



Proceedings from the final workshop

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Proceedings from the final workshop of the Beacon project

Date and time: 17 May 13.00-19.00, 18 May 09.00-17.45 and 19 May 09.00-15.00

Place: Imperial College London

Participants see attached participant list. It is not quite complete regarding the online participation but accurate regarding the persons attending in person.

The meeting agenda is Appendix 1.

The 5th Annual meeting and General Assembly Meeting was held together with the final workshop of Beacon. The minutes from the 5th Annual meeting and General Assembly Meeting are available in deliverable D8.14 and therefore not present here.

All presentations from the workshop can be accessed in <u>this folder in Projectplace</u> as well as the book of abstracts. They will also be accessed on <u>www.beacon-h2020.eu</u>. The book of abstracts is Appendix 2.

The meeting opened at 13.00 the 17th May with a short welcome from the Executive Board of the project (Olivier Leupin, Simon Norris, Antonio Gens, Klaus Wiezcorek, Jean Talandier, Johan Swahn, Juan Carlos Mayor, Susanna Maanoja, Patrik Sellin and Mary Westermark, as Irena Hanusova had not yet arrived) followed by a welcome and meeting practicalities session by Professor Lidija Zdravkovic of ICL. The Project Officer, Seifallah Ben Hadj Hassine, gave a short introduction to Beacon and its context among EC projects.

Patrik Sellin gave a general introduction and background to the project, and during day 1 and the beginning of day 2 all WP leaders of WPs 1-6 (not the dissemination and management/coordination WPS) presented the work performed in the project and put it into a context.

Further to put Beacon into a context the EB had invited Sebastia Olivella of UPC to give an invited talk about geomechanical coupled models involving unsaturated clays. It was followed up day two by Enrique Romero Morales also from UPC giving an invited talk on experimental insights into pellet-based and granular bentonite buffer materials. Both invited talks were very appreciated.

At the end of day 1 was a poster session preceded by short poster introductions which were mentioned specially by the EARB as very appreciated.

During the poster session, and the breaks, a film was screened that explains the Swedish KBS3 concept of final repository for radioactive waste, and puts the bentonite mechanical evolution into a context. It can be downloaded <u>here</u>.

Plenary presentations (see the attached agenda) were given by Maria Victoria Villar, CIEMAT, Antonio Gens, UPC, Robert Charlier, ULiege, Caroline Graham, BGS, Liliana Gramegna, ULiege, Darius Justinavicius, LEI, Joni Tanttu, JYU, Klaus Wiezcorek, GRS,

Beacon





Heini Reionen, GTK, Matias Alonso, Andra, Marcelo Sanches, Texas A&M University, Marcelo Lavina, Amphos21, Jose A. Bosch, EPFL, Rebecca Newson, Quintessa,Steffen Beese and Vinay Kumar, BGR, Jiri Svoboda, CTU, Daniel Malmberg, Clay Technology and Heidar Gharbieh, ex VTT,

Chairs for the plenary presentations were Juan Carlos Mayor (JCM), Enresa, Susanna Maanoja (SM), Posiva, Simon Norris (SN), RWM, Olivier Leupin (OL), Nagra, Irena Hanusova (IH), SURAO, and Patrik Sellin (PS), SKB.

The EARB gave their input to the project, its deliverables during the last year and the workshop. Their expert feedback is available in their presentation and in the deliverable D8.15.

The work package work was summarized by the WP-leaders of WPs 3-5; Antonio Gens, Klaus Wiezcorek and Jean Talandier.

The project was summarized by Patrik Sellin and Olivier Leupin.

The EARB's overall opinion of the project is quoted below and the workshop seems to have been very appreciated.

"This research project has been smoothly initiated and successfully carried out. The approach of the project is systematic and the coverage is extensive.

Disturbances by the pandemic has been well handled even if the interactions between partners could not be maximised for the comparison and interpretation of the results.

The objectives of the project have been well formulated in the beginning and achieved at the end of the project.

Compared to other similar projects, the integration between work packages has been wellorganized and implemented.

The outcomes from this project are highly relevant to the design and the safety analysis of different types of final disposal facilities that apply bentonite as an engineering barrier in relatively large dimensions.

Project achievements and additional research needs have been well identified."



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Agenda Beacon Final Workshop

This is also the 5th and last Annual Meeting and General Assembly Meeting of the Beacon project

Date, time: 17 May 13.00 - 19 May 15.00 Place: Imperial College London. Skempton Building - Depo

lace: Imperial College London, Skempton Building - Department of Civil and Environmental Engineering, Lecture theatre 201, Imperial College Road, South Kensington, London

Beacon partners have nametags that are marked with post-its.

Pink for WPs 3 & 5 Model development and testing

Green for WP4 Experimental

Yellow for WP1 Assessment cases, WP2 Collection of existing data/models and WP6 Civil society Orange for management and coordination

If you have Beacon related questions, don't hesitate to ask anyone of the involved. They will be able to answer or point towards someone who can.

Tuesday	17 May Chair
13.00 -13.10	Welcome to Beacon final workshop, 5 th Annual Meeting and General Assembly (Beacon Executive Board)
13.10 -13.20	Welcome to Imperial College London (Lidija Zdravkovic, ICL)
13.20 -13.30	Seifallah Ben Hadj Hassine, EC (online)
13.30 -13.50	Beacon general introduction and background (Patrik Sellin, SKB)
13.50 -14.35	Geomechanical coupled models involving unsaturated clays (Invited PS speaker Sebastià Olivella , UPC)
14.35 -15.05	Break
15.05 -15.25	WP1 Definition and application of assessment case (Olivier Leupin, Nagra)
15.25 -15.55	WP4 Laboratory testing (Klaus Wiezcorek, GRS)
15.55 -16.25	WP3 Model development (Antonio Gens, UPC)
16.25 -16.55	WP5 Testing, verification and validation of models (Jean Talandier, Andra)
	Questions PS
17.00 - 17.20	 Poster introduction - 3 slides each: 1 for title and two describing, white background, 2 min/ poster Hydro-mechanical properties of compacted bentonites GMZ and MX80 (Chun-Liang Zhang/Klaus Wieczorek, GRS/BRIUG) Estimation of the buffer homogenisation in the prototype repository (Mattias Åkesson, SKB) Implementation of an advanced constitutive model for bentonite using MFront for safety and performance assessments of HLW-repositories in the numerical code OpenGeoSys (Eric Simo, BGE Technology) Description of the hysteresis based material model (Ola Kristensson, Clay) Modeling of initially heterogen systems using the hysteresis based material model (Alex Spets, Clay) Hypoplastic modelling of bentonite homogenisation (David Mašín, CU) Numerical modelling of an inhomogeneous bentonite barrier for radioactive waste disposal applications (Giuseppe Pedone (Lidija Zdravkovic), ICL) Downscaled tests for studying the influence of the temperature in the homogenization process (Xavier Pintado, Mitta Engineering)
17.20 -	Poster session. Snacks/finger food served.
17.30 -	A 6 min animation that puts the bentonite into a context of a final MW repository will be shown on the screen in the lecture hall. Can be shown again on request.



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Wednesday	18 May	Chair
09.00-09.05	Welcome back	SN
09.05-09.25	WP2 Collection and compilation of existing data and available models (Simon RWM/NWS)	Norris,
09.25-09.45	WP6 Dissemination to civil society (Johan Swahn MKG)	
	Questions	
09.55-10.40	Experimental insights into pellet-based and granular bentonite buffer	JT
	materials (Invited speaker Enrique Romero-Morales, UPC)	
10.50-11.20	Break	
	Plenary presentations (15 min per person/team + 5 for questions and change of speaker)	
11.20 - 11.40	Microstructural evolution of binary barriers during saturation (Maria Victoria Villar, Ciemat)	JCM
11.40 – 12.00	Bentonite homogenization and microstructure evolution modelled using a double structure constitutive law (Antonio Gens , UPC)	JCM
12.00 - 12.20	How does wall friction drive bentonite heterogeneity? (Robert Charlier , ULiege)	JCM
12.20 -13.20	Lunch served, hosted by the project	
13.20 -13.40	Swelling into a void as function of sample/void ratio, temperature and salinity (Caroline Graham , BGS)	SM
13.40 -14.00	Microstructure evolution in pellet based bentonite hydration: focus on pore size distribution characteristics (Liliana Gramegna , ULiege)	SM
14.00 -14.20	Prediction of bentonite behaviour using hydro-mechanical model developed in COMSOL Multiphysics (Darius Justinavicius , LEI)	SM
14.20 -14.40	Simultaneous determination of deformation and liquid content in swelling clay using X-ray radiography (Joni Tanttu , JYU)	SM
14.40-14.50	Future Beacon related work (Jiri Svoboda , CTU)	
14.50 – 15.20	Break	
15.00 15.40	Presentations of work performed outside Beacon	CNI
15.20 - 15.40	Large-scale festing of a sanawich shaft seal (Kiaus wieczorek , GRS)	SIN
15.40 – 16.00	Long-term aspects of bentonite self-healing and self-sealing via the IBL- project (Heini Reijonen , GTK)	SN
16.00–16.20	Hydration survey of a large scale sealing experiment (Bure, France) (Matías Alonso, Andra)	SN
16.20 - 16.40	Study of coupled gas migration phenomena through clay barrier systems intended for the isolation of high-level nuclear waste (Marcelo Sánchez , Texas A&M University)	IH
16.40 - 17.00	Hydro-chemo-mechanical modelling of bentonite sealing components	IH
	(Marcelo Laviña, Amphos21)	
18.00	Dinner hosted by the project	



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Thursday	19 May	Chair
09.00-09.05	Welcome back	KW
09.05 - 09.25	Analysis of the mechanical behaviour of a heterogeneous bentonite backfill upon non-isothermal saturation (Jose A. Bosch , EPFL)	KW
09.25 – 09.45	Applications of a thermo-hydro-mechanical internal limit model to bentonite experiments (Rebecca Newson , Quintessa)	KW
09.45 – 10.05	Double porosity model for bentonite in thermo-hydro-mechanical processes (Steffen Beese and Vinay Kumar, BGR)	IH
10.05 – 10.25	Investigation of BCV bentonite (Jiri Svoboda, CTU/CU)	IH
10.25-10.55	Break	
10.55-11.10	Putting Beacon into context (Olivier Leupin , Nagra)	
11.10-11.25	Modelling of the SKB assessment case using the HBM model (Daniel Malmberg , Clay Tech)	OL
11.25-11.40	Sensitivity analysis of bentonite block-pellet tunnel backfill mechanical evolution during saturation (Heidar Gharbieh , DSA ex. VTT)	OL
11.40-11.50	PEP serious games (Frédéric Bernier, EARB/FANC)	
11.50-12.20	EARB: Input towards submitted deliverables, the workshop contents and the project as a whole	
12.20-13.10	Lunch served, hosted by the project	
13.10-13.25	WP3, summary and conclusions (Antonio Gens, UPC)	
13.25-13.40	WP4, summary and conclusions (Klaus Wieczorek, GRS)	
13.40-13.55	WP5, summary and conclusions (Jean Talandier, Andra)	
13.55-14.20	Summary discussion of WPs 3-5	AG, KW, JT
14.20 - 14.45	Summarizing Beacon. Impact on the treatment of the mechanical evolution of bentonite barriers in future assessments. (Olivier Leupin, Nagra/Patrik Sellin, SKB)	
14.45 – 14.55	How to move forward/ideas for future work (Jiri Svoboda, CTU)	
14.55 – 15.00	Any remaining decisions for Beacon Annual meeting and General Assembly	MW
15.00	End of workshop, 5 th Annual Meeting and General Assembly	

AG – Antonio Gens JCM - Juan Carlos Mayor JT – Jean Talandier IH – Irena Hanusová KW – Klaus Wieczorek MW – Mary Westermark OL – Olivier Leupin PS – Patrik Sellin SM – Susanna Maanoja SN – Simon Norris

SWELLING INTO A VOID AS FUNCTION OF SAMPLE/VOID RATIO, TEMPERATURE AND SALINITY

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ABSTRACT

We present a suite of experiments carried out within the BEACON project, examining the evolution of swelling and pore pressures in compacted bentonite, with varying degrees of permitted axial swelling into a void. The resulting degree of homogenisation was investigated under both ambient conditions and elevated temperatures and salinities.

After 100 days, almost all samples had completely swelled into the void and differential swelling pressures had reduced substantially. The larger the degree of axial swelling permitted, the smaller the swelling pressures that were measured along the sample length, as might be expected due to the resulting reduction in dry density. Swelling pressures across the entire sample length were higher at elevated temperatures of 90 and 100°C, but a substantial reduction in values was apparent at 150°C. At elevated salinities, clay that swelled into the void failed to generate significant swelling pressures during the testing period.

In almost all tests, differential pressures along the sample were still relatively significant at day 100, despite the overall rate of pressure decline having reduced to low levels. This was also reflected in axial variation in geotechnical data collected from post-test subsamples. Pore pressure evolution in all tests occurred in a staggered fashion along the length of the vessel, with hydraulic equilibrium being reached last at the higher density end, where the compacted clay sample was initially situated. The time period to reach hydraulic equilibrium along each sample was shortest in cases where the greatest degree of axial strain was experienced. This

is consistent with observations of residual heterogeneity, which was found to be highest for those samples that experienced the smallest axial swelling strains (Figure 1). The larger the void present, the greater the capacity for the clay to reach hydraulic equilibrium and the faster the homogenisation of swelling pressures. Additional testing at low strains will help to confirm whether this relationship is truly linear and the degree to which environmental conditions have an impact in the case of smaller voids. Such information is key to assessing whether any residual heterogeneity is significant or can be tolerated in Geological Disposal Facility (GDF) design. The data generated by these experiments also provide a suitable resource parameterisation for and validation of numerical models that can further assess the long-term homogenisation behaviour of bentonite in GDFs.



Figure 1. Residual swelling pressure differential after 100 days of testing, as a function of axial strain.

LARGE-SCALE TESTING OF A SANDWICH SHAFT SEAL

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⁵ Technische Universität Bergakademie Freiberg (TUBAF), Freiberg, Germany

ABSTRACT

Shaft sealing systems for a nuclear waste repository are constructed to limit the fluid inflow from the adjacent rock after closure and to delay the release of potentially contaminated fluids from the repository at later stage. Current German concepts of shaft seals contain the hydraulic Sandwich sealing system as a component of the lower seal in the host rock. The KITdeveloped Sandwich sealing system consists of alternating sealing segments (DS) of bentonite and equipotential segments (ES) that are characterized by a high hydraulic conductivity. Within the ES fluid is evenly distributed over the cross section of the seal. Water bypassing a DS via the excavation damaged zone, or penetrating the DS inhomogeneously, is contained and a more homogeneous hydration and swelling of the DS is obtained. Functionality of such a system was proven in laboratory and semi-technical scale experiments. A large-scale experiment to demonstrate feasibility and effectiveness of the Sandwich shaft sealing system in interaction with the host rock was launched at the Mont Terri rock laboratory in July 2019 with partners from Germany, Switzerland, Spain, UK, and Canada. It consists of two experimental shafts of 1.18 m diameter with depths of 10 and 12 m, respectively, constructed using a core drilling technique with a custom-made drill rig in a new niche in the sandy facies of the Opalinus Clay. The seal in Shaft 1 consists of four DS (Calcigel) of 1 m thickness and five ES (fine-grained guartz sand), each 30 cm thick. Since May 2021 the sealing system in Shaft 1 is hydrated from a pressure chamber located at the shaft bottom via an inclined lateral feeding borehole. The seals and the surrounding rock are intensely monitored. Measurements in the rock (geophysics, pore pressure and total stress) were started before shaft sinking. Measurements inside the shaft comprise water content, relative humidity and temperature, pore pressure, stress, and displacements. Shaft 2 will host a slightly modified system integrating experience obtained during the early operation phase of Shaft 1 and providing complementary data. Shaft 2 installation is planned for the second half of 2022. The in-situ work is supported by laboratory testing and model simulation. The experiment is funded by the German Federal Ministry for Economic Affairs and Energy under contract 02E11799.



HOW DO WALL FRICTION DRIVE BENTONITE HETEROGENEITY?

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ABSTRACT

Hydration of bentonite with an initial high suction involves an important swelling. Numerous tests are performed under isochoric condition, and large swelling stresses are observed. Bentonite seals for underground nuclear waste disposal are generally designed in order to develop such large stresses and also to limit volumetric strains in order to maintain permeability at a very low level.

Bentonite hydration is always non uniform. it starts usually from one side of the sample in lab tests, and from the host rock for in situ seals or EBS. Therefore, swelling upon the hydration beginning is heterogeneous due to local water saturation gradient. Most of the time swelling tests are performed in isochoric cells and only high axial stresses are measured on one side. When initial voids or two-component bentonite samples such as bentonite block and pellets are initially introduced in the cell, large strains may develop in the hydration direction, parallel to cell wall. So friction appears at the sample boundary and induces heterogeneous swelling (Abed & Solowsky, 2019). Similarly, for in situ seals, friction on the tunnel wall, concrete liner or rock, plays an important role in final density distribution and swelling.

In this presentation, we will focus on friction induced heterogeneity, using FE numerical modelling. In a first section, finite element dedicated to large strain contact and friction will be presented.

Following, two different lab tests and one actual seal will be analysed. In the two lab tests, the samples are composed of two parts with different densities, the lower density being in one case very low (Villar et al, 2021). The numerical modelling put in evidence the major role of friction in the stress evolution and in the final bentonite densities. A seal designed for an underground large gallery is then analysed. It is confined radially by the tunnel liner, while longitudinally it is only supported by a backfill plug, which stiffness is low. Again, it appears the longitudinal strain is constrained by friction and that a part of the seal near the backfill has a significantly lower density compared to its central part.



Figure 1: final density of a two-layers bentonite isochoric hydration test. Numerical simulation.

A. Abed, W.T. Solowski - Simulation of swelling pressure evolution during infiltration in a bentonite block-pellet laboratory scale test. Japanese Geotech. Society Special Publication, 7 (2) (2019), pp. 323-330, 10.3208/jgssp.v07.05

M. V. Villar, R. J. Iglesias, C. Gutiérrez-Álvarez, B. Carbonell, Pellets/block bentonite barriers: Laboratory study of their evolution upon hydration, Engineering Geology, Volume 292, 2021

HYDRO-MECHANICAL PROPERTIES OF COMPACTED BENTONITES GMZ AND MX80

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ABSTRACT

As the potential buffer material for safe isolation of high-level radioactive waste in the granite in China, two types of GaoMiaoZi (GMZ) bentonite were investigated and compared with the well-known MX80 bentonite. These bentonites consist predominately of montmorillonite in different fractions of $f_m = 56-90\%$. Parallel experiments were carried out on GMZ and MX80 specimens with dry densities of $\rho_d = 1.3-1.8$ g/cm³ to investigate their hydro-mechanical properties such as water uptake and retention, swelling pressure, water permeability, and gas penetration. The experiments showed that the properties of the bentonites are strongly determined by the montmorillonite fraction and dry density. Main findings include: (1) the amount of water uptake increases with increasing the montmorillonite fraction and the environment humidity (fig. 1); (2) the swelling pressure reached at full saturation increases exponentially with the increase of montmorillonite fraction and dry density (fig. 2); (3) threshold hydraulic gradients were identified for advective water flow through the compacted MX80 bentonite and beyond that, the water permeabilities of the bentonites decrease exponentially with the increase of montmorillonite fraction and linearly with swelling pressure (fig. 3); (4) gas penetration through water-saturated bentonites needs high gas pressure exceeding the local total stress σ and tensile strength σ_T for creating micro-fissures (fig. 4) and the gas flow is characterised by a cyclic pressure rising/dropping process due to pathway closing/opening.





ANALYSIS OF THE MECHANICAL BEHAVIOUR OF A HETEROGENEOUS BENTONITE BACKFILL UPON NON-ISOTHERMAL SATURATION

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ABSTRACT

Predicting the response of bentonite upon saturation is of outmost importance in most designs of nuclear waste repositories. In this context, very few modelling efforts have been directed towards the Thermo-Hydro-Mechanical (THM) analysis of buffers involving granular bentonite mixtures (GBM) in addition to bentonite blocks. Experimental evidence from laboratory and field scale experiments, shows that after saturation, the dry density distribution differs from the initial state, even if the overall volume of bentonite remains constant.

To better understand the implications of the initial heterogeneous layout, a buffer consisting of bentonite blocks and GBM has been numerically studied with a recently developed hydromechanical constitutive model extended to non-isothermal conditions. One of the key elements of the model is a two-way coupling between the degree of saturation and the deformation. The water retention model incorporates explicitly the contribution of adsorbed water to the total water content. The material parameters can be calibrated following a robust procedure based on conventional laboratory tests. The constitutive model has been implemented in the finite element software LAGAMINE.

The repository design that will be discussed in this presentation corresponds to the Swiss concept for radioactive waste disposal (Figure 1). It is based on the field scale FE experiment at the underground laboratory Mont Terri. The model considers a case of GBM segregation due to emplacement in order to examine its consequences on the mechanical performance of the buffer. The buffer is predicted to reach saturation after 80 years and a fairly homogeneous state in terms of void ratio is reached at the end of the saturation phase (Figure 1). The model predicts the initial settlement of the canister measured in the field scale FE experiment as a result of the temperature emitted by the canister. As hydration proceeds, due to the different swelling experienced by the block pedestal and the granular backfill, the canister is subjected to upward displacements. While the initial segregation of the GBM appears not to affect the mechanical homogenisation, it might reduce canister displacements.



Figure 1. Evolution of void ratio and saturation.

LONG-TERM ASPECTS OF BENTONITE SELF-HEALING AND SELF-SEALING VIA THE IBL-PROJECT

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ABSTRACT

The International Bentonite Longevity (IBL) project Phase A has been finalised recently (Reijonen & Alexander 2022). IBL studies middle Miocene (~12 to 16 Ma old) bentonite deposits that are sourced also for commercial Kunigel bentonite. During this first project phase, several locations were identified in the Tsukinuno bentonite mine where originally homogenous bentonite beds have been deformed by later fault movements. Two main types of deformation features have been identified to date: 1) bentonite deformation via shearing along the bentonite bedding, 2) bentonite deformation via faulting cross-cutting across bentonite beds. Preliminary characterisation of bentonites with deformation structures has been made, but no detailed assessment on the properties of the fault planes and the related degrees of self-healing or self-sealing has been undertaken yet. This topic will be a potential target in the IBL Phase B studies. We will present the overall advancement of the IBL-project with existing examples of the natural bentonite deformation and specifically explore the potential to expand the natural analogue approach to mechanical behaviour of bentonites over long time scales relevant to repository performance.

Reference

Reijonen, H.M. & Alexander, W.R.2022. Sealing Deep Site Investigation Boreholes: Phase 3: International Bentonite Longevity (IBL) project Report - Phase A. Jacobs Report to NWS, Ref. 207314_R_05, Issue 1, January 2022. Jacobs, Harwell, UK (*in press*).

Microstructure evolution in pellets based bentonite hydration: focus on pore size distribution characteristics

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ABSTRACT

Bentonite-based materials are used to seal underground galleries and shafts in some nuclear waste disposal concept designs. The fundamental goal of a majority of experimental campaigns and constitutive model development has been to assess the transition between a dry to hydrated state and estimate long-term material behavior. All of these investigations have shown that the multi-porosity bentonite structure has a significant impact on the highly coupled hydro-mechanical processes that occur during water saturation.

As a result, many traditional experimental investigations on unsaturated soils have been conducted in combination with multi-scale observation approaches in recent years (for instance MIP or μ -CT). Despite their well-known limitations, such observation approaches provide fascinating quantitative observations in terms of pore diameter families that differ by many orders of magnitude, as well as their distribution with regard to distinct assembly types (namely pellets mixtures and compacted bentonite blocks). On the other side, very few studies have focused on the effect of such pore size distributions in the hydro-mechanical response, both experimentally and numerically.

The goal of this article is to introduce the experimental campaign as well as the numerical modeling strategy used to identify the effect of different pore size distributions characterizing MX-80 bentonite in different forms (32 mm pellets mixture, 7 mm pellets mixture, and compacted sample surrounded by gap) with the same overall dry density during isochoric hydration tests. The hydro-mechanical response of these bentonite assemblies is investigated using multisensor-equipped cells and post-mortem analysis performed by CEA, as well as the finite element code LAGAMINE built at the University of Liege. The experimental and numerical results are in good agreement and provide complementing information about the characteristics of each assembly type.

Characteristics of the considered samples and boundary conditions of the model.



MICROSTRUCTURAL EVOLUTION OF BINARY BARRIERS DURING SATURATION

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ABSTRACT In the last two decades the waste disposal concept based on the horizontal placement of canisters on a rigid support made of highly compacted bentonite blocks and the filling of the reminder of the gallery with granular bentonite material (GBM, i.e. pellets) has been tested in large-scale tests such as the EB and FE carried out at the Mont Terri URL (NAGRA 2019). These binary barriers are a source of bentonite heterogeneity, since the initial dry density and structure of the two components noticeably differ. CIEMAT carried out in the framework of BEACON a series of tests in cells to obtain information about the evolution, at laboratory scale, of initially inhomogeneous bentonite samples (pellets/blocks) upon hydration under isothermal conditions. The tests were performed with FEBEX bentonite in a large-scale oedometer and in a transparent cell and were described and jointly analysed in Villar et al. (2021). The materials used were the same as in the EB in situ test.

Bentonite water content and dry density gradients were observed at the end of the tests. 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 different even after full saturation and, unlike with water content or dry density, there was not a smooth change between the microstructural parameters of pellets and block. The most notable change in the pellets parts was the overall drastic decrease in size and volume of macropores, whereas the mean size of the pores smaller than 200 nm increased with respect to the original values. This increase was related to the increase in the smectite basal spacing as a result of the hydration of the interlayer cations, which is the driving mechanism for crystalline swelling. In fact, the basal spacing of the smectite was higher in pellets samples than in block samples, although it also increased in the latter. As well, because of the overall dry density decrease of the block subsamples, the volume and size of the macropores tended to increase in them, except in the shorter, less saturated tests. Nevertheless, the volume and size of macropores continued to be higher in the pellets than in the block parts.

These results have been compared with the postmortem analyses of the bentonite samples from the EB in situ test, dismantled after full saturation. Similar trends were found, but the samples from the in situ test presented a much broader range of dry densities and water contents, which was reflected in their pore size distribution. In both kinds of samples, for a given water content the basal spacing of pellets samples was higher than for block samples.

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SIMULTANEOUS DETERMINATION OF DEFORMATION AND LIQUID CONTENT IN SWELLING CLAY USING X-RAY RADIOGRAPHY

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ABSTRACT

Non-intrusive method based on X-ray radiography was used to measure deformation and local liquid content in swelling clay materials. In the measurements, cylindrical compacted clay sample is placed in a custom-built sample holder cell (Fig. 1 a)). Saturation of the sample and its swelling into a limited void space is monitored by taking consecutive X-ray projection images. The measurement setup is intended to mimic a situation where planned geological repository buffer clay material swells and homogenizes into bedrock cracks filled with liquid.

Numerical image analysis yields time development of one-dimensional displacement field throughout the swelling process by tracking tracer particles added to the sample. These displacements are used together with sample-specific calibration to compute temporally and spatially resolved dry clay and liquid contents during the homogenization process (Fig. 1 b)). Furthermore, the axial swelling pressure is monitored for more detailed information on the hydro-mechanical process in the clay.

The method was applied to several clay-liquid material combinations including three different montmorillonite-containing clay materials with varying dry densities, and seven different salt water solutions with varying chemical composition and salinity. The now collected comprehensive data shows that the method has good repeatability and coherence with validation data acquired by gravimetrical methods. In addition, the results show that as the salinity of the water solution increases, the swelling rates increase and swelling pressure decreases. This indicates that hydro-mechanical properties of montmorillonite-containing clay materials depend on the chemical composition of the wetting liquid. The obtained data is aimed to help in parametrization and validation of safety- and hydro-mechanical models of spent nuclear fuel repository concepts.



Figure 1 a) Sample holder cell schematic and b) dry bentonite clay (solid dotted red line) and water (solid dotted blue line) content as a function of time and position. Gravimetrically measured validation data (red and blue dots) and X-ray radiographs corresponding to the wetting times are included in the figure.

DESCRIPTION OF THE HYSTERESIS BASED MATERIAL MODEL

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ABSTRACT

A hydromechanical material model for bentonite, called the Hysteresis Based Material (HBM) model, has been developed within the Beacon project. The reason for developing yet another model describing bentonite clay comes from our experiences when using available geomechanical material models for representing bentonite. Commonly available models often belong to a framework suitable for a large class of geomaterials but not necessary bentonite, in some sense an extreme geomaterial.

It should, however, be said that we have in the past used available models, for example variants of the Barcelona Basic Model, with good results. Still, when pushed, the common type models show a limit in their generality and predictive capability for bentonite. To get reasonable results, we often have been forced to predict the result of the simulation to calibrate the material model used within the simulation, a less than optimal situation.

Much of bentonite's characteristic properties at full saturation have their origin in the osmotic nature of the material, i.e. the ability of the montmorillonite interlayers to take up water. With this in mind, HBM was formulated in the thermodynamical framework where this phenomenon is expressed macroscopically. In doing so, the clay water chemical potential and its pressure dependence are considered, and from this a relation appears which couples the hydraulic and mechanical processes. The obtained relation is linked to characteristic behaviour of bentonite such as retention properties, swelling pressure curves, and deviatoric stress at failure. During Beacon the formulation was changed and generalised in several aspects. The major developments were to enable general stress states and unsaturated conditions.

One of the main findings when testing the model's capabilities is that the HBM model agrees well with how bentonite behaves for a variety of different scenarios using a single set of parameters. There is no need to adjust or recalibrate the parameters for different scenarios to obtain representative responses.

This indicates that a suitable coupling between mechanical and hydraulic variables, here obtained from the thermodynamical starting point, give a versatile model. Versatile in the sense that different material characteristics such as retention, swelling pressure and deviatoric stress at failure relates to each other properly and thereby enables the material to be viewed from different aspects or to be exposed to very different conditions, without the representation losing validity.

The formulation can also be characterised as being rigid in the sense that it does not invite the user in excessive manipulations. This rigidness is of course positive from a perspective of performing predictive analyses. Once set up properly, the same parameterisation can be used to perform calculations of very different cases.

MODELING OF INITIALLY HETEROGEN SYSTEMS USING THE HYSTERESIS BASED MATERIAL MODEL

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ABSTRACT

Task 3 of work package 5 within the Beacon Project focused on simulating the hydromechanical evolution, water uptake and mechanical homogenisation, of three experimental setups of Febex bentonite. The three experiments were initially heterogenic and consisted of two separate bentonite volumes, a low-density volume (granular filling/crushed pellets) and a high-density volume (compacted block). The setup for the three experiments differed in how the volumes were stacked and/or how water was added to the bentonite volumes.

At Clay Technology, the opportunity to simulate these experiments have been used to apply and continue the development of the Hysteresis Based Material model. In this work, the initial modelling strategy was to make as few changes as possible to the representation of the unsaturated Febex block compared to what was used in previous simulations. The work was instead focused on the development of a new representation for the granular filling by introducing some modifications to the model of the block. Two of these modifications were to introduce a higher permeability and lowering of the relative load bearing area function, the latter modification resulting in a softer material at unsaturated states.

In a first realisation the axial compressive stress was overestimated, see the curve labelled FIRST in left graph below. But the obtained final dry density profile, see the curves labelled FIRST in the right graph below, agreed well with the experiment. It should be noted that the simulation, starting from an averaged dry density of 1.45 g/cm³, never will match the experimental data perfectly if solid mass is conserved.

There could be several reasons for the mismatch in vertical stress between model and data, for instance significant friction between the clay and the container wall, or unsuitable calibration of the material properties. In a second realisation the calibration of a core relation in the material model, the clay potential, was updated using more data points.

Using the second parameter set resulted in the curves labelled SECOND in the graphs below. The agreement in terms of vertical stress was improved, the overestimation was decreased, but the agreement regarding the dry density profile worsened, the profile show less homogenisation. This indicates that the representation of the granular material is too stiff and that it might be beneficial to lower the relative load bearing area function even more.



MODELLING OF THE SKB ASSESSMENT CASE USING THE HBM MODEL

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ABSTRACT

Within the BEACON project Clay Technology has implemented the so-called Hysteresis Based Material (HBM) model in Comsol Multiphysics. The HBM model has been used extensively by Clay Technology in other modelling assignments within the BEACON project with good results. At the core of the HBM model is the clay water chemical potential, which is parameterised using the fundamental hydro-mechanical behaviour of bentonite clay, e.g. swelling pressure, retention behaviour and deviatoric stress at failure.

As part of BEACON a predictive modelling exercise was to be carried out, and we selected the SKB assessment case. This case considers the thermo-hydraulic evolution in a backfilled tunnel in the Swedish KBS-3V concept for the final storage of spent nuclear fuel. The models were simulated using a 2D axisymmetric geometry in COMSOL which included highly compacted bentonite blocks and the surrounding pellets material. The water transport through the surrounding rock mass was not included in the model. Instead, water inflow to the bentonite clay was handled using a liquid flow boundary condition, simulating both free access to water and a flux-limited case.

The mechanical behaviour at the interface between the buffer and the rock should realistically be handled using wall friction as the clay moves along the tunnel surface. However, at the time of modelling it was not possible to include friction and thus two sets of models were simulated, roller (e.g. free movement along the rock wall) and locked (e.g. infinite friction) to study the bounding effects of friction.

The results of the models showed a significant homogenisation of the buffer components, with the highly compacted bentonite blocks swelling up and compressing the pellet filled outer column due to water uptake. An example of the change in dry density is shown in the left graph in Figure 1 below, where the dry density at the start and end of the simulation are shown in two points of a model with roller conditions on the tunnel wall and free access to water. The right graph in Figure 1 shows the stress evolution in the same model. One conclusion to be drawn from the modelling is that the influence of friction is probably rather small while the rate of water uptake can have a very significant effect on the final state of the buffer components.



Figure 1. Dry density at the start and end of the simulation (left) and net mean stress evolution (right) in a model of the SKB assessment case with free access to water and roller boundaries on the tunnel wall.

BENTONITE HOMOGENIZATION AND MICROSTRUCTURE EVOLUTION MODELLED USING A DOUBLE STRUCTURE CONSTITUTIVE LAW

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ABSTRACT

The microstructure of the bentonite undergoes significant changes during hydration and subsequent saturation even under quite confined conditions. Those changes are likely to affect the hydromechanical behaviour of the bentonite in a substantial way. To take into account the evolution of the microstructure in an approximate way, a double structure constitutive law has been developed that distinguishes two structural levels: a microstructure that considers the basic phenomena occurring at particle level and a macrostructure that refers to the overall arrangement of the porous medium. The behaviour of the microstructure is assumed to be non-linear, reversible and independent of the macrostructure. In contrast, the behaviour of the macrostructure is irreversible and influenced by the deformation of the microstructure. The effects of the microstructure on the macrostructure are expressed by suitably defined interaction functions.

The constitutive law used in the BEACON project is a development of the previously existing BExM model where a number of significant enhancements have been incorporated. The main ones are: a more rigorous definition of the porosity levels in terms of volume fractions; the microstructure may be unsaturated; negligible advective fluxes through micro-pores are considered based on the very low mobility of water and gas in this structural domain; and hydraulic equilibrium between microstructure and macrostructure is not assumed. The potential local difference of the water potential in macro- and micro-pores controls the mass of water exchanged between both pore domains.

The performance of the double structure constitutive law has been demonstrated in the modelling of the laboratory tests that constitute step 3 of the project's WP5. The tests have been carried out by CIEMAT to explore the behaviour of binary barriers during saturation. For this purpose, the oedometer sample subject to isothermal hydration is composed of two parts: bentonite block and bentonite pellets. A large degree of homogenisation in terms of dry density is observed at the end of the tests that it is satisfactorily reproduced by modelling (see Figure, left). The tests have also yielded important information concerning the evolution of the microstructure through the performance of MIP tests before and at the end of the tests. In this way they provide essential information to check the performance of the double structure model in this regard. By and large, the modelling results correspond well to the observations. (see Figure, centre and right)



Observations vs, modelling results of the distributions of dry density (left), micro void ratio (centre) and macro void ratio (right) at the end of test MGR22.

DOUBLE POROSITY MODEL FOR BENTONITE IN THERMO-HYDRO-MECHANICAL PROCESSES

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ABSTRACT

Bentonite plays a central role in the safety concepts for nuclear waste disposal in crystallineand clay-rock formations. Because of its low permeability, its capability to swell under water uptake and due to its radionuclide attenuation potential, it is currently regarded as the most suitable material for geotechnical barriers. Bentonite is used as buffer material, as well as in sealing constructions. The successful design of an emplacement site in different host rock formations crucially relies on an accurate description of the thermo-hydro-mechanical behaviour of the geotechnical barrier. Within the BEACON project, experts in different disciplines of bentonite mechanical behaviour are brought together to collect experimental data, validate their models and discuss the strategies to effectively model its thermo-hydromechanical behaviour in nuclear waste emplacement sites by numerical codes.

During the project, the THM implementation in OpenGeoSys was enhanced in all involved processes. The deformation process now involves an inelastic constitutive approach based on a modified Cam-clay constitutive law, thus increasing process complexity compared to linear elasticity used at the beginning. For the hydraulic process, a multiscale porosity model was introduced in order to take the different water uptake behaviour of large and small pores into account. Therefore, the porosity evolution on the micro- and macro-scale is incorporated into the mass balance equation of the fluid. A swelling model, which depends on the water saturation on the microscale is an additional enhancement. The transport equation involves the flow of liquid and its corresponding vapour, as well as its phase transition between both physical states. It is postulated, that the gaseous phase can move freely in the porous medium and there is no mass exchange between the constituents air, liquid and solid.

In this contribution the resulting model will be presented. Its capabilities and restrictions are tested with examples (see e.g. **Fel! Hittar inte referenskälla.**) of the different BEACON tasks and the potential strategy to further improve the model will be sketched.



Figure 1: Line plots of porosity and saturation at different times within the pedestal. Simulation results of the Nagra assessment case conducted with OpenGeoSys.

PREDICTION OF BENTONITE BEHAVIOUR USING HYDRO-MECHANICAL MODEL DEVELOPED IN COMSOL MULTIPHYSICS

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ABSTRACT

Within the BEACON project several bentonite materials (MX-80, FEBEX) of different forms (block, pellets, pellet-powder mixture) were investigated experimentally and numerically. Tests of different scale, configuration and hydration mode has been performed. The Lithuanian Energy Institute (LEI) participated in the modelling activities of the BEACON project. A non-linear elastic hydro-mechanical model for representation of behaviour and interaction between different forms of bentonite was developed in COMSOL Multiphysics (USA) and validated against experiments performed by the project partners (SKB, CEA, POSIVA, CIEMAT, EPFL). The model is based on Richard's equation to represent water flow through unsaturated material and elastic deformation to represent wetting induced swelling. The model includes couplings to consider the impact of mechanical deformations on porosity change and subsequently on change of water balance, specific moisture capacity, storage coefficient and permeability. LEI modelling results of three laboratory experiments are presented in this study:

- Hydration of compacted MX-80 bentonite block at constant volume condition with subsequent increase of volume for swelling (Test1a01) performed by SKB, Sweden;
- Large scale oedometer tests under confined volume conditions performed by CIEMAT, Spain (layers of compacted block and pellets of FEBEX bentonite);
- High-pressure oedometer tests, performed by EPFL, Switzerland (granular MX-80 bentonite).

Modelling results were compared to the available experimental data. In general, a satisfactory agreement between the modelling results and the experimental data were obtained, especially for hydraulic parameters (water intake to the samples and degree of saturation). Results of mechanical behaviour (swelling pressure, dry density and void ratio) varied to some extent compared to the experimentally measured values.

Current model formulation includes some parameters (e.g. swelling coefficient) which depend on bentonite type, sample form, density, porewater composition, experimental conditions (confined volume, unconstrained swelling conditions), etc. Due to lack of consistent experimental database covering a full range of these important aspects, it was difficult to derive functional relationships thus the parameter values were calibrated when modelling the particular test. In order to increase the predictive capacity of the model, the hydro-mechanical behaviour of bentonite under different material layouts and hydration conditions should be explored further experimentally and numerically. Future model developments are needed with the main focus on the consideration of friction (for laboratory scale experiments) and the representation of irreversible strains.

Despite the highlighted shortcomings, a valuable knowledge on modelling coupled hydromechanical processes has been gained by LEI team during the cooperation with partners within the project. Sharing the knowledge on main processes, aspects and challenges in numerical assessment paved the way for further competence development in the prediction of bentonite material behaviour.

SENSITIVITY ANALYSIS OF BENTONITE BLOCK-PELLET TUNNEL BACKFILL MECHANICAL EVOLUTION DURING SATURATION

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ABSTRACT

A sensitivity analysis was performed to study the relative importance of factors affecting the mechanical evolution of KBS-3 bentonite block-pellet tunnel backfill during saturation. A double porosity hydromechanical model was used for the bentonite blocks, whereas the model was extended to include a third porosity level for pellets. The model geometry consisted of an axisymmetric cut cone (length: 7 m, minimum and maximum radii: 2.50 and 2.86 m), which was filled with compacted bentonite blocks (cylinder with 2.31 m radius) surrounded by bentonite pellets.

The sensitivity analysis followed Definite Screening Design (DSD) with six three level input parameters (with low end, high end, and centre values) and one categorical input parameter, which required 16 model runs in total. The three level parameters were design parameters (the block and pellet dry densities), bentonite swelling capacity (the state function in the model), mechanical model parameters (the block and pellet elastic stiffness) and a hydraulic model parameter (the intrinsic permeability). The hydraulic boundary condition was varied between two options (categories), which were water inflow either through the whole bedrock boundary or through a single vertical fracture at the middle level of the tunnel section.

Using the DSD input parameter combinations and the simulation results, regression models were fitted for three output variables to capture different aspects of the mechanical evolution. To measure the density homogeneity of the tunnel backfill after saturation, the pointwise deviation from the average dry density was integrated either over the whole model area or over the tunnel section mid-plane at the fracture. The mean stress after saturation was selected as the third output variable to represent the swelling stress state of the tunnel.

The statistical tests of the regression models suggest that the sensitivity analysis is statistically valid for the intended screening purposes. The results indicate that the most important input parameters for the mechanical evolution are the hydraulic boundary condition, the swelling capacity, and the intrinsic water permeability. The hydraulic boundary condition and the intrinsic water permeability were important especially for the density homogeneity, whereas the swelling capacity affected the mean stress the most. The results could be used to guide future experiments and simulations on the topic.

The work was performed in Euratom Beacon project, which receives funding from the Euratom research and training programme 2014-2018 under grant agreement No 745 942.

APPLICATIONS OF A THERMO-HYDRO-MECHANICAL INTERNAL LIMIT MODEL TO BENTONITE EXPERIMENTS

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Bentonite is used in components of the Engineered Barrier System in many European geological disposal concepts for high-level radioactive waste and spent fuel. 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. Coupled models of the thermo-hydro-mechanical response of bentonite are used to demonstrate understanding of bentonite behaviour in experiments and to predict the response of bentonite in a repository environment. One such model is the Internal Limit Model, which has been further developed and tested as part of the Beacon project.

The Internal Limit Model is based on the Modified Cam Clay model and uses the observation that, for a given dry density of bentonite, there is a limiting stress that the sample can support, be that stress due to swelling, compaction or suction, to explicitly couple the hydraulic and mechanical models. In the Beacon project, the model has been applied to a series of laboratory experiments conducted with MX-80 and FEBEX bentonites, using a single set of parameters for each bentonite type. Models were built in QPAC, a general-purpose finite volume code. Model developments were required to represent void and friction boundaries, pellets and granular bentonite. Friction has been shown to have a significant impact on swelling behaviour and stresses in small-scale experiments.

The model has also been applied to larger-scale experiments, including the FEBEX in-situ experiment, and used to represent a bentonite plug seal in the ILW disposal cells of Andra's repository concept. The complex geometry of the disposal concept required development of a pre-processor to allow unstructured grids developed using the Gmsh mesh generator to be used in QPAC. These applications have demonstrated the ability of the model to reproduce and predict the evolution of bentonite components with minimal calibration.

ESTIMATION OF THE BUFFER HOMOGENISATION IN THE PROTOTYPE REPOSITORY

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ABSTRACT

The Prototype Repository is a full-scale field experiment in crystalline rock at a depth of 450 m in the Äspö Hard Rock Laboratory (Äspö HRL). The experiment aims to simulate conditions largely relevant to the Swedish/Finnish KBS-3V disposal concept for spent nuclear fuel. The experiment consists of six deposition holes with copper canisters (with electrical heaters) and with bentonite (MX-80) buffer. The buffer was installed as compacted blocks and by filling the outer slot between the blocks and the rock wall with bentonite pellets. The test-tunnel was divided into two separate sections and backfilled and finally sealed by two reinforced concrete dome plugs. The inner section, with four deposition holes, was installed in 2001, whereas the outer section, with two deposition holes, was installed in 2003 and subsequently retrieved in 2010/2011. The inner section will be retrieved beginning in 2023, and different pre-modelling activities are currently ongoing as part of the planning of this operation.

The aim of this work is to estimate the buffer homogenisation in the Prototype Repository. An extensive and detailed analysis regarding the water content and the density of the buffer was performed during the course of the dismantling of the outer section (SKB, P-13-14). These measurements demonstrated that the buffer had homogenised to a large extent, but also that a remaining heterogeneity could be noted between the inner and outer parts of the buffer. Differences between the dry density in different directions could also be observed. If this was due to differences in the installed density in different directions, or if it was caused by localized water entry and horizontal displacements of the canister is not known. The buffer in the inner section has been exposed to conditions with water uptake for a duration almost three times as long as for the buffer in the inner section. It can therefore be anticipated that the dry density distribution of the buffer in the inner section will display a larger extent of homogenisation in comparison with the outer section.

The estimation is being performed through numerical modelling. For this purpose, a set of COMSOL models of the buffer at canister mid-height is analysed. The Hysteresis Based Material (HBM) model is used for this work. This was first defined during the course of the homogenisation project (SKB TR-19-11) and the related modelling task (SKB P-18-05). The definition and the implementation of this has been further developed within the framework of the BEACON project.

It is not possible to make predictions of any specific part of the buffer, since "*the uncertainties in the measured inflows to the deposition holes were too large to make a precise calibration of the rock surrounding the deposition holes*" as was noted for the TH modelling of the outer section (SKB, TR-13-22). Different generic 1D axisymmetric model cases are therefore analysed: with fast or slow hydration, and (due to the failure of some of the heaters) with or without a thermal gradient. This will thus address the issue of the rate of hydration and how this influences the extent of remaining heterogeneity at full saturation. The issue of horizontal movements of the canister caused by the uneven wetting of the buffer is analysed with HM models with a circular 2D geometry.

Please send abstracts to <u>beacon@skb.se</u> Deadline 15 April 2022. Response will be given 30 April 2022

INVESTIGATION OF BCV BENTONITE

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ABSTRACT

Deep geological repository (DGR) concept for radioactive waste is based on system of barriers. Those are natural and manmade. Important part on manmade barrier is bentonite buffer and backfill. To safely design those barriers a knowledge of their behaviour and reliable dataset of material properties is needed.

Within WP4 of BEACON project hydromechanical properties and behaviour of bentonite was investigated as an input into development of mathematical models describing behaviour of engineered barrier system (EBS).

At Czech Technical University (CTU) and Charles University (CU) laboratories an extensive laboratory test programme was carried out on Czech bentonite (BCV) from Černý vrch deposit (north western region of the Czech Republic). This material was chosen as it is reference research material in the ongoing development of the Czech deep geological repository (DGR) concept.

The hydraulic and mechanical properties of BCV bentonite were investigated using: Constant load tests, Constant volume tests, Stress path investigation, Water retention curves, MIP, ESEM. This was complemented by set of small physical models investigating Swelling into limited void and Homogenisation of dual density samples.

The tests were performed on one batch of BCV material in both CTU's and CU's laboratory using different equipment allowing to cross check the procedures and results. The resulting comprehensive dataset was used to support development and verification of hypoplastic material model for BCV.

The results of Stress path investigation using oedometric tests on powder material and pellets shows that there is a strong stress/saturation path dependency and stress at saturation is important. It indicates that there is continuous development of macro- & micro-structure of material. However, after full load and unload cycle in saturated state stress path stabilises.

Multiple sets of dual density experiments, each combining two different initial dry densities, were carried out. Within each set, two identical samples were tested with different directions of saturation. A significant homogenisation was observed in all dual density samples and evaluated in comparison with swelling pressures of the individual layers. A study of homogenisation in vertical profile was carried out by direct determination of dry density in vertical profile on selected set of samples. A considerable degree of homogenisation was observed in all experiments. The final inhomogeneities may be partially attributed to the boundary conditions, especially wall friction, during the homogenisation process.

The laboratory experiments performed were modelled using hypoplastic material model using single element (Triax software) and finite element (SIFEL FEM package) simulations. This

allowed to perform calibration of the model and at the same time to get a better insight into processes taking place in the experiments.

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HYPOPLASTIC MODELLING OF BENTONITE HOMOGENISATION

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ABSTRACT

The presentation is aimed to describe progress in bentonite simulation using THM hypoplastic model implemented in coupled THM finite element code achieved during the BEACON project. The double structure hypoplastic model defined within coupled THM framework is introduced first. Its evolution during the BEACON project is demonstrated by single and finite element simulations of experimental data on BCV bentonite using the original and updated version of the model, which includes, for example, more advanced smooth formulation of water retention curve. The talk will focus not only on the constitutive aspects of the model (prediction of soil behaviour), but also on the critical aspects of the model implementation, which do not affect element test predictions but significantly affect robustness of finite element simulations. This includes, among others, the way the model stiffness matrix is calculated and the way how negative/positive suction transition is handled.

Second, the aspects of coupled finite element model formulation are discussed. Differences between fully coupled and staggered approaches for simultaneous solving mechanical and transport equations are introduced and differences in their predictions is demonstrated using hypoplastic model simulation of some boundary value problems. Also, the effect of permeability dependence on state variables (constant permeability vs. density- and saturation-dependent permeability) is demonstrated.

Finally, predictions of hypoplastic model obtained throughout the benchmark exercises within WP3 and WP5 of BEACON project are shown. Predictions of benchmark element test (Task 3.3), benchmark laboratory tests using finite element simulations focused on bentonite homogenisation (MGR tests of WP5) and benchmark full-scale Mock-up experiment (CRT test) are shown. Predictions of experiments on BCV bentonite performed by CU & CTU teams, including the homogenisation dual density experiments, are shown along with the common benchmark simulations performed by all team members.

Finally, conclusions are drawn regarding predictive capabilities of the constitutive model and robustness of finite element simulations. While significant progress has been achieved during the BEACON project, there are still important aspects of bentonite behaviour to be studied in subsequent research. This includes most importantly modelling pellet material. From the finite element modelling perspective, the critical issue is fully coupled simulation of highly deforming specimens with significant pore water pressure evolution and dissipation due to sample displacements.

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HYDRATION SURVEY OF A LARGE SCALE SEALING EXPERIMENT (BURE, FRANCE)

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ANDRA has designed a large scale sealing experiment which is called NSC (French acronym for Noyau de SCellement). The main objective of the NSC experiment is to verify the general performance and evaluate the equivalent hydraulic permeability of a sealing core as well as the near field of the seal. Given the long time associated to the natural hydration process of a repository seal (thousands of years), the core of the NSC test is artificially hydrated using six hydration membranes embedded in the core. Then, once saturation is achieved, an overall permeability test will be performed between upstream and downstream of the seal to estimate the equivalent permeability of the seal.

The NSC experiment is located at the end of the GES gallery of the Andra's URL. The seal has a length of 5 m, a diameter of 4.6 m, and it is supported at its ends with two concrete plugs. The core is made by bricks (300 x 200 x 100 mm) composed by a mixture of 40% of bentonite MX80 and 60% sand (representing 95% of the core material) and a mix of pure bentonite powder and pellets filling the spaces between the blocks (representing the 5% of the core material). Regarding the measurements, 420 sensors were installed along with 23 instrument boreholes, giving 866 measurement points (Figure 1). Inside the core and the concrete plugs, sensors are distributed along different cross sections. In the seal and at the interface with the concrete plugs (upstream and downstream), is monitored with 319 sensors (humidity sensors: 64 capacitives, 64 psychrometers and 16 FDR; pore pressure sensors: 99; total pressure sensors: 76).



Figure 1 General layout of the NSC experiment in the Andra's URL (a) and location of the sensors inside the core and the concrete plugs (b)

The first phase of this experiment is the artificial hydration of the core until it is saturated. The second phase corresponds to a performance test which aims to assess the overall permeability of the seal. A third phase will consist of injecting gas into the seal to get the performance of the seal to gas percolation.

The GES drift was excavated in 2012 and all the instrumentation inside GES drift and S/B mixture was installed during 2013. During the construction of the S/B seal, volume and mass of the S/B mixture was controlled. Those measurements were used to estimate the dry density of the clay material in the seal, which is close to 1.45 kg/m³. The artificial hydration started in January 2014. After 8 years, the amount of water injected is approximately 23 m³. Relative

humidity measurements indicate that full saturation has not yet been reached. Artificial hydration is currently ongoing.

ANDRA and UPC-CIMNE have identified the interest of carrying out a project related to the improvement of expansive clay-based materials models and simulate this NSC experiment. For that purpose, first hydro-mechanical simulations have been carried out in an axisymmetric configuration with CODE_BRIGHT. Specific constitutive models were implemented to cope with the behaviour of the Callovo-Oxfordian formation, and the expansive bentonite-based core material. For the definition of the simulation phases, the actual registered schedules of the excavation, construction and artificial hydration processes were taken into account. Nine simulations were performed, considering three different values for the initial porosity of the core and three different values for the power law parameter of the liquid phase relative permeability equation. The simulations were able to reproduce in general the artificial hydration procedure. Results of relative humidity evolution within the core show a good agreement with experimental data, except for the fact that in all the simulation the fully saturation state is eventually reached at some time (Figure 2).



Figure 2 Simulation: a) Model geometry, materials and mesh and b) Relative humidity evolution: sensitivity to the power law parameter of the liquid phase relative permeability equation

Works of the next stages will focus to the following aspects:

- Include the gas phase in the formulation to analyze the effect of eventual gas trapping on the reach of full saturation in the core.
- Implement the hydraulic interaction between the micro and macrostructure within the framework of the BExM model, in order to cope with the observed delay between hydration and swelling processes.
- Create 3D simulations to further analyze effects not considered in the axisymmetric simulations and provide insight into the representativity of the latter ones.

STUDY OF COUPLED GAS MIGRATION PHENOMENA THROUGH CLAY BARRIER SYSTEMS INTENDED FOR THE ISOLATION OF HIGH-LEVEL NUCLEAR WASTE.

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ABSTRACT

The main safety function of a Geological Disposal Facilities (GDFs) for High-Level nuclear Waste (HLW) and Spent Fuel (SNF) is to confine the pollutant waste, preventing or delaying (as much as possible), the release of radionuclides to the biosphere. Complex Thermo-Hydro-Mechanical and Chemical (THMC) phenomena will take place in the Engineered Barrier System (EBS) as a result of the heating (generated by the HLW/SNF radioactive decay) and the hydration (induced by the host rock) under highly confined conditions. The GDF's fundamental functions can be seriously jeopardized by the presence of evolving or pre-existing discontinuities and interfaces between materials in the EBS, which will serve as preferential pathways for the flow of water and gas.

In this study we present a-state-of-the-art automated cell developed to study the evolution of EBS prototypes under repository conditions (**Fig. 1a**). The scaled prototype (**Fig. 1b**) is composed of a cylindrical clay barrier surrounded by a rock (5cm diameter, 10 cm height). Six microprocessor-controlled syringe pumps for the precise regulation and measurement of fluid pressure and volume change assist the operation of cell. A high accuracy mass flowmeter monitors the gas volume and flow rate permeating through the EBS. A heating unit enables conducting tests up to T ~150°C. Several sensors allow tracking the evolution of pressure, temperature, stresses and displacements during testing.

The cell was used to investigate the evolution of a clay barrier system during hydration. The sample was made up of a clay mixture with a 67/33 ratio (by dry mass %) pellet/powder of MX-80 bentonite hosted by an argillite rock. Gas breakthrough tests were conducted at different stages of the experiment involving several hydration and rehydration stages (**Fig. 1c**). We observed that the rock-clay interface offers potential pathways for gas release through the EBS. The experiments also show a reduction in the gas breakthrough pressure during successive gas breakthrough pressures when the EBS is not re-hydrated. Further insight into the behaviour of this type of system was achieved by means of an updated fully coupled THMC finite element code able to handle both pre-existing and evolving discontinuities in geological media.



Fig. 1. *a) Multipurpose automated cell, b) EBS prototype, and c) EBS gas breakthrough tests.* The financial support from the Nuclear University Energy Program (NEUP), Department of Energy (DOE), USA, is acknowledged. Award DE-NE0008762 (Project #18-15585).

NUMERICAL MODELLING OF AN INHOMOGENEOUS BENTONITE BARRIER FOR RADIOACTIVE WASTE DISPOSAL APPLICATIONS

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ABSTRACT

Disposal of high heat generating radioactive waste in deep geological formations generally includes bentonite barriers, the latter installed to shield the surrounding host rock from the canister containing the waste. The evolution of the hydro-mechanical properties of bentonite barriers over time has to be carefully assessed by designers, in order to satisfy the repository safety criteria in the long-term (i.e. several hundreds of years after installation).

When installed, bentonite barriers are unsaturated and, therefore, the evolution of their mechanical properties over time depends on the transient seepage processes regulating water flow from the surrounding host rock to the bentonite. Engineered barriers are usually formed of compacted bentonite blocks, often employed in combination with bentonite pellets, the latter used to fill the gaps between blocks and the host rock interface. Compacted bentonite blocks are characterised by very low hydraulic conductivity, hence their saturation can take from several decades to several hundreds of years. Predicting the bentonite behaviour over such long time frames represents a significant challenge for design engineers, given that fully representative laboratory or field experiments are unfeasible. In this scenario, numerical tools, such as finite element (FE) codes, enable predictive assessments of the barrier performance in the long term.

The present work reports the results of isothermal hydro-mechanically coupled FE analyses, conducted at Imperial College London as part of the BEACON project to assess the long term performance of an inhomogeneous bentonite barrier employed in a radioactive waste repository. The numerical simulations reproduce the KBS-3 design scheme developed in Sweden by SKB, that envisages the combined use of MX-80 bentonite high-density blocks and pellets for tunnel backfilling.

Two-dimensional (2D) axisymmetric FE analyses were conducted, accounting for the variability of the tunnel cross-sectional area (i.e. the thickness variability of the pelletised bentonite layer). Two bentonite hydration scenarios were considered, related to two hydraulic boundary conditions imposed by the host rock on the barrier: (i) application of pore water pressures at the rock/bentonite interface, representative of repository depth; and (ii) a low water inflow allowing for full saturation to take place over around 4000 years (aimed at reproducing the scenarios of free and restricted access to water, respectively). The simulations were conducted with the Imperial College Finite Element Programme (ICFEP), employing an advanced constitutive model capable of simulating the hydro-mechanical behaviour of unsaturated expansive soils characterised by a dual porosity structure.

The analyses allowed to verify the long-term safety requirements of the inhomogeneous blockand-pellet bentonite barrier employed as part of the KBS-3 design scheme (i.e. in terms of minimum and maximum swelling pressures developing during hydration). The two FE simulations showed that, even when free access to water is considered, steady state conditions may be achieved in over a century. The analyses also show that, during hydration, the pellets tend to compress and the blocks tend to swell, always resulting in a more homogeneous final void ratio distribution across the engineered barrier, with a more pronounced homogenisation likely to be achieved with slower hydrations.

Implementation of an advanced constitutive model for bentonite using MFront for safety and performance assessments of HLW-repositories in the numerical code OpenGeoSys

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Argillaceous formations are currently being considered in several countries as a possible host medium for deep geological disposal of high- and intermediate-level and long-lived nuclear waste (Delage et al., 2010). In such formations, bentonite materials are considered as the main sealing component of the engineered barrier system. This is particularly due to their swelling capacity upon hydration, which helps to close remaining gaps and voids at the sealing location, and thus ensure confinement of the disposed radioactive waste.

In repository conditions, bentonite materials will be subjected to coupled thermo-hydro-mechanical loads, which can potentially compromise their sealing capacity if certain tolerances are exceeded. The understanding of the complex thermo-hydro-mechanical behaviour of bentonite is therefore necessary for the safety assessment of repository systems. Constitutive models able to reproduce such material behaviour are needed for the numerical based safety and performance assessments of repository systems.

The development of material models for bentonite-based materials has been addressed in the past two decades by several researchers; see for instance Alonso et al. (1999), Mašín (2012, 2017), Dieudonné (2016), Darde (2020) or Ruiz (2020). The approaches proposed by Mašín (2012, 2017) have been selected by the authors for further development and implementation in the numerical code OpenGeoSys (Kolidtz et al. ,2012; Bilke et al. ,2019). The implementation will be carried out in MFront, a code generation tool for constitutive modelling (Helfer et al., 2015; Helfer et al., 2020). The complexity of the considered material behaviour requires addressing several numerical challenges. For instance, a new concept has been developed to use MFront as a wrapper to integrate an existing implementation of a constitutive equation in a solver supported by MFront (Helfer et al., 2020a). The concept has been successfully validated for the hypoplastic model for bentonite by Mašín (2012, 2017). The present contribution intends to give an overview to the implementation strategy for the selected models within the MFront framework and the first results obtained so far.

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HYDRO-CHEMO-MECHANICAL MODELLING OF BENTONITE SEALING COMPONENTS

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ABSTRACT

Bentonite-based seals will be used for the closure of galleries, ramps and shafts of the Cigéo project, the future deep geological disposal facility for radioactive waste in France. Their main function is to limit the water flow within the repository. This implies the development and stability of swelling pressure that ensures a complete filling of technologic voids and an effective contact with the surrounding materials and host rock. The engineering performance of these seals in the long term involves hydro-chemo-mechanical coupled processes which can result in changes in the swelling pressure of bentonite. The objective of this work is to evaluate and quantify the impact of hydrogeochemical processes at seal scale on its mechanical performance (fig.1). To this end, a set of hydro-chemo-mechanical models are implemented that explicitly consider two-phase flow, reactive transport, and non-linear solid mechanics. The geochemical alteration of the seal due to the interaction with the surrounding materials (concrete plugs, concrete liner, and the surrounding Callovo-Oxfordian claystone) and its effects on swelling pressure evolution are assessed for various sealing concepts and scenarios.

A coupled hydro-chemo-mechanical (HCM) model for swelling clays has been developed [1]. The HM performance of bentonite is assessed by means of a nonlinear-elastic approach based on the Barcelona Basic Model (BBM). The impact of chemical processes on the swelling capacity of bentonite is included by the explicit consideration of (1) montmorillonite dissolution, (2) porewater salinity, and (3) cation exchange reactions in the constitutive law. Parameterization and validation are based on existing swelling pressure tests on different clay-sand mixtures and a dedicated experimental modelling study [2].

The HCM models were implemented in iCP [3], an interface between Comsol Multiphysics and Phreeqc. Initially, the bentonite constitutive law was included by adapting the Comsol implementation of the BBMx. This approach showed to be suitable to represent swelling pressure development under confined conditions and enabled the implementation of fully-coupled HCM models for long-term assessments (100,000 years). However, some limitations were detected in this approach linked to the integration scheme used to solve the constitutive relation. To overcome these, a dedicated implementation of the bentonite constitutive law based on the use of the External Material Model (ExtMat) functionality in Comsol has been developed. This functionality enables the user to implement a custom constitutive relation in Comsol by means of an external library programmed in C. The new HM implementation solves the constitutive relation incrementally and has been validated with CODE_BRIGHT results for confined and unconfined bentonite test cases.

In this contribution, we present results of the HCM evolution of different Cigéo sealing systems (fig. 1) with special focus on the swelling pressure changes due to hydraulic and chemical processes (fig. 2). The mechanical response of the system is governed by the seal resaturation, the pore pressurization and partial desaturation due to hydrogen overpressures, host rock drying, COx and concrete creep, and long-term geochemical processes.

Acknowledgements

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Fig. 1. Concept of sealing component in Cigéo (source: Andra).



Fig. 2. Potassium fraction in bentonite interlayer (left) and swelling pressure evolution (right).

DOWNSCALED TESTS FOR STUDYING THE INFLUENCE OF THE TEMPERATURE IN THE HOMOGENIZATION PROCESS

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ABSTRACT

The buffer will be under strong thermal gradients during the first 200-300 years before the decay of the spent nuclear fuel activity reduces significantly the temperature. The influence of the thermal gradients was studied in past in tests for assessing the vapour transport (Pintado et al. 2002; Pintado et al., 2013a) and the shrinkage – swelling due to the movement of vapour and liquid water (Pintado et al. 2011).

In order to study the behaviour of the blocks and pellets at similar conditions as expected in the deposition holes, new test cells were developed at larger scale. Some of these cells were constructed in plastic in order to be able to observe directly the behaviour of the pellets and the evolution of the piping channels in erosion tests. The size of the samples was 269 mm diameter and 800 mm heigh. These cells were also instrumented for measuring the swelling pressure directly with load cells and pressure transducers and indirectly gluing strain gauges on the plastic cell (Pintado et al. 2013b; Bendito and Pintado, 2016). The tests were carried out in isothermal conditions at laboratory temperature (22°C). These tests allowed to study the hydration of the buffer – pellets system and also the mechanical erosion when water was pumed into the cell. The final density distribution was measured after the tests.

In order to study the influence of the temperature, two different sets of tests were carried out with these cells. The first set of tests was carried out adding a heater at the axis of the test cell, so a radial thermal gradient was fixed along the sample. The temperature of the heater was 98°C and the cell wall temperature was around 30°C. The second set of tests were carried out at a smaller thermal gradient, where the core temperature of the sample was 65°C and the cell wall and pumped water temperatures were 50°C.

The results of downscaled tests showed that the mechanical erosion was not affected by the temperature but tests at elevated temperature in isothermal conditions showed less homogenization.

The plastic cells allow to observe the tests directly and they are quite useful for studying the tests under qualitative point of view, observing the evolution of the large pores between the pellets or the evolution of the channels during the erosion process but the measurements should be considered with caution due to the creep of the plastic materials, so the expansion measured with the strain gauges might be overestimated and the radial swelling pressure might be underestimated.

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