraulic component of the formulation. Variations of permeability depend only on the macro porosity, a more realistic assumption that, in addition, allows to examine the effect of evolving microstructure. This is consistent with the assumption that advective flow takes place in the macrostructure. The exchange of water (or gas) between micro and macro levels occurs at a local level only; this has the added advantage that the potential (or suction) at micro level becomes a local variable, reducing in this way the number of global degrees of freedom. Also, separate retention curves are defined for each structural level, as the microstructure may now be unsaturated.

Finally, there has been continuous work on the model implementation in the computer code (that it is still ongoing) to improve the convergence performance of the calculations. This is especially necessary when thermal effects are incorporated. Special attention has been given to the precise calculation of the Jacobian under a variety of conditions. The numerical algorithm requires still improvements for the non-isothermal model.

WP3 also includes a Task (3.3) devoted to the verification of the basic features of the models against simple benchmarks. For this purpose, a set of oedometer laboratory tests on MX-80 bentonite performed by EPFL were selected that included MIP porosimetry determinations at various stages of the experiments. The constitutive model has been able to represent correctly most of the observed features of behaviour: development of large swelling strains at low confining stresses, occurrence of a sharp yield during saturated compression, stress path dependency and a realistic value of swelling pressure. However, the model does not yield the convergence of consolidation lines at large stresses. The evolution of micro and macro porosity obtained from the model appears consistent with porosimetry results, although it also highlights the difficulty of defining precisely the boundary between the two levels of porosity.

The application of the model developed to the solution of boundary value problems constitutes the UPC contribution to WP5. WP5 is organized in four successive steps; UPC has contributed to all of them. All analyses have been performed using the computed code CODE_BRIGHT.

Step 1 includes a series of deceptively simple laboratory tests structured in three different sets of tests: bentonite swelling into a void performed by Clay Technology (1a), a constant-volume swelling test on a pellets mixture carried out by CEA (1b) and the hydration of a specimen composed by pellets poured on top of a bentonite block, performed by POSIVA (1c). The performance of the model was generally highly satisfactory not only in terms of the final state of the sample but also regarding its transient evolution. The main exception is the axial pressure of case 1c. As friction was not included in the analysis, the different axial pressures at both ends of the sample measured in the test could not be reproduced.

Step 2 refers to large scale tests; UPC selected the EB experiment for analysis. The EB test involves the artificial hydration of an engineered barriers that include bentonite blocks and granular bentonite (pellets). The practically complete homogenization between blocks and pellets is successfully reproduced by the analysis. There are more differences between observations and model results regarding the transient hydration period. However, it should be pointed out that the degree of control of the process of artificial hydration was not high and the level of instrumentation in the barrier was rather sparse. In addition, a sensitivity analysis was performed to check on the effects of two of the most uncertain components of the formulation: retention curve and interaction functions.

Step 3 is based on a series of isochoric oedometer hydration tests performed by CIEMAT on samples constituted by bentonite pellets and a compacted bentonite block. Different hydration conditions were applied. Three tests were selected for the step, two of them intended for calibration and the third one for blind prediction. The UPC work in this step was delayed because of the Covid-19 pandemic. It coincided with a change of personnel and the necessary training of new researchers was hindered by lockdown restrictions. For this reason, the UPC results of this step were only partially reported in Deliverable 5.6; the analyses of this step have now been completed and are fully reported in Deliverable 5.7. The spirit of blind prediction has been kept by using for test MGR27 the same parameters as for the two calibration tests without any modification. In all cases, there has been a quite large degree of axial homogenization between pellets and block that has been well captured by the analyses. The type of evolution and final value of the swelling pressure is also well reproduced by the model but there are significant departures concerning the time evolution of the hydration and of the pressure development during the transient period. Also, the non-consideration of lateral friction prevents a good prediction of the swelling pressure value in the MGR27 test. The development of interface formulations for friction modelling is under way, based on thin finite elements, but they are not fully implemented yet. Micro and macro porosity results obtained from the double structure model appear largely consistent with observations.

Finally, Step 4 refers to the analyses of assessment cases; UPC has analysed that proposed by NAGRA. It involves an engineered barrier made up of bentonite blocks and pellets subjected to heating and natural hydration from the rock. The goal is to examine the evolution of the dry density of the barrier during the initial thermo-hydro-mechanical transients. Because of the non-isothermal nature of the case, the model including thermal effects has been used. Because the development of the formulation is still not fully complete, there are a number of convergence difficulties and the final time of the analysis (10000 years) has not been yet achieved at the time of writing this contribution.

What have been the main learning points from the work described above? (What have you learned from experiments or from modelling of experiments about the mechanical evolution and homogenization of bentonite?)

The double structure model appears to fulfil most of the criteria required for adequate modelling of the bentonite mechanical behaviour, as identified in WP3. It also seems to have a good capability to reproduce most experimental results proposed for analysis in the project. It seems that the same

basic constitutive model can be used for bentonite pellets and bentonite blocks, by choosing appropriate parameters. In general, dry density distributions and swelling pressures have been more successfully modelled than transient hydraulic behaviour. This may simply reflect the sensitivity of the hydration process to uncertain parameters such as retention curves and saturated and unsaturated hydraulic permeability, but it may also indicate more fundamental limitations of the formulation concerning hydraulic phenomena. It has also been possible to identify some shortcomings of the model that may require further developments: - the adoption of Bishop effective stress for the microstructural behaviour links closely the effects of suction and stress changes when, in fact, the material response may be quite different, - a more constrained manner to determine and calibrate the interaction functions is required - the variation of permeability with fabric changes should be reviewed and the formulation modified accordingly - the use of a double structural model introduces a considerable level of complexity in the analyses and requires more computing power. The need for such an approach should be carefully evaluated for each particular case analysed. This appears to be especially relevant in non-isothermal problems - friction has proved to be significant, at least in some laboratory tests. It should be introduced in the analyses It should also be mentioned that the predictive power of the model is largely unproven. The only prediction exercise involved calibration tests quite similar to the test to be predicted. It is uncertain how the predictive power may differ across a wider range of conditions.
What are the main outstanding uncertainties regarding mechanical evolution and homogenization of bentonite? Do you have any recommendations for how these could be investigated in future work? It is apparent that a large degree of homogenization is achieved in many of the cases examined in then project but full homogeneity is not ensured. It has not been established the dependence of the degree of homogenization on boundary conditions (hydraulic and/or thermal), geometry, type of materials) on a sufficiently firm basis. Because of the uncertainty concerning the predictive capability of the models, the knowledge acquired may not be sufficient to provide reliable predictions on he likely homogenization of new or different designs. A more complete assessment of the predictive power of the existing models would appear advisable. There is also uncertainty in the determination of hydraulic parameters and their variation when the fabric of the material evolves. This may underlie the shortcomings exhibited by a number of analyses regarding the modelling of transients. The double structure model attempts to follow, in some way, the evolution of the microstructure by tracking the changes in macro and micro porosity but does not include the all-important (for permeability) variations of pore size. It seems evident that models that incorporate changes of bentonite fabric should have an advantage when predicting bentonite behaviour. The difficulties of such an approach, however, should not be underestimated such as, for instance, establishing a criterion for distinguishing between porosity levels. The tempting possibility of increasing the number of porosity levels is likely to lead to formulations of excessive complexity.
Are you aware of any external work since the start of the Beacon project which could feed into the Beacon project? The WP7 of the EURAD project contains a Task (3) devoted to bentonite material. However, the focus is on the effects of high temperature on bentonite and therefore not really aligned with the main objectives of BEACON

The SKB Task Force on Engineered Barriers has an ongoing task on unsaturated homogenization based on tests performed by CIEMAT within the BEACON project. No results have been reported yet.

A.13 VTT

Description of the work your organisation has undertaken during the Beacon project (in Work Packages 3, 4 and/or 5) WP3: limited input in the form of participating deliverable D3.1 with working time moved from Posiva. WP4: no particapation WP: Modelling the WP5.1tests and performing sensitivity analysis of SKB assessment case WP5.4. Also simulation of CRT in WP5.2 which was not initially planned.
What have been the main learning points from the work described above? (What have you learned from experiments or from modelling of experiments about the mechanical evolution and homogenization of bentonite?) Use of sensitivity analysis in modelling gives rational means to identify the most important parameters with respect to specific applications. The performed sensitivity analysis in WP5.4 was useful in identifying the key parameters for the bentonite mechanical evolution in the SKB tunnel case. The progressing complexity in WP5.1 test cases from blocks to pellets and their mixtures resulted in realization that a third porosity level is needed for 1) the model concept to better match the experiments and 2) double porosity model parameters to remain physically meaningful.
What are the main outstanding uncertainties regarding mechanical evolution and homogenization of bentonite? Do you have any recommendations for how these could be investigated in future work? Uncertainties in the basic model parameters and their statistics, in model concepts and related to differently processed materials (e.g. granular fills). For example, more detailed data would be needed for better sensitivity analysis and the time evolution of the wetting profiles is not well captured by the current models.
Are you aware of any external work since the start of the Beacon project which could feed into the Beacon project? Work performed in EC EURAC Hitec and in the Finnish Research Programme on Nuclear Waste Management (KYT)

Appendix C: Experiment Database

Appendix B Reference No	Name/title	Organisation	Name of contact	Start and end dates	Duration	Bentonite type	Bentonite form	Availability of material parameters: Swelling	Retention curve	Shear strength	Tensile strength	Hydraulic conductivity	Microstructur	Other	Scale	Purpose of experiment	Evidence of heterogeneity	Boundary Conditions	Water Chemistry
1.1	Analysis of microstructural images of bentonite samples	Hokkaido University													Lab				
1.2	Artificial wetting tests	VTT, Posiva	Veli-Matti Pulkkanen	2011-2012	3-57 days	MX-80, (Cebogel pellets in some tests)	Blocks (uniaxially and isostatically compacted), pellets (different types), slurry	Mx-80 (Y)	Mx-80 (Y)	Mx-80 (partially)	Mx-80 (partially)	Mx-80 (Y)	Mx-80 (Y)		Lab (cylinder with 36 cm radius, 39 or 47 cm height)	Swelling and homogenisation of bentonite in downscaled buffer geometry including compacted blocks and different installation gap fillings (pellets, slurry)	Density and water content profiles in post-mortem analyses	Stainless steel chamber, wetting from bottom valve (flooding of the installation gap)	Different water salinities, (tap water, groundwater, groundwater simulants)
1.3	Bentogaz	CEA, Andra	Jean Talandier			MX-80	Blocks (Mx80/ sand mixture)/ pellets (pure MX-80)/ interfaces	Y	Y	Y	Y	Y			Lab	HM-Gas behaviour	Differences in radial and axial responses during hydration	Constant volume cell/slow water saturation	Synthetic Bure water
1.4	Bentonite homogenisation	BGS	Jon Harrington	3 experiments performed between 01-10-2014 to 02/12/2016	146 – 347 days	MX-80	Single block	Y	N	N	N	Y	N	Complete	Lab (cylindrical sample dimensions: length =120 mm, diameter = 60 mm)	Hydration behaviour of bentonite examining the spatial and temporal development of porewater pressure, stress and permeability	Yes in both stress and porewater pressure data	Constant volume, 1D flow	DI water
1.5	Bentonite re-saturation project	Radioactive Waste Management Funding and	Patrik Sellin	?	164 days	Na Bentonite (Kunigel V1)		Y	N	N	N	N	N		Lab	Homogenization of a block-pellet system	Yes, both in swelling pressure and final dry density	Flooded with water at low head	Distilled water as well as 0.5 M NaCl

Appendix B Reference No	Water Content: Initial	Final	Time Series	Spatial	Pore pressure /suction: Initial	Final	Time Series	Spatial	Relative humidity: Initial	Final	Time Series	Spatial	Strain: Initial	Final	Time Series	Spatial	Dry density: Initial	Final	Time Series	Spatial	Stress: Initial	Final	Time Series	Spatial	Radial	Axial	Other	Data quality	Modelled?
1.1																													
1.2	Y	Y	N	Y	N	N	N	N	N	N	N	N	N	N	N	N	Y	Y	N	Y	Y	Y	Y	Y	Y	Y	Axial displacement of the top lid	Good	Yes (some tests in the series have been modelled)
1.3	Y	Y	Y		Y	Y	Y	Y	N	N	N	N	N	N	N	N	Y	Y			Y	Y	Y	Y	Y	Y	Axial swelling pressure, gas transfer	Good (well-defined geometry, material already characterized during ESDRED project. Swelling pressure, liquid and gas pressures recorded)	Yes (for some of them-HM)
1.4	Y	Y	N	N	Y	Y	Y	Y	N	N	N	N	N	N	N	N	Y	Y	N	N	Y	Y	Y	Y	Y	Y	Swelling pressure, porewater pressure, permeability	A number of highly instrumented tests have been at different hydraulic gradients. All tests performed under controlled temperature (isothermal) conditions, with inflow (and where appropriate outflow) monitored with time.	Yes (limited)
1.5	Y	Y	Y	N	N	N	N	N	N	N	N	N	N	N	N	N	Y	Y	N	Y	Y	Y	Y	Y	Y	N	Swelling pressure, resistivity	Good (well-defined geometry, THM material characterisation, large number of sensors to	Yes (scoping calculations)

Appendix B Reference No	Name/title	Organisation	Name of contact	Start and end dates	Duration	Bentonite type	Bentonite form	Availability of material parameters							Scale	Purpose of experiment	Evidence of heterogeneity	Boundary Conditions	Water Chemistry	Availability of material parameters																										Data quality	Modelled?
																				Water Content				Pore pressure /suction				Relative humidity				Strain				Dry density				Stress						Other		
								Swelling	Retention curve	Shear strength	Tensile strength	Hydraulic conductivity	Microstructur	Other						Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Radial	Axial			
		Research Centre, SKB																																													follow HM evolution, has not been used before as benchmark)	
1.6	Block-pellet homogenization in KBS-3V buffer	Posiva	Veli-Matti Pulkkanen			MX-80									Lab																					Y	Y		Y							Swelling pressure		
1.7	Buffer homogenisation project	Clay Technology AB, SKB	Mattias Åkesson /Ann Dueck	2008 to now	months - 2.5 years	MX-80, Calcigel	Blocks (block and powder - only Calcigel)	Y						Friction*	Lab (cm-dm)	Study the homogenisation processes	Initial voids, initial density contrast	Confined conditions	De-ionized water	Y	Y	N	Y	Y	Y	Y	N	N	N	N	N					Y	Y	N	Y	Y	Y	Y	Y	Y	Y		Good (small scale, simple geometries, well defined boundary conditions, suitable for modelling)	Yes (HM)
1.8	Centrifuge physical modelling test	CRIEPI				Na Bentonite									Lab experiment using reduced physical model																	Y	Y	Y	Y													Yes (THM)
1.9	Characterization of material properties	Clay Technology AB, SKB	Mattias Åkesson /Ann Dueck	1995-2013	weeks - months	MX-80	Blocks or powder	Y	Y	Y				*	Lab (compilation) (cm-dm)	Compile material model parameters for HM modelling		Mainly confined conditions	De-ionized water	Y	Y	N	N	N	N	N	N	N	N	N	N					Y	Y	N	N	Y	Y	N	N	Y	Y	Oedometer tests considered only	Good (suitable for characterization, evaluation of model parameters and modelling)	No
1.10	Clay hydration characterisation using microfocus x-ray CT	SCK-CEN													Lab																																	
1.11	CTU lab experiments	CTU	Jiří Svoboda			Ca-Mg	Blocks, Pellets, Powder	Y	Y				?Y		Lab - cylinder d=30mm (or 120mm), h=20m	Permeability and swelling pressure measurement in constant volume cell	Pellet samples; Heterogenous samples (dual density) planned as	Artificial saturation, constant volume cell	Distilled water or Natural ground water (Josef URL)	Y	Y	N										N	N	N	N	Y	Y	N	N	Y	Y	Y	N	N	Y	Swelling pressure. Spatial dry density can be measured	Good (great calibration and validation tool for material models. Highly controlled boundary conditions	Yes (some of them)

Appendix B Reference No	Name/title	Organisation	Name of contact	Start and end dates	Duration	Bentonite type	Bentonite form	Availability of material parameters: Swelling	Retention curve	Shear strength	Tensile strength	Hydraulic conductivity	Microstructur	Other	Scale	Purpose of experiment	Evidence of heterogeneity	Boundary Conditions	Water Chemistry	Availability of material parameters: Water Content: Initial	Final	Time Series	Spatial	Pore pressure /suction: Initial	Final	Time Series	Spatial	Relative humidity: Initial	Final	Time Series	Spatial	Strain: Initial	Final	Time Series	Spatial	Dry density: Initial	Final	Time Series	Spatial	Stress: Initial	Final	Time Series	Spatial	Radial	Axial	Other	Data quality	Modelled?
															m (typically for D30)		part of other WP																													in future tests.	and well defined material.)	
1.12	CUNI laboratory test	Charles University	David Mašín			B75 Czech Ca-Mg		Y	Y	N	N	Y	Y		Lab	Swelling under constant load, free swelling experiments, oedometric compression curves	Element tests, no heterogeneities	Oedometric	Natural groundwater	Y	Y											Y	Y	Y	N	Y	Y	Y	N	Y	Y	Y	N	N	Y		Good	Yes (intermediate model calibration, not all data available yet, calibration to be finalised)
1.12	CUNI laboratory test	Charles University	David Mašín			B75 Czech Ca-Mg		Y	Y	N	N	Y	Y		Lab	Vapour equilibrium water retention curves	Element tests, no heterogeneities	zero stress	Natural groundwater	Y	Y	Y		Y	Y	Y		Y	Y	Y		Y	N	Y	N	Y	Y	Y	N	Y	Y	Y	N	Y	Y		Good	Yes (intermediate model calibration, not all data available yet, calibration to be finalised)
1.13	Effects of heterogeneities on the hydromechanical behaviour of bentonite	Andra	Jean Talandier			MX-80	pellets/ blocks	Y	Y	Y	Y	Y	Y		Lab	HM-Gas behaviour	heterogeneities in pellets mixture + initial voids															Y	Y	Y	N		Y	N										Yes
1.14	Experimental characterization of cement bentonite	University of Bern				MX-80									Lab																																	

Appendix B Reference No	Name/title	Organisation	Name of contact	Start and end dates	Duration	Bentonite type	Bentonite form	Availability of material parameters							Scale	Purpose of experiment	Evidence of heterogeneity	Boundary Conditions	Water Chemistry	Availability of material parameters																										Other	Data quality	Modelled?
																				Water Content				Pore pressure /suction				Relative humidity				Strain				Dry density				Stress								
								Swelling	Retention curve	Shear strength	Tensile strength	Hydraulic conductivity	Microstructur	Other						Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Radial	Axial			
	interaction																																															
1.15	FORGE	Clay Technology AB, SKB	Mattias Åkesson /Ann Dueck	2009-2013	days - weeks	MX-80, Wyoming Na/ Ca	Blocks or powder	Y				Y		*	Lab (mm-cm)	Study response in bentonite due to external fluid/gas pressurization	Density re-distribution in compacted bentonite	Controlled pressurized fluid/gas, confined conditions	Water (initially de-ionized)	Y	Y	N	N	Y	Y	Y	N	N	N	N	N					Y	Y	N	Y	Y	Y	Y	N	N	Y	Gas transfer	Good (small scale, simple geometries, well-defined boundary conditions so tests with applied water pressures suitable for modelling)	Yes (analytical)
1.16	FSS laboratory tests+mock-up	CEA, Andra	Jean Talandier			WH2 MX-80	Pellets	Y	Y	Y	Y	Y			Lab/ mock-up	HM-Gas behaviour	Initial dry density variable	Slow water flow to saturate	Synthetic Bure water/cementeous water	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	N	N	N	N	Y	Y			Y	Y	Y	Y	Y	Y	Swelling pressure	good (data available at several scales from few centimeters to meter scale)	No
1.17	Gas release of bentonites	GRS	Klaus Wieczorek	Jan. 2015, ongoing	3 years (planned)	Various	Bentonite powder	N	N	N	N	N	N		Lab	Quantify gas release capacity and verify origin of released gases for 15 bentonites	No	Powder and solution in gastight containers at 120 °C, fully confined	Diluted caprock solution, 150 g/l salinity	Y	Y	Y	N	Y	Y	Y	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	Temperature, gas pressure, swelling pressure (post-mortem)	Not applicable for Beacon purposes	No
1.18	Microstructure and anisotropic swelling behaviour of compacted bentonite /sand mixture	IRSN, Laboratoire Navier				MX-80									Lab																																	
1.19	Microstructure of saturated bentonites	Hokkaido University				?									Lab																																	
1.20	Physico-chemical controls on	University of California				?									Lab																																	

Appendix B Reference No	Name/title	Organisation	Name of contact	Start and end dates	Duration	Bentonite type	Bentonite form	Availability of material parameters							Scale	Purpose of experiment	Evidence of heterogeneity	Boundary Conditions	Water Chemistry	Availability of material parameters																										Other	Data quality	Modelled?
								Swelling	Retention curve	Shear strength	Tensile strength	Hydraulic conductivity	Microstructur	Other						Water Content				Pore pressure /suction				Relative humidity				Strain				Dry density				Stress								
																				Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Radial	Axial			
	initiation and evolution of desiccation cracks																																															
1.21	Re-saturation of bentonites	GRS	Klaus Wieczorek	Oct. 2001 - Sep. 2003	25 months	MX-80	Compacted powder	N	N	N	N	N	N		Lab	Gather detailed data on the transient water content distribution in the bentonite	No	Artificial saturation, ambient temp., fully confined	Äspö solution	Y	Y	Y	Y	N	N	N	N	N	N	N	N	N	N	N	N	Y	N	N	N	N	N	N	N	N	N		Good - but no mechanical data	Yes
1.22	SB (laboratory tests)	GRS, Nagra	Klaus Wieczorek	Jan. 1995 - Dec. 2007		Calcigel	Granular sand/bentonite mixture	Y	N	N	N	Y	N		Lab	Qualify sand/bentonite mixtures as material for engineered barriers			Pearson water																											gas breakthrough pressure		Yes
1.23	SEALEX laboratory tests	IRSN				MX-80	Powder and pellets								Lab					Y	Y	Y	N	Y	Y	Y	Y													Y	Y	Y		Y	Y			Yes
1.24	Sealing Site Investigation Boreholes Phase II: laboratory program	Clay Technology AB, RWM	Mattias Åkesson /Ann Dueck	2016	weeks - months	Wyoming Na, MX-80	Blocks or powder	Y				Y		*	Lab (cm)	Study impact of different saline solutions on swelling pressure and hydraulic conductivity		Controlled saline conditions, confined conditions	De-ionized water and saline solutions with different ions and strength	Y	Y	N	N	N	N	N	N	N	N	N	N					Y	Y	N	N	Y	Y	Y	N	N	N	Hydraulic conductivity, swelling pressure	Good (small scale, simple geometry, well-defined boundary conditions with different cat ions and ion strengths, suitable for MC modelling)	No
1.25	Swelling pressure development of compacted bentonite	LEMTA, BRGM, LIEC	Jean Talandier			Kunipia-G	block	Y	Y			Y	Y		Lab	Microstructure evolution on wetting path			Aqueous solutions with different ionic strength	Y	Y	Y	Y													Y	Y											Yes
1.26	Swelling pressure material test	CRIEPI				Na-type + Ca-type									Lab					Y	Y	N	N	Y								Y	Y		N											Swelling pressure		No
1.27	THEBES	JyU, Aalto University	Markku Kataja	1.2.2015-ongoing	4	MX-80 + purified	Small scale samples	Y	N	N	?	Y	N		Lab	Non-intrusive measurement of time evolution of dry	Sample heterogeneit	Simple	NaCl solution	Y	Y	Y	Y	N	N	N	N	N	N	N	N	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	N	Y		Good (Time series data of strain (displacement), dry	Yes. Modelling

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								Swelling	Retention curve	Shear strength	Tensile strength	Hydraulic conductivity	Microstructur	Other						Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Radial	Axial			
						(BP Biomedicals)	compacted from powder									density and water content for model validation purposes.	y directly measured																														density and water content inside the sample during wetting process)	efforts ongoing.
1.28	Transu	Posiva Oy, Saanio & Riekkola Oy	Veli-Matti Pulkkanen	2011	32-133 days	MX-80	Compacted blocks, pellets	Mx-80 (Y)	Mx-80 (Y)	Mx-80 (partially)	Mx-80 (partially)	Mx-80 (Y), Ibeco RWC (Y)	Mx-80 (Y)		Lab	Study of saturation behaviour of buffer	Initial density heterogeneity between block and pellets	Artificial hydration	?	Y	Y	Y	Y	Y	Y	Y	Y	N	N	N	N	Y	Y	Y	Y	N	N	N	Y	Y	Y	Y	Y	Y	Y			
1.29	Water retention behaviour of compacted bentonites	Andra	Jean Talandier			Various	Pellets								Lab																									Y	Y	Y	Y	Y	Y			Yes
1.30	X-Boy	Posiva Oy, Saanio & Riekkola Oy	Veli-Matti Pulkkanen	2010-2011	69-122 days	MX-80	Compacted blocks, pellets	Mx-80 (Y)	Mx-80 (Y)	Mx-80 (partially)	Mx-80 (partially)	Mx-80 (Y), Ibeco RWC (Y)	Mx-80 (Y)		Lab	Study of early saturation behaviour of buffer	Initial density heterogeneity between block and pellets	Artificial hydration	?	Y	Y	Y	Y	N	N	N	N	N	N	N	N	N	N	N	N	Y	Y	N	Y	Y	Y	Y	Y	Y	Y	Temperature		
1.31	X-ray CT visualization of a clay liner	Kumamoto University				Na bentonite	Granular								Lab					Y	Y	Y		N	N	N	N					N	N	N	N					N	N	N	N	N	N	Temperature		
1.32	Microstructural and hydro-mechanical behaviour of bentonite pellets and powder mixtures	Universitat Politecnica de Catalunya		2020		MX-80	Pellets and powder	Y	Y	Y	Y	Y	Y		Laboratory	Describing the initial state of a MX-80 and bentonite powder mixture and the main microstructural features.	Mixture of pellets and powder			Y	Y	N		N	N	N	N	N	N	N	N	N	N	N	N	Y		N	Y	Y	Y			N	Y	Porosimetry		
1.33	Swelling behavior of	Laboratoire Navier/CER		2019	1 year	MX-80	Compacted powder	Y	Y	Y	Y	Y	Y		Laboratory	Investigating the influence of a rock fracture on the	Heterogeneous hydration	Hydration through rock fracture at		N	N	N	N					Y	Y	Y	Y	Y	Y	Y	N	Y	Y	N	Y	Y	Y	Y	Y					

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								Swelling	Retention curve	Shear strength	Tensile strength	Hydraulic conductivity	Microstructur	Other						Water Content				Pore pressure /suction				Relative humidity				Strain				Dry density				Stress						Other		
																				Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Radial	Axial			
	compacted bentonite with the presence of rock fracture	MES, Hobai University														swelling behaviour of compacted bentonite	(artificial fracture)	constant pressure, constant volume																														
1.34	X-ray computed tomography, pellet swelling	Geological Survey of Finland		2020		Cypriot Kato Moni bentonite, Tsukinuno bentoniote, Dobuyama bentonite, MX-80	Pellets and Blocks								Laboratory	XCT is applied to improve the textural and structural characterisation of natural and man-made bentonite samples	Micro fracturing, initial density variation		MilliQ water																											XCT		
2.1	BBI	VTT, Posiva	Veli-Matti Pulkkanen	5.5.2015-6.7.2015	2 months	MX-80, Ibeco RWC, Cebogel	Blocks, pellets	Mx-80 (Y)	Mx-80 (Y)	Mx-80 (partially)	Mx-80 (partially)	Mx-80 (Y), Ibeco RWC (Y)	Mx-80 (Y)		Lab (1/6 scale)	Interaction between the buffer and the backfill, formation of flow paths, erosion	Density and water content profiles in post-mortem analyses, flow channels	Single point-wise water inlet in buffer, flow rate 0.1 l/min, several water outlets in backfill, plexi-glass walls in steel frame, isothermal conditions (ambient temperature)	Salinity of 1 % (NaCl solution)	Y	Y	N	Y	N	N	N	N	N	N	N	N	Y	Y	Y	Y	Y	Y	N	Y	Y	Y	Y	Y	Y	Y	Water sampling at outlet (eroded mass), video monitoring of flow paths, wetting patterns	Good	No
2.2	FEBEX mock up	CIEMAT	María Victoria Villar	Feb-97	>18 years	FEBEX	Blocks	Y	Y			Y	Y	Solid & pore water chemical composition	Mock up (large-scale test)	Research on bentonite barrier behaviour	RH and P sensors	Artificial saturation, two reduced-scale heaters	Granitic low-salinity	Y		N	N	Y	Y	Y	Y	Y	Y	Y	Y			N	N	Y		N	N	Y	Y	Y	Y	Y	Y	Temperature	Very good	Yes
2.3	Mock-up-CZ	CTU	Jiří Svoboda			Czech Ca-Mg + sand +	Blocks, Powder	Y	N (Febex or	Y		Y	?Y		Mock up (lab test)	Halfscale deposition place test	Initial void, Blocks and Powder parts	Artificial saturation	Artificial granitic	Y	Y	Y	Y									N	N	N	N	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Swelling pressure, temperat	Good (finished, comprehensive analysis of final state,	Yes (limited, no fully

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								Swelling	Retention curve	Shear strength	Tensile strength	Hydraulic conductivity	Microstructur	Other						Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Radial	Axial			
						graphite			B75 can be used instead)																																					ure, mineralogical changes, corrosion	geometry and boundary conditions clearly defined, rich dataset for input/ benchmarking/verification of models	coupled analysis)
2.4	OPHELIE	EURIDICE, NIRAS/ONDRAF	Geert Volckaert			Fo Ca	bentonite precompacted blocks	Y				Y			Large scale mock-up	simulation of real HLW disposal "old design"		imposed hydraulic and thermal boundaries	controlled	Y	Y	Y	N		Y	Y	Y					Y	Y	Y	Y	Y	Y	N								Temperature	Good (well-characterised, many sensors, has been dismantled)	Yes (THM, 1D)
2.5	REM	Andra		2014-ongoing	ongoing	MX-80	powder/pellets								Surface experiment	Study the water saturation of pellet/powder mixture of FSS	(Relatively homogeneous mixture)	Artificial saturation, confined in cylinder	?	Y	-	Y	N	Y	-	Y	Y	Y	-	Y	Y	N	N	N	N											Total pressure, temperature	Good (well-defined geometry, material HM characterised, large no. of sensors)	Yes (H, code_bright)
2.6	SB (mock up)	GRS, Nagra	Klaus Wieczorek	Jan. 1995 - Dec. 2007		Calcigel	Granular sand/bentonite mixture	Y	N	N	N	Y	N		Mock up	Qualify sand/ bentonite mixtures as material for engineered barriers	not at full saturation	Artificial saturation, ambient temp.	Pearson water																												Limited (only deals with sand-bentonite mixtures)	
3.1	40% scale buffer tests	VTT, Posiva	Veli-Matti Pulkkanen	Test 1: Nov '11-Sep '13, Test 2: Nov '11-ongoing	Test 1: 22 months, Test 2: ongoing (status 3.11.17, >6 year)	MX-80	Blocks, pellets	Mx-80 (Y)	Mx-80 (Y)	Mx-80 (partially)	Mx-80 (partially)	Mx-80 (Y), Ibeco RWC (Y)	Mx-80 (Y)		URL (40% scale)	In-situ buffer demonstration at early state, distribution of heat, rate of saturation from the pellet-filled gap to the middle of the buffer block, artificial watering effects, piping and erosion, swelling and buffer uplift.	Test 1: density and water content profiles in post-mortem analyses	Test 1: natural water inflow through bedrock fractures, test 2: artificial wetting (inflow rate 8-10 l/min), heater (up to 90 degC), natural bedrock surrounding the buffer	Test 1: natural groundwater, Test 2: salinity of 10-12 g/l TDS (natural groundwater)	Y	Y	N	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	N	Y	Y	Y	Y	Y	Y	Y	Temperature, swelling pressure	Good	No
3.2	BACCHUS I	CEA/DRDD, ANDRA, ONDRAF/NIRAS				Fo Ca									URL					Y	Y	Y	N	Y	Y	Y	Y					N	N	N	N											Swelling pressure, temperature	Good but ended suddenly	Yes
3.3	BACCHUS II	SKN/CEN, ENRESA, ANDRA, CEA				Fo Ca									URL					Y	Y	Y	N	Y	Y	Y	Y					N	N	N	N											Temperature, thermal conductivity		
3.4	BRIE	Clay Technology AB,	Mattias Åkesson			MX-80									URL																																Not suitable for mechanical modelling in Beacon (experiment	Yes

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								Swelling	Retention curve	Shear strength	Tensile strength	Hydraulic conductivity	Microstructur	Other						Water Content				Pore pressure /suction				Relative humidity				Strain				Dry density				Stress								
																				Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Radial	Axial			
		Chalmers University of Technology, SKB																																													designed to minimise influence of mechanical processes)	
3.5	CRT	SKB	Mattias Åkesson / Ann Dueck	1999-2005	5 year	MX-80	Blocks and pellet	Y		Y		Y			Full scale field experiment	To demonstrate technique for retrieving emplaced canisters and to monitor processes during the operational phase	Initial inner slot, initial outer gap with pellet	Artificially hydrated, heater, confined condition	Äspö local groundwater	Y	Y	N	N	Y	Y	Y	Y	Y	Y	Y	Y					Y	Y	N	Y	Y	Y	Y	Y	N	Y	Temperature	Good (well-defined geometry, defined boundary conditions, initial conditions, water uptake and final conditions measured accurately)	Yes
3.6	DOPAS EPSP	CTU, SURAO	Jiří Svoboda			B75 Czech Ca-Mg	Pellets	Y	Y				?Y		Mock up (in situ)	Repository plug test	Voids between pellets, Two types of pellets deposition	Artificial and natural saturation	Natural groundwater	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	N	N	N	N	Y				Y	Y	Y	Y	Y	Y		Good (can serve as a benchmarking tool, provides data on transient effects and gradual saturation of pellets)	Yes (limited, not fully coupled)
3.7	EB	Enresa, CIEMAT	Antonio Gens	2002-2013	10.5 years	Serrata	Pellets and Blocks	Y	Y	N	N	Y	Y		Full scale field experiment	Study of the hydration of a possible EBS design	Both pellets and blocks used in the same EBS section	Artificial hydration	?	Y	Y	N	Y	N	N	N	N	Y	Y	Y	N	N	N	N	N	Y	Y	N	Y	N	N	Y	N	Y	N	Swelling pressure	Probably suitable as dismantling data available. Artificial hydration process not well controlled	Yes (HM)
3.8	FE (Full-scale Emplacement)	Nagra	Olivier Leupin			Na Bentonite									URL					Y	Y	Y	Y	Y	Y	Y	Y					Y	Y	Y	Y											Temperature, swelling pressure, geophys, corrosion	Good (initial conditions well-documented, ongoing measurements of material properties evolution)	Yes
3.9	FEBEX in situ	Enresa	María Victoria Villar	Feb-97	18 years	FEBEX	Blocks	Y	Y			Y	Y	Solid & pore water chemical composition	Full scale	Demonstration and study of near-field components	Y	Natural saturation, two full-scale heaters	Natural granitic groundwater	Y	Y	N	Y	Y	Y	Y	Y	Y	limited	limited	limited			N	N	Y	Y	N	N	Y	Y	Y	limited	limited	limited	Temperature	Good, but limited in final stages	Yes
3.10	GAST	ANDRA, KORAD,	Olivier Leupin			MX-80									Large scale					Y	Y	Y	Y									N	N	N	N											Geophysical	Good but ongoing (initial conditions well documented, mock-up	Yes

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																				Water Content				Pore pressure /suction				Relative humidity				Strain				Dry density				Stress								
								Swelling	Retention curve	Shear strength	Tensile strength	Hydraulic conductivity	Microstructur	Other						Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Radial	Axial			
		Nagra, NWMO																																												measure ments	experiment allows for detailed studies, ongoing geophysical measurements)	
3.11	HE-B	BGR, ENRESA, GRS, NAGRA	Klaus Wieczor ek	May 1999 - Dec. 2003	Satura tion: 34 month s, heatin g: 18 month s	Serrata	Blocks	Y	Y	Y	Y	Y	Y		URL	Study of THM properties in the near field of a heat source	higher dry density / lower water content close to heater	Artificial saturation, max. temp. 100 °C, initial gaps heater/block and blocks/rock	Pearson water	Y	Y	Y	Y	N	N	N	N	Y	N	N	N	N	N	N	N	Y	Y	N	Y	Y	N	N	N	N	N	Gas, geotechni cal measure ments	Not great (most instruments immediately failed so limited data, leak in injection system)	Yes
3.12	HE-E	NAGRA, GRS, BGR, ENRESA	Klaus Wieczor ek	June 2011, ongoing	ongoi ng	MX-80	Blocks and granular	Y	Y	N	N	Y	N		URL	Investigate early non-isothermal re-saturation period of the buffer and its impact on the THM behaviour	initially two bufer types (blocks/granu lar) with different density	Natural saturation, max. temp. 140 °C	Opalinus clay water	Y	N	N	N	Y	Y	Y	Y	Y	Y	Y	Y	N	N	N	N	Y	N	N	N	N	N	N	N	N	N	Seismicity , resistivity, temperat ure	Potentially interesting (ongoing, heterogeneities evolving, but missing data since it has not been dismantled yet)	Yes
3.13	ITT	AECL				MX-80									Large scale in situ						Y	N	Y									Y	Y	Y	N		Y	N	Y	Y	Y	Y	Y					Yes (HM)
3.14	LASGIT	SKB, Posiva, BGS	Jon Harringt on	01/02/2 005	ongoi ng	MX-80	Blocks and pellets	Y	N	N	N	Y	N		Field scale mock up	Hydration of the clay and subsequent gas migration behaviour	Yes in the time-dependent development of porewater pressure, stress, suction, canister movement and gas flow behaviour	In-situ test in an Äspö deposition hole, capped with a concrete plug and retaining steel lid which itself is rock anchored to floor.	Combination of in-situ water and local tap water have been used at different times in the experiment	Y	N	N	N	Y	N	Y	Y	Y	N	Y	Y	Y	N	Y	N	Y	N	N	N	Y	N	Y	Y	Y	Y	Swelling pressure, porewate r pressure, temperat ure, suction, permeabil ity, displacem ent	Good (high level of instrumentation, detailed initial characterization of host rock and bentonite => well defined boundary conditions) Ongoing so spatial data not currently available. Strain data relates to measured displacement of the canister and deformation of the steel retaining lid.	Yes (limited)
3.15	LIT	CFM Project (GTS Phase IV	Bill Lanyon	12/05/2 014	Until early 2018	Serrata	16 2.5cm high rings (1.65 g/cm3)	Y							In situ	Colloid formation and migration	Uneven axial load	Confined in borehole interval	GGW Natural groundwater	Y	-	-	-	Y		Y	Y									Y	-	-	Y	Y	Y	Y	Y		Y	Swelling pressure, erosion, tracer		No

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								Swelling	Retention curve	Shear strength	Tensile strength	Hydraulic conductivity	Microstructur	Other						Water Content				Pore pressure /suction				Relative humidity				Strain				Dry density				Stress						Other		
																				Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Radial	Axial			
		experimen t)					Inner diameter 43mm outer 82 mm																																									
3.16	MCJ	SURAO / CTU	Jiří Svoboda			B75 Czech Ca-Mg	Blocks	Y	Y	Y		Y	?Y		Field-scale (half-scale)	Halfscale deposition place in-situ test	Initial voids	Natural saturation	Natural groundwater	Y	N	Y	Y					Y	N	Y	Y	N	N	N	N	Y	Y	Y	N	Y	N	Y	Y	Y	Y	Temperature		No
3.17	NSC	Andra	Jean Talandier			MX-80	Bricks (Mx80/ sand mixture)/ pellets	Y	Y			Y			Field scale (half-scale)	Water saturation/hydraulic tests at field scale	Initial void,initial dry density distribution	Artificial water injection/direct contact with host rock	Water from Bure site	Y	N	N	N	Y	N	Y	Y	Y	N	Y	Y	N	N	N	N	Y	N	N	Y	Y	N	Y	Y	Y	Y	Swelling pressure, EDZ transmissivity	Good (well-defined geometry, initial THM characterisation of all materials involved, large number of sensors monitoring HM evolution, heterogeneities, not used as a benchmark/ modelling exercise before)	Yes (scoping calculations)
3.18	PGZ2	Andra	Jean Talandier			MX-80	Blocks (MX-80/ sand mixture)/ pellets (MX-80)	Y	Y	Y	Y	Y			In situ (borehole test)	Water saturation/gas transfer	initial void + heterogeneous distribution of total pressure	Natural re-saturation/direct contact with host rock	Water from Bure site	Y	N	N	N	Y	Y	Y	Y	N	N	N	N	N	N	N	N	Y	N	N	N	Y	N	Y	Y	N	Y	Gas transfer		Yes
3.19	PRACLAY	EURIDICE	Robert Charlier	01/01/2010	15 years	MX-80	Blocks	Y	Y	N	N	y	N		Full scale	seal for a heating experiment with increase of pore pressure	divergence of stresses measured in different points	artificial and natural hydration, constant volume swelling, complex shape		Y	N	N	N	Y	N	Y	Y	Y	N	Y	Y	Y	Y	Y	Y	Y	N	N	N	Y	N	Y	Y	Y	Y	Temperature, swelling pressure	Good (well-characterized bentonite, lots of sensors, strong THM coupling, could be considered as a special in-situ test)	Yes (blind)
3.20	Prototype	SKB	Mattias Åkesson /Ann Dueck	II: 2003-2011 (I: 2001 - ongoing)	8 years	MX-80 and Milos (backfill)	Blocks, pellets and bentonite /crushed rock (backfill)	Y		Y		Y			Full scale field experiment	To gain experience in designing and constructing a repository in crystalline rock, and to test engineered barriers	Initial inner slot, initial outer gap with pellet, developing heterogeneity on re-saturation.	Natural hydration from the host rock, heater, confined condition	Äspö local groundwater	Y	Y	N	Y	Y	Y	Y	Y	Y	Y	Y	Y					Y	Y	N	Y	Y	Y	Y	Y	N	Y	Temperature	Good (rock and bentonite well characterised)	Yes (THM)

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3.21	RESEAL II	SCK-CEN	Antonio Gens	1999-2007	8 years	Fo Ca	Pellets + Powder	Y		N	N		Y		Lab + URL	Study of a seal hydration	Local heterogeneity: powder pellets	Artificial hydration		Y	N	N	N	Y	Y	Y	N	Y	Y	Y	N	N	N	N	N	N	N	N	N	Y	Y	Y	N	Y	Y		Good well-defined geometry and hydration b.c. Limited number of sensors. Not dismantled	Yes (HM)
3.22	SB (in situ)	GRS, Nagra	Klaus Wieczorek	Jan. 1995 - Dec. 2007	13 years	Calcigel	Granular sand/bentonite mixture	Y	N	N	N	Y	N		In situ	Qualify sand/bentonite mixtures as material for engineered barriers	not at full saturation	Artificial saturation, ambient temp.	Pearson water	Y	Y	N	Y	Y	Y	Y	Y	N	N	N	N	N	N	N	N	Y	Y	N	Y	Y	Y	Y	Y	N	N			
3.23	SEALEX	IRSN	?	2012	ongoing	MX-80 sand mixture	blocks	Y	Y	?	?	?	?		In situ	Testing different ways to make seals	Technological void around blocks	Artifical saturation	?					Y	Y	Y	Y	Y	Y	Y	Y									Y	Y	Y	Y	Y	Y			Yes (decovalex)
3.24	TBT	ANDRA, SKB, Clay Technology AB	Mattias Åkesson			MX-80									URL																																Not suitable for mechanical modelling in Beacon (high temperature)	Yes
4.1	Dual density tests	CU	Jan Najser	2020		Czech Ca-Mg	Blocks	Y	Y	N	N	Y	Y		Laboratory	Study of homogenisation	Initial density hetereogeneity - two blocks	constant volume, artificial saturation from one base	De-ionized water	Y	Y	N	N	Y	Y	N	N	N	N	N	N	Y	Y	N	N	Y	N	N	N	Y	Y	Y	N	N	Y		good	Yes, CU (hypoplastic model)
4.2	PCT (Pellet-Cluster Test)	GRS	Klaus-Peter Kröhn	2021	ongoing	MX-80	Pellets	Y							Laboratory	Swelling behaviour of a pellet cluster	Inherent initial heterogeneity	Constant volume, artificial hydraion	Pearson water	Y		Y														Y				Y		Y			Y		OK	Useful for calibrating a constitutive model
4.3	Influence of pellet granulometry on final state	EPFL	Alessio Ferrari	2018-2019		MX-80	Granular	Y	Y			Y	Y		Laboratory	Determine the ifluence of initial granulation on the final state after saturation		Oedometric	Distilled	Y	Y	Y	N	Y	Y	N	N	Y	Y	N	N	Y	Y	Y	N	Y	Y	Y	N	Y	Y	Y	N	N	Y	PSD from MIP and SEM	Good	No
4.4	Saturation of pellet/block systems under isochoric conditions	CIEMAT	María Victoria Villar	2017-2021	14-278 days	FEBEX	pellets mixture/compacted block	Y	Y			Y	Y	Solid and pore water chemical composition	Laboratory	evolution of bentonite swelling, fabric and microstructure upon hydration and factors affecting them	water content and density gradients	Constant volume cell/slow water saturation	deionised	y	y	y	y	N	N	N	N	Y	N	N	N	Y	Y	Y	N	y	y	N	y	Y	Y	Y	N	N	Y	water intake, microstructure	good	yes

Appendix B Reference No	Name/title	Organisation	Name of contact	Start and end dates	Duration	Bentonite type	Bentonite form	Availability of material parameters							Scale	Purpose of experiment	Evidence of heterogeneity	Boundary Conditions	Water Chemistry	Availability of material parameters																										Other	Data quality	Modelled?
								Swelling	Retention curve	Shear strength	Tensile strength	Hydraulic conductivity	Microstructur	Other						Water Content				Pore pressure /suction				Relative humidity				Strain				Dry density				Stress								
																				Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Radial	Axial			
4.5	Saturation of pellet/block systems under isochoric conditions	CIEMAT	María Victoria Villar	2019-2021	>700 days	MX-80	pellets-powder mixture/compacted block	Y	Y			Y	Y		Laboratory	evolution of bentonite swelling, fabric and microstructure upon hydration and factors affecting them	different radial pressures	Constant volume cell/slow water saturation	deionised	y	y	y	y	Y	Y	Y	N	Y	Y	Y	Y	N	N	N	N	Y		N		Y	Y	Y	Y	Y	Y	water intake, microstructure	good	no
4.6	Shear strength of interface steel-bentonite at different w/c	EPFL	Alessio Ferrari	2018-2019		MX-80	Granular		Y	Y					Laboratory	Determine the shear strenght of the interfaces bentonite-steel and bentonite-bentonite		Direct shearing	Vapour saturation	Y	Y	N	N	Y	Y	N	N	Y	Y	N	N	Y	Y	N	N	Y	Y	N	N	Y	Y	N	N	N	Y		Good	No
4.7	Influence of stress path on final state	EPFL	Alessio Ferrari	2018-2019		MX-80	Granular	Y	Y			Y	Y		Laboratory	Determine the influence of stress path on the final state after saturation		Oedometric	Distilled	Y	Y	Y	N	Y	Y	N	N	Y	Y	N	N	Y	Y	Y	N	Y	Y	Y	N	Y	Y	Y	N	N	Y	PSD from MIP and SEM	good	Yes (see task 3.3 in the final BEACON deliverable D3.3)
4.8	Swelling into limited void	CIEMAT	María Victoria Villar	2017-2021	4-466 days	FEBEX	compacted block	Y	Y			Y	Y	Solid and pore water chemical composition	Laboratory	effect of initial gaps on homogeneity	water content and density gradients	uniaxial swelling into gap	deionised	y	y	y	y	N	N	N	N	N	N	N	N	N	N	N	N	y	y	y	y	N	N	N	N	N	N	microstructure	good	yes
5.6	Oedometer compression	CIEMAT	Villar	published 2005	1072 days	MX-80	compacted in the cell		Y			Y		1D compression & swelling coefficients	Lab	Characterisation for MX-80 bentonite as part of the Prototype repository project.	no	laterally confined swelling in oedometer+ load at constant suction	unknown	Y	Y					Y								Y				Y							Y		ok	Useful for calibrating a constitutive model
5.6	Isotropic cell compression	ENPC	Tang	published 2008	unknown	MX-80	compacted in the cell							isotropic compression & swelling coefficients	Lab	Investigate isotropic behaviour under mechanical, hydraulic and thermal loads. Thermal effects are not modelled.	no	laterally unconfined swelling in isotropic cell + loading at constant suction	unknown	Y				Y	Y											Y										mean stress, void ratio in time	ok	Useful for calibrating a constitutive model

Appendix B Reference No	Name/title	Organisation	Name of contact	Start and end dates	Duration	Bentonite type	Bentonite form	Availability of material parameters							Scale	Purpose of experiment	Evidence of heterogeneity	Boundary Conditions	Water Chemistry	Availability of material parameters																										Other	Data quality	Modelled?
								Swelling	Retention curve	Shear strength	Tensile strength	Hydraulic conductivity	Microstructur	Other						Water Content				Pore pressure /suction				Relative humidity				Strain				Dry density				Stress								
																				Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Initial	Final	Time Series	Spatial	Radial	Axial			
	BPT					MX-80																																										
	GMT					Serrata																																										
	KEY					MX-80																																										
	LOT					MX-80									?																																	
	ABM	SKB, Posiva, Clay Technology AB	Mattias Åkesson			11 types																																									Not suitable for mechanical modelling in Beacon (focussed on mineralogical stability)	
	LpHSP					Serrata																																										
	BMT					MX-80																																										
	S&TP					MX-80																																										
	EZ-A					MX-80																																										
	BCE	AECL				Na Bentonite																																										
	TSX	AECL				Kunigel V1									Full scale																																	
	CSE					Kunigel V1									?																																	
	ESP	AECL				Kunigel V1 + MX-80									Full scale																																	
	RESEAL I					Fo Ca + Serrata									Lab																																	Yes
	CHINA mock up					GMZ																																										
	KENTEX					Jinmyeong Mine																																										
	BIG-BEN	CLAY (SKB), CNWRA (NRC), KPH				Kunigel V1									Large scale lab																																	
	KISE					OT-9607																																										

*MX-80: Karnland et al. 2006, Åkesson et al. 2010, Dueck et al. 2010 and 2011, Dueck and Nilsson 2010, , Karnland et al. 2000, Olsson et al. 2013

Calcigel: Svensson et al. 2011