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REVIEW ARTICLE

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Modelling of the long-term evolution and performance of engineered barrier system

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Abstract. Components of the so-called "multiple-barrier system" from the waste form to the biosphere include a combination of waste containers, engineered barriers, and natural barriers. The Engineered Barrier System (EBS) is crucial for containment and isolation in a radioactive waste disposal system. The number, types, and assigned safety functions of the various engineered barriers depend on the chosen repository concept, the waste form, the radionuclides waste inventory, the selected host rock, and the hydrogeological and geochemical settings of the repository site, among others. EBS properties will evolve with time in response to the thermal, hydraulic, mechanical, radiological, and chemical gradients and interactions between the various constituents of the barriers and the host rock. Therefore, assessing how these properties evolve over long time frames is highly relevant for evaluating the performance of a repository system and safety function evaluations in a safety case. For this purpose, mechanistic numerical models are increasingly used. Such models provide an excellent way for integrating into a coherent framework a scientific understanding of coupled processes and their consequences on different properties of the materials in the EBS. Their development and validation are supported by R&D actions at the European level. For example, within the HORIZON 2020 project BEACON (Bentonite mechanical evolution), the development, test, and validation of numerical models against experimental results have been carried out in order to predict the evolution of the hydromechanical properties of bentonite during the saturation process. Also, in relation to the coupling with mechanics, WP16 MAGIC (chemo Mechanical AGIng of Cementitious materials) of the EURAD Joint Programming Initiative focuses on multi-scale chemo-mechanical modeling of cementitious-based materials that evolve under chemical perturbation. Integration of chemical evolution in models of varying complexity is a major issue tackled in the WP2 ACED (Assessment of Chemical Evolution of ILW and HLW Disposal cells) of EURAD. WP4 DONUT (Development and improvement of numerical methods and tools for modeling coupled processes) of EURAD aims at developing and improving numerical models and tools to integrate more complexity and coupling between processes. The combined progress of those projects at a pan-European level definitively improves the understanding of and the capabilities for assessing the long-term evolution of engineered barrier systems.

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1 Introduction

The concept of geological disposal of radioactive waste emerged in the late 1950s [1–4] to ensure long-term containment and isolation of the waste from the biosphere and ensure the safety of future generations. A multi-barrier system of engineered (near field) and natural barriers (near and far field) is foreseen in most of the repository designs. The Engineered Barrier System (EBS) comprises various components, such as the waste form itself, waste canisters, backfill, seals, and plugs. Materials, designs, and safety functions of the EBS depend on the host rock and the concept developed in each country.

The Strategic Research Agenda (SRA; https://www.ejp-eurad.eu/publications/eurad-sra) of the European Joint Programme on Radioactive Waste Management (EURAD; https://www.ejp-eurad.eu/) describes the scientific and technical domains and sub-domains and knowledge management needs of common interest between EURAD participant organizations [5]. The SRA scope is structured by seven scientific themes. Theme number 3 is entitled "Engineered barrier system properties, function, and long-term performance". A list of RD&D priorities and activities of common interest to be addressed within EURAD for theme 3 has been established. Amongst others, the following priorities have to be considered:

- improved understanding of the interactions occurring at interfaces between different barriers, including waste packages in the disposal facility.
- Characterized bentonite/clay-based material evolution under specific conditions to provide data on hydromechanical, thermal and chemical behavior.
- Improved quantification and understanding of cement-based material evolution to improve long-term modeling and assessments.
- Improved understanding of the performance of plugs and seals.
- Improved description of the spatial and temporal evolution of transformations affecting the porous media and degrading materials in the near field of HLW and ILW disposal systems.

Tackling these R&D priorities will help to understand the EBS system evolution and the interactions within the repository near field environment, which support the design and optimization of the EBS system. Independently of the waste package, backfill, and buffer materials under consideration, a need for an improved understanding of the mechanical/chemical evolutions at the interface between the EBS components and the host rocks has been identified in the SRA. Indeed, the EBS properties will evolve with time in response to the thermal, hydraulic, mechanical, radiological, and chemical gradients and interactions between the various constituents of the barriers and the host rock. Therefore, assessing how these properties evolve over long time frames is highly relevant for evaluating the performance of repository systems and for evaluating their safety functions in a safety case. For this purpose, mechanistic numerical models are increasingly being used to make predictive multi-physics assessments at larger time frames (e.g. 10 000 to 100 000 years) and space scales (e.g. hundreds of meters) than the ones covered by laboratory or field experiments. New trends and developments in numerical analysis allow for solving more and more complex problems. Such models provide an excellent way for integrating into a coherent framework a scientific understanding of coupled processes and their consequences on different properties of the materials in the engineered barrier system. Their development and validation are supported by R&D actions within either ongoing HORIZON 2020 European projects or within EURAD R&D work packages supporting its SRA and roadmap. For example, the HORIZON 2020 project BEACON (Bentonite mechanical evolution; https://www.beacon-h2020.eu/) aims to develop, test, and validate numerical models against experimental results to predict the evolution of the hydromechanical properties of bentonite during the saturation process. On the other hand, in relation to chemo-mechanical coupling, WP16 MAGIC (chemo Mechanical AGIng of Cementitious materials; https://www.ejp-eurad.eu/implementation/chemo-mechanical-aging-cementitious-materials-magic) of the EURAD Joint Programming Initiative focuses on multi-scale chemo-mechanical modeling of cementitious materials that evolve under chemical perturbation (including bacterial impact). Integration of chemical processes in models at different scales and of varying complexity (from complex description to their abstraction) is a major issue tackled in the WP2 ACED (Assessment of Chemical Evolution of ILW and HLW Disposal cells; https://www.ejp-eurad.eu/implementation/assessment-chemical-evolution-ilw-and-hlw-disposal-cells-aced) of EURAD. WP4 DONUT (Development and improvement of numerical methods and tools for modeling coupled processes; https://www.ejp-eurad.eu/implementation/development-and-improvement-numerical-methods-and-tools-modelling-coupled-processes) of EURAD aims at developing and improving numerical models and tools to integrate more complexity and coupling between processes. The combined progress of those projects at a European level will definitively improve our understanding of and our capabilities for assessing the long-term evolution of engineered barrier systems and will enhance collaboration between scientific communities.

In this manuscript, first, how the different projects contribute to the EBS thematic is explained. Then the models used to describe some of the most important coupled processes occurring within EBS are discussed in detail, and relevant examples are given.

2 Projects contributed to the scientific basis for EBS evolution and modeling of their evolution

The four R&D projects mentioned above contribute to a better understanding of EBS behavior in radioactive waste disposal. It is worth keeping in mind that they do not have the same level of maturity as they did not start at the same time. BEACON started in June 2017 and has finished in May 2022, while ACED and DONUT were launched in June 2019, and MAGIC only in June 2021.

2.1 Mechanical evolution of bentonite barriers (BEACON)

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

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

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

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

The overall objective of the BEACON project has been to develop, test, and improve models that can predict the mechanical evolution of installed bentonite components. Their application is both to support the handling of the barriers in the safety case and to give feedback on the design and the engineering of the barrier components.

2.2 Development and improvement of numerical methods and tools for modeling coupled processes (DONUT)

Understanding multi-physical Thermo-Hydro-Mechanical-Chemical coupled processes (THMC) occurring in the EBS is a major and permanent issue supporting the optimization of design and safety case abstraction. Numerical simulations are necessary to make predictive multi-physical analyses for time periods and space scales larger than experiments can cover. These numerical simulations require integrating, in a consistent framework, the increasing scientific knowledge acquired for each of the individual components of the EBS. This implies the integration of couplings of different and non-linear processes, covering a wide range of heterogeneous materials with evolving properties in time and space. The development of cutting-edge and efficient numerical methods is thus necessary for the scope of having useful, powerful, and relevant numerical tools for assessments as well as for process understanding. It is also necessary to manage the uncertainties associated with the input data feeding the models, to assess the model responses, and to identify the main parameters and processes driving the behavior of the systems of interest. Managing uncertainties in these complex systems require the improvement and development of innovative, appropriate and efficient numerical methods. According to these needs, a work package called Development and Improvement Of NUmerical methods and Tools for modeling coupled processes (DONUT) has been launched within the EURAD project to develop relevant, performant, and cutting-edge numerical methods that can easily be implemented in existing or new tools, in order to carry out high-performance computing to facilitate the study of highly coupled processes in large systems. These methods and their implementation in tools will be mainly applied to reactive transport, two-phase flow, and THM modeling in porous and fractured media. In addition, numerical scale transition schemes are developed to upscale coupled processes from pore scale to continuum scale in order to support the study of specific multi-scale couplings such as chemo-mechanics. Numerical development is also addressing innovative methods (e.g. surrogate models) to carry out uncertainty and sensitivity analyses. Last but not least, the setup and the achievement of benchmark exercises on representative test cases allow us to evaluate the efficiency of developed methods and tools (robustness, accuracy, time computational).

2.3 Assessment of the chemical evolution at disposal cell scale (ACED)

Within a disposal system for intermediate or high-level radioactive waste (ILW/HLW), a particular subsystem is the waste packages and their immediate surroundings (near field), which is the focus of the EURAD ACED work package. These subsystems consist of engineered materials with sometimes distinct different geochemical properties. Depending on the radioactive waste type and the disposal system, the materials considered in ACED consist of vitrified waste, cemented waste, steel, cementitious barriers, and the host rock (clay or granitic rock). Undoubtedly, interstitial pore water of the different porous materials will mix and induce geochemical alterations within the materials leading to, amongst others, dissolution and precipitation of primary and secondary phases with changes in microstructure and transport parameters. Moreover, nonporous material (e.g., steel) may corrode or dissolve as well. Within the perspective of the lifetime of a repository, simulating the chemical evolution is relevant for assessing the durability of different materials and the speciation of the chemical environment as input for radionuclide fate and transport; therefore, its assessment is one of the key elements for the basis of the evaluation of the long-term performance and safety of a repository.

Assessing the chemical evolution is challenging because of the many orders of magnitude in scale to be considered – both in time because, even if geochemical processes are sometimes very slow, they proceed for ten thousand years and in space, with interactions at μm scale, especially at interfaces, influencing the system behavior at scales of several meters. ACED addresses this by considering three scales – interface, waste packages, and disposal cell scale – via dedicated experimental and modeling studies. The experimental studies combine new approaches for studying steel-concrete and steel-clay interfaces under different conditions and enhanced characterization of long-lasting experiments allowing for time scales spanning from one year to a few decades. These studies form the basis for scientific understanding of processes at interfaces between two materials or interactions between two or more materials. In addition, thermodynamic data, specifically for iron phases, and other variables are collected as input for numerical modeling.

The other pillar is numerical modeling from the interface scale to the disposal cell scale. Modeling in ACED is based on so-called continuum modeling, in which the flow and transport of solutes (and possible gases) by diffusion and advection are coupled with thermodynamic and kinetic models to represent the geochemical state. Such models are typically called coupled reactive transport models [6], and although they have already been available for several decades, their recent capabilities now allow them to handle complex environmental and engineering problems, including radioactive waste disposal [7,8]. Beside the reactive transport codes themselves, and the variety of geochemical processes under different conditions (e.g. ionic strength, temperature,...) they can simulate, thermodynamic databases are also a cornerstone for such simulations. Recent relevant databases are e.g., Thermoddem [9], ThermoChimie [10], and CEMDATA [11], amongst others. Models for some kinetic reactions are well-established (e.g. clay minerals [12]), but the incorporation of kinetic models for some engineered barriers, such as steel and glass, in a reactive transport code remains challenging. However, these are essential for the chemical assessment of the disposal cell scale, and approaches are developed in ACED.

ACED describes the processes at different scales but always uses a continuum model. The basic idea is to perform detailed modeling of relevant processes at one scale and extract information as input to a larger scale in which some processes cannot be described with the same level of detail (mainly due to computational time or because it is not a possibility to include sufficiently small timesteps or spatial discretization at a larger scale). By integrating knowledge and information, ACED simulates the chemical evolution at relevant spatial and temporal scales related to the cell disposal scale. The last step is to abstract these complex models to enable sensitivity and uncertainty analyses of the chemical evolution – a key aspect here is that the abstracted models reproduce the aspects of interest of the chemical evolution in a sufficiently accurate way.

2.4 Chemo-mechanical evolution of concrete barriers (MAGIC)

Concrete, mortars, and grouts are used for structural, containment, and isolation purposes in high-level and low-intermediate-level radioactive waste repositories. For example, cement-based backfill materials are envisaged for a large number of disposal facilities for intermediate-level wastes across Europe and are already used as liners in disposal cells or as part of waste containers in many Member States' existing facilities for low-level waste near-surface disposal facilities. Knowledge and feedback on concrete durability are available through the return of experience from civil engineering. However, a specific approach during the design and construction of a repository in terms of stringent safety requirements is of paramount importance. In addition, further understanding is required to support their use as a backfill material for high-level wastes under geological disposal conditions, particularly to understand their contribution to the overall system performance during late post-closure time frames. This is especially the case for concrete with low-pH cement-based material formulation, where less knowledge is available.

The mechanical behavior of cementitious materials is strongly influenced by the boundary conditions imposed by the geo-technical system and the host rock (i.e., water saturation, temperature, etc.) during both the operational phase and the post-closure transient period. To assess the performance of the cementitious components, studies must be extended-for long time periods (several years), also considering the operating period in unsaturated conditions. Cementitious materials are planned to be used as disposal barriers (i.e., buffer, plugs, and waste matrices) and structural systems, which require further understanding of their long-term behavior, considering the initial mechanical state and including the impacts of microbes on their degradation. Furthermore, over the long term, ground- and pore waters, with aggressive chemical ions, are a key driving factor for cementitious materials' deterioration. The mineralogical and microstructural changes generated by these aggressive environments might have consequences for the mechanical behavior of the cement matrix.

Cement and concrete are heterogeneous materials containing different constituent phases, pores, cracks, and inclusions at various scales. Their macroscopic thermo-hydro-mechanical (THM) behavior is intimately related to its multi-scale structure. Under THM loading and chemical processes, their microstructures are modified such as porosity variation, calcium dissolution, calcite formation, corrosion product expansion, crack initiation and propagation etc. Consequently, the macroscopic behaviors are affected by such microstructural evolutions. It is crucial to develop multi-scale experimental and modeling approaches to establish inherent relations between short- and long-term macroscopic behaviors of cement and concrete and their microstructural evolutions. On the other hand, there is also a strong spatial variability and uncertainty in the microstructure and the macroscopic properties in large-scale concrete structures. Despite significant advances performed during the last decades, the development of an efficient modeling strategy of concrete materials and structures by considering multi-scale microstructures evolution, uncertainty, and variability is still a pending issue.

The MAGIC WP aims to increase confidence in Chemo-Mechanical numerical models by reducing uncertainties in input data and understanding key coupled processes (for both young (not early-age) and aged materials). Specific conditions for waste disposal (microbial activity, chemical and mechanical stress, variable saturation, etc. . .) are taken into account by addressing implementation needs and safety aspects, e.g., regarding the selection of materials, dimensioning, and (long-term) behavior of seals and plugs.

This WP is improving the knowledge of the mechanical transformations of concrete in EBS (from the container to the massive plug in the sealing area) exposed to various disturbances (mechanical, chemical stresses, microbial activity. . .). Several laboratories, mock-ups, and in situ experiments (mainly existing) dedicated to identifying the mechanical behavior of concrete under various stresses are developed/exploited. Furthermore, multi-scale models describing the chemical and microbial impacts on the concrete mechanical properties under real repository conditions are developed.

Particular attention is paid to reinforced concrete. To control crack propagation in civil engineering concrete structures in the short term (during the construction of repository structures and their exploitation phases), steel reinforcement is efficient. The ability of rebars to limit crack openings is well controlled for usual reinforced concrete structures in contact with the atmosphere and the expected service life duration of classical constructions [13]. However, in the context of nuclear waste repositories, the transfer of chemical species into the micro cracks and the localized opened cracks created in the short term could either lead to the healing or the propagation of these cracks, depending on the chemical environment and the mechanical loading. Among the different parameters controlling these phenomena, the two most important ones are the evolution of the concrete matrix mechanical properties and the concrete-rebar bonds (stiffness, strengths, swelling or shrinkage, and creep for both). These aspects are treated experimentally and numerically in the present project to provide homogenized behavior laws for plain and reinforced concrete usable in finite element codes. These codes are then used at the structure scale. The coupling between chemical reactions at the micro-scale, rebars consideration at the meso scale, and loading at the structural scale, enables envisioning a large variety of scenarios by practitioners to examine the safety of these installations during the medium-term (exploitation phase) and the long-term (post sealing phase).

This WP strives for scientific excellence using novel approaches, including microbial effects and nanoscale process understanding under variably-saturated conditions. Moreover, it enhances the quantification and understanding of cement-based material evolution to improve long-term modeling and assessments.

3 Examples of EBS modelling performance and evolution

3.1 Mechanical evolution of bentonite barriers (BEACON)

The scientific part of BEACON was divided into five actions. The first dealt with the application of the results from the project in safety cases and design. The purpose of the second was to collate and share knowledge on the available information about bentonite mechanical evolution. The third handled the development of models. The objective of the fourth was to provide experimental data to support the model development and testing. The core activities of BEACON were, however, performed in the fifth action, where numerical models describing the mechanical evolution of bentonite barriers were tested, verified, validated, and finally applied in relevant assessment cases. The originality of work performed in this work package was to propose test cases in which heterogeneities in the bentonite-based component were initially present or to revisit large-scale experiments to follow heterogeneities evolution and the capacity of the model to predict the final state. The following section will focus on some of the achievements gathered during BEACON.

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

To overcome this issue, modeling activities were carried out either in a test case built on experiments performed within BEACON and included a blind prediction of an experiment or on assessment cases proposed by waste management organizations (WMO) based on specific components taken from actual repository designs.

In detail, calibration/validation of the models was carried out using three sets of laboratory tests. These latter were chosen based on the initial heterogeneity of the materials or the introduction of perturbations during the test to induce some heterogeneities. These tests were complementary and represented relevant situations encountered in a repository when installing an EBS. The dispersion of the numerical results was rather large. This was especially true regarding the calculated stresses. For the final

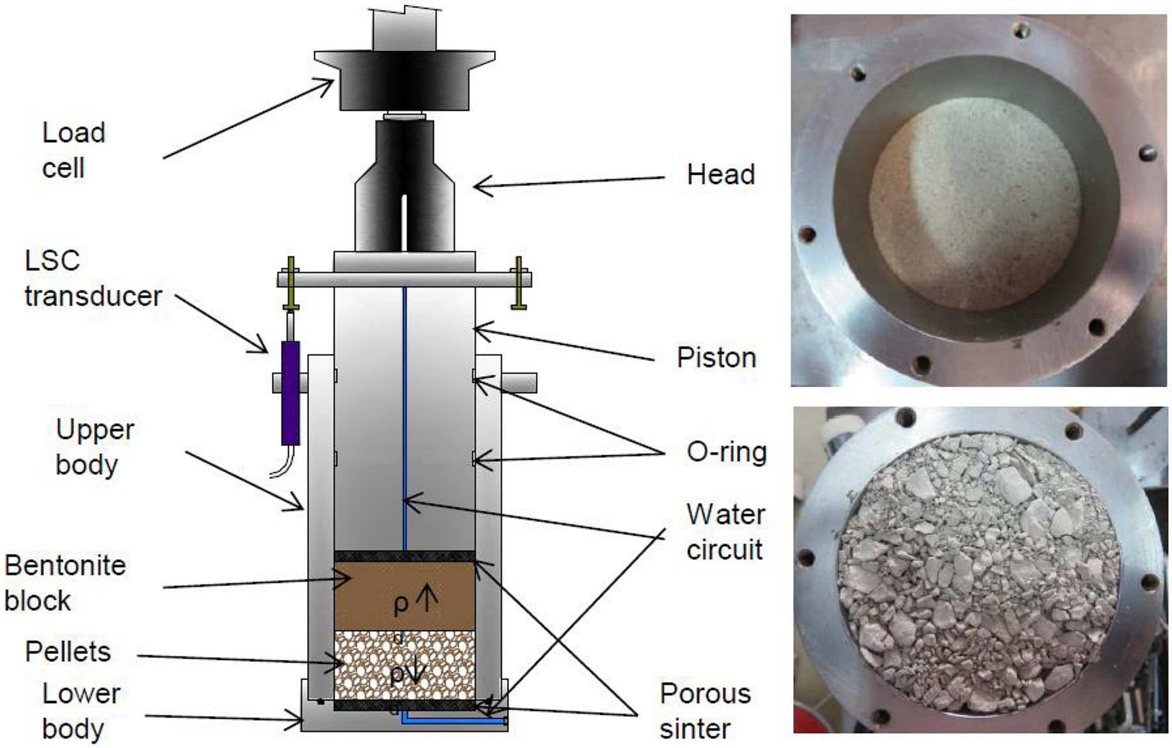


Fig. 1. Schematic representation of the test cell and images of the block (upper right) and pellets (lower right). In the predictive test, the block was placed at the bottom of the cell (Villar et al. [14]).

dry density in the test, the calculated values were in better agreement with the measured values. At this point, many teams were also rather inexperienced with this type of issue.

Regarding large-scale experiments, to show the capacity of the models to reproduce in situ experiments, three experiments were selected:

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

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

One of the main challenges in modeling 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. Tests performed within the BEACON project were simulated to evaluate the ability of the models to predict the hydromechanical evolution of bentonite. Two tests were already finished at the beginning of the project. All the data available on these tests were given to the partners. The purpose was to have a first calibration step. For these tests, the bottom part of the cell was filled with bentonite pellets with an average dry density close to 1.30 g/cm^3 and the top part with a bentonite block with a dry density of 1.60 g/cm^3 (Fig. 1). Hydration with deionized water took place through the bottom. In the first case, constant pressure was imposed, and in the second, a constant flow was imposed. One test was

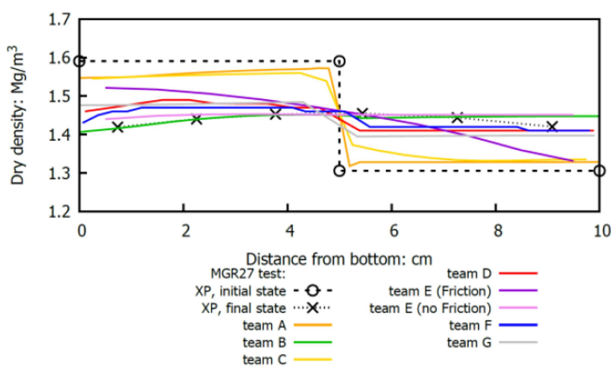


Fig. 2. Dry densities at saturation for the experiment used for predictive modelling.

Table 1. Mechanical constitutive models used in the benchmark.

Team	Model
A	Bishop effective stress; modified CamClay
B	Hysteresis Based Material (HBM) model
C	Double-structure hypoplastic model for expansive clays
D	ACMEG – TS elastoplastic model
E	Internal Limit Model (ILM)
F	Modified Barcelona Basic Model (BBM) elastoplastic model
G	Elastic with modulus depending on water saturation
H	Modified BBM with double structure ICDSM
I	Modified Barcelona Expensive Model BExM

selected for predictive modeling. The results of this test were not given to the participants. The conditions of the test were similar to the first test, except that the pellets layer was located in the upper part of the cell and the block in the lower part. Predictive simulations of water intake, dry densities, gravimetric water content, and stresses were expected on this test case. The results from the predictions of dry densities as well as the experimental results, can be found in Figure 2.

The water intake with time was well modeled by most teams. However, one may observe a number of variations or divergences. Moreover, prediction is less easy for early times of hydration. These globally good results may be surprising considering the large range of permeability used in the simulations by the different teams. As seen in Figure 2, the final (at saturated state) dry densities are well reproduced by many of the models. They do not depend significantly on the mechanical models (including law and friction aspects). It was very difficult to predict the stress's final value and time evolution. Stress evolution showed much variation between teams. Comparing mechanical behavior is not an easy task. Each team has a different conceptual model, and few parameters are comparable. A short synthesis of the mechanical constitutive models used by the different teams is presented in Table 1.

Two teams modeled friction at the cell wall–bentonite interface. These teams managed to satisfactorily blind-predicted the evolution of axial stress in the test.

Direct application to real assessment cases in actual repository systems has also been tackled. 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, and (3) the KBS-3 deposition tunnel backfill (SKB, POSIVA). These are representative of the primary areas of uncertainty in density homogeneity. Here, the teams divided the cases, and only 3−4 teams modeled a particular case. The results from the modeling showed a rather strong divergence in results for the final dry density distribution for all three cases. For the Andra and SKB cases, the calculated values were still within the range acceptable for repository performance, but that was less true for the Nagra case. This shows that there are challenges to moving from modeling laboratory and field experiments, where results are available, to simulations of repository performance.

3.2 Development and improvement of numerical methods and tools for modeling coupled processes (DONUT)

In addition to the specific R&D work that will be conducted, a specific outcome of DONUT is the definition of a well-described benchmark problem that can be used to validate the newly developed simulator capability. While international benchmarks initiatives exist [15–17], the goal here is to define benchmarks of methods and tools to quantify efficiency and added value in terms of:

- increase of knowledge (e.g., better physical representation, integration of couple processes).
- Accuracy, robustness, computational cost.
- Robustness of scale-transition approaches.
- Ability to manage uncertainty and sensitivity analyses.

Recently, Bildstein et al. [17], in a guest editorial to the subsurface environmental simulation benchmarks special issue, mentioned emerging benchmarking opportunities. Amongst others, machine learning was identified. Indeed, it is considered a recent disruptive technology in the field of reactive transport and will possibly unlock the next generation of simulation that requires highly demanding CPU time [18,19]. The high computing cost associated with chemical equilibrium calculations is typically the most demanding one in comparison to fluid flow or heat transfer. To circumvent this issue, the use of surrogate models is promising, with first implementations providing an impressive speed-up between one and four orders of magnitude without loss in accuracy [20–22]. The observed speed-up depends on the chemical system, simulation code, application, and problem formulation [20–22]. These developments have been possible due to technological and scientific advancements both in terms of the available increasing computing power and the recent breakthrough of machine learning algorithms and relevant open-source software. Therefore, the need for a benchmark that tackles these emerging technologies is timely and will serve as the basis for future developments in the field. Within this context, DONUT defines a benchmark related to machine learning and geochemistry. It aims at mainstreaming and catalyzing the use of machine learning in reactive transport by providing a point of reference for testing and addressing the challenges relevant to (i) producing high-quality training datasets, which will be possible to be used by all available machine learning techniques, (ii) implementing several machine learning algorithms to learn from the generated data such as deep neural network learning, Polynomial Chaos Expansion and Gaussian processes, among others, (iii) testing the accuracy of predictions for geochemical calculations, reactive transport, and uncertainty analysis. Joint efforts across EURAD have resulted in the definition of two nuclear waste management relevant benchmark cases. The first focuses on uranium sorption in claystone, and the second is relevant to the temporal evolution of cementitious systems. While the first one is more related to the long-term/far-field radionuclide migration, the second one tackles the behavior of cementitious materials, which is one of the major construction materials commonly found across all EBS concepts. The test cases are designed with increasing complexity in terms of system dimensions in order to identify the limitations of these techniques relevant to the computational cost of training, efficiency, and accuracy during runtime. The uranium sorption case considers surface complexations. The cementitious system includes the precipitation of CSH-phases and the formation of solid solutions. Both cases will consider the presence of CO_2.

The thermodynamic modeling is done using the major geochemical solvers, which are currently used across EURAD (PHREEQC, GEMS, ORCHESTRA), and an excellent agreement between the solvers is observed. The use of open-source software is pursued across the benchmark, and the dissemination of training datasets and the release of the jointly developed algorithms for generating the training datasets and testing the accuracy is foreseen.

3.3 Assessment of the chemical evolution at disposal cell scale (ACED)

One of the central elements in ACED is modeling the chemical evolution at the disposal cell scale. This aspect is presented here as an example of the modeling studies in ACED. Although each country program in Europe has its own particularities, some common features in their designs can be identified [23]. Figure 3 shows the four generic disposal cells representing some of the main features of disposal cells throughout Europe. For a high-level waste representative disposal cell, there is a 30 cm Portland-based concrete or a 75 cm bentonite buffer between the vitrified waste (borosilicate glass type) surrounded by a 5-cm thick carbon steel canister and the clay or granitic host rock. The intermediate disposal cell consists mainly of different types of cementitious materials ranging from high-quality functional concrete for waste container walls to backfill mortar. Waste containers are filled with cemented organic waste or bulk steel waste backfilled with mortar. A disturbed excavation zone is considered in the clay host, whereas the granitic host rock has fracturated.

Depending on the disposal cell, some of the following geochemical processes are included: (i) aqueous complexation, (ii) redox reactions, (iii) cation exchange, (iv) surface complexation, (v) mineral dissolution and precipitation (kinetic/equilibrium), (v) solid solutions, (vi) kinetic corrosion of the steel components with the formation of corrosion products and interaction with cement or bentonite, and (vii) kinetic glass dissolution models. In the case of the high-level waste, 2 periods were considered: (i) transient thermal and/or hydric stage assuming an intact canister, (ii) period after canister failure with glass dissolution and interaction with corrosion products.

Simulations were performed with advanced state-of-the-art coupled reactive transport codes such as CORE^{2D}V5 [24], iCP [25], HYTEC [26], and the latest version of OpenGeoSys [27].

Because of symmetry reasons, the high-level waste disposal cells are simulated in a 1D-radial geometry (Fig. 4, top left). For the transient stage (Period II) and the period after canister failure (Period III), a base case simulation and sensitivity cases are performed. Figure 4 shows some selected results. Model results for the HLW disposal cell in granite (Fig. 4, top right) show that after 25 000 years before the canister breached, magnetite, siderite, and greenalite precipitated in the bentonite near the canister. Small amounts of siderite and greenalite precipitate 0.1 and 3 dm in the bentonite at 25 000 years. The calculated concentrations of exchanged and sorbed Fe^{2+} in the bentonite increase near the canister interface. After the canister breaching, H_4SiO_4 diffuses from the glass into the bentonite, causing the precipitation of greenalite. Magnetite redissolves, and greenalite and siderite precipitate. The pH values are 8.2 in the glass, 8.8 in the canister, and 8 in the bentonite. Figure 4 (bottom left, HLW disposal cell in clay) shows the evolution of minerals and pH in the grout cell next to the canister in case of a transient temperature evolution (purple line) for a sensitivity case considering a thin young cement (5 cm). Temperature influences the effective diffusion coefficient and the solubility of the minerals. In this specific case, complete portlandite dissolution occurs faster compared to a case with a constant temperature at 25°C (100 y compared to 300 y). The modeling of the full system (Fig. 4, bottom right) showed that the driving force is the chemical destabilization of the concrete buffer by the clay rock. This perturbation (decalcification, sulphate attack, carbonation) slowly propagates by diffusion towards the steel overpack with a pH decrease. Overpack water tightness is set as long as the pH is larger than 10.5, then steel corrosion increases significantly, forming magnetite and Fe(II)-silicates. The precipitation of the latter seems to sustain glass dissolution as long as the remaining steel still corrodes.

A two-dimensional model was selected for the intermediate waste simulations in clay rock, although axis symmetry was also applied Figure 5 (top left) to save computational time. Geochemical interactions in a fully saturated system are simulated for 10^5 y. The model does not consider the waste inside the package but only the walls of the container. However, the geochemical evolution

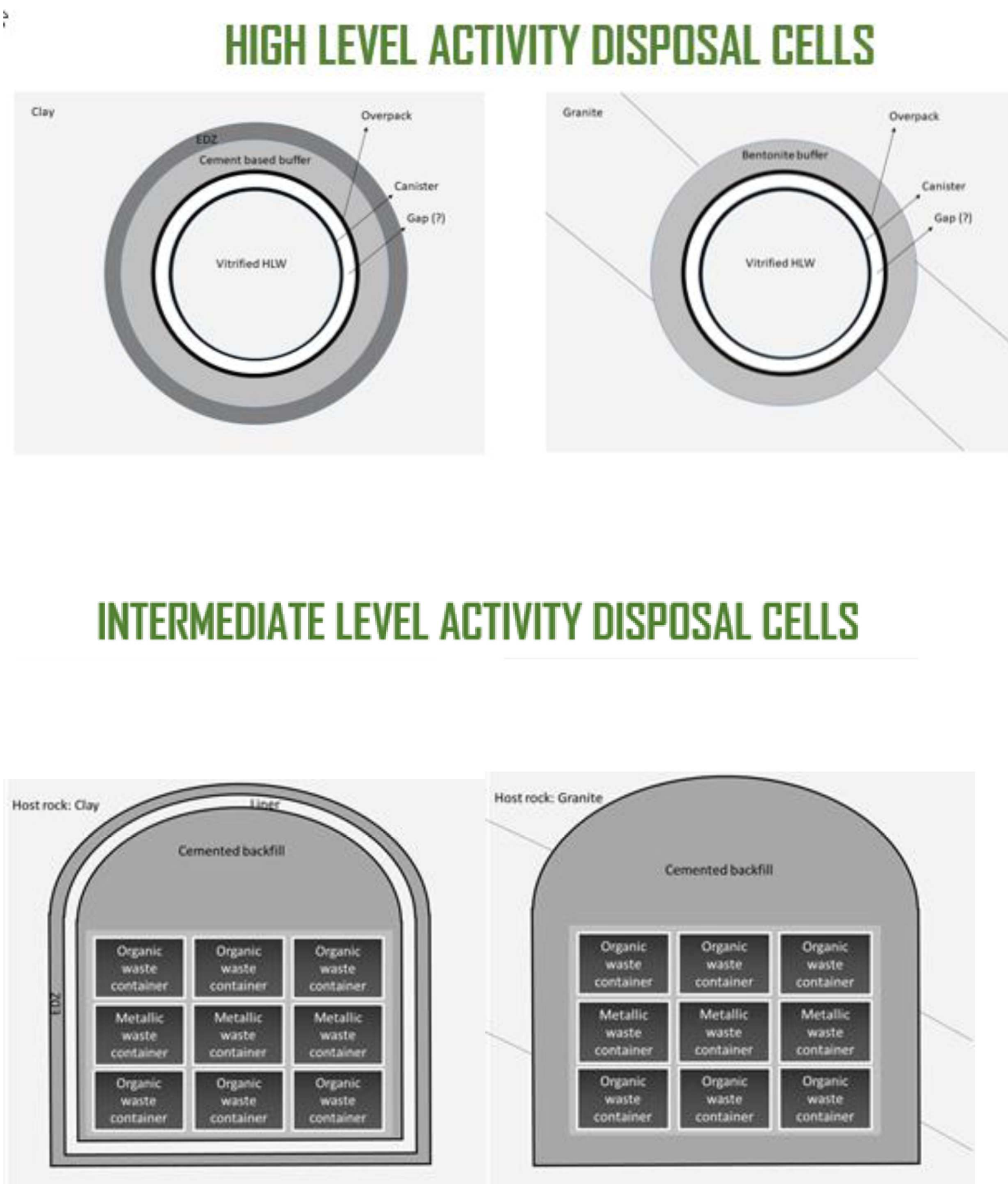


Fig. 3. Schematic representations of the four generic disposal cells considered in ACED for high level radioactive waste (top) and intermediate radioactive waste (bottom) in clay (left) and granite (right) rocks.

and gas generation of one organic waste drum inside the container was simulated by Huang et al. [28] for 150 years and open to the atmosphere – this information from the waste package scale will be incorporated at the disposal cell scale at a later stage. Figure 5 (top–right) shows the spatial distribution of portlandite after 10^5 y. Due to the geometry of the disposal cell, a space-dependent dissolution pattern of portlandite is observed, with significant amounts of portlandite remaining at the concrete walls. On the other hand, precipitation of the calcite at the host rock at the interface occurs more uniformly (Fig. 5); bottom, one observes darker red zones around the disposal cell with increasing interaction time). Also, other geochemical variables (pH, pore water composition), as well as microstructure (porosity), and corresponding transport properties, evolve in a complex space-time manner [29].

In the case of the intermediate waste simulations in crystalline rock, the 1D model considering water inflow to the disposal cell from the left side is assumed at the present moment (Fig. 6) in analogy to the work performed by Idiart et al. [30] which will be extended to a 2D model.

The models illustrated above are cost computing demanding. Therefore, model abstraction will help reduce these complex models to their essential components and processes while preserving the validity of the model for the specific purpose [31]. The following two broad families of abstracted models are envisaged: (i) construction of lower-fidelity numerical models by using (a) a predefined

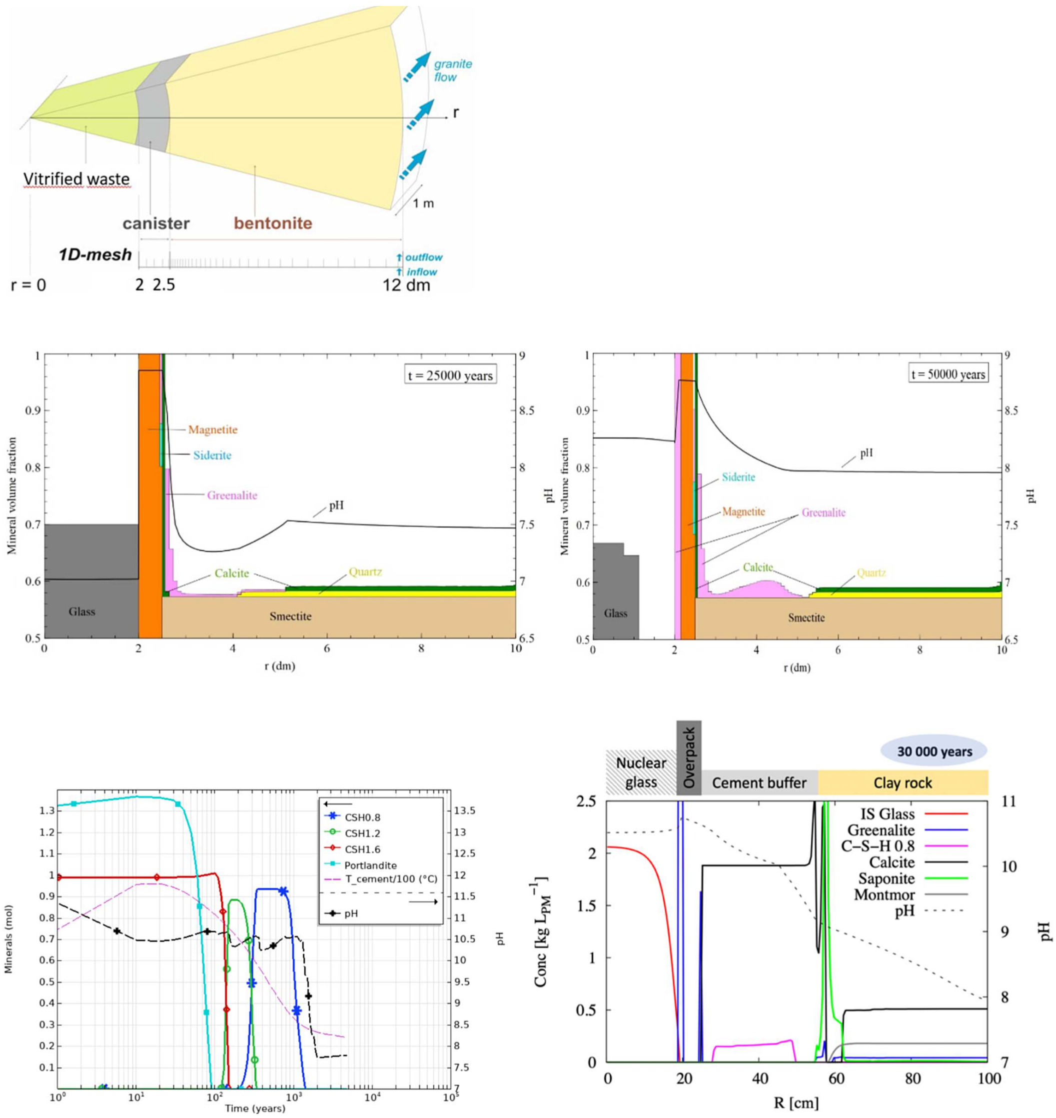


Fig. 4. (Top) 1D radial geometry of the HLW disposal cell in granite, (middle) CORE 2D modelling of the geochemical evolution in a HLW disposal cell in granite, (bottom left) HLW disposal cell in clay: transient stage with variable temperature in cement (first cell next to liner), (bottom right) HLW disposal cell in clay: HYTEC modelling of the evolution of the mineralogy of the full disposal cell components after 30 000 years of interaction.

hierarchy of models, (b) delimiting the input domain, (c) scale change by upscaling or aggregation, or (d) reducing numerical accuracy, and (ii) using response surface surrogates of (a) input-output relations of the whole model, (b) the geochemical calculations, or (c) process models.

3.4 Chemo-mechanical evolution of concrete barriers (MAGIC)

As MAGIC started recently and results are not available yet, we describe here the strategy in model development in view of the WP objectives. Modeling activities within MAGIC consider all relevant scales from the nano (cement paste) to the safety structure scale (i.e., reinforced concrete). Keeping in mind that the general objective of the modeling activities is to obtain long-term chemo-mechanical models for Portland and low-pH concrete-based material degradation exposed to relevant deep disposal environments.

Concrete degradation, in the time frame of deep disposal, embraces the conjunction of multi-scale coupled processes, occurring from the excavation and construction of the repository until the disposal of the waste for 1 million years (see Fig. 7). Many coupled processes occurring during concrete degradation are inherently multi-scale due to dynamic localization effects (i.e., deformation, reactions, or micro-cracking), which require special constitutive models and numerical methods. Individual processes are often best described on different scales depending on their phenomenology and the scales of their experimental characterization. Consequently, different processes,

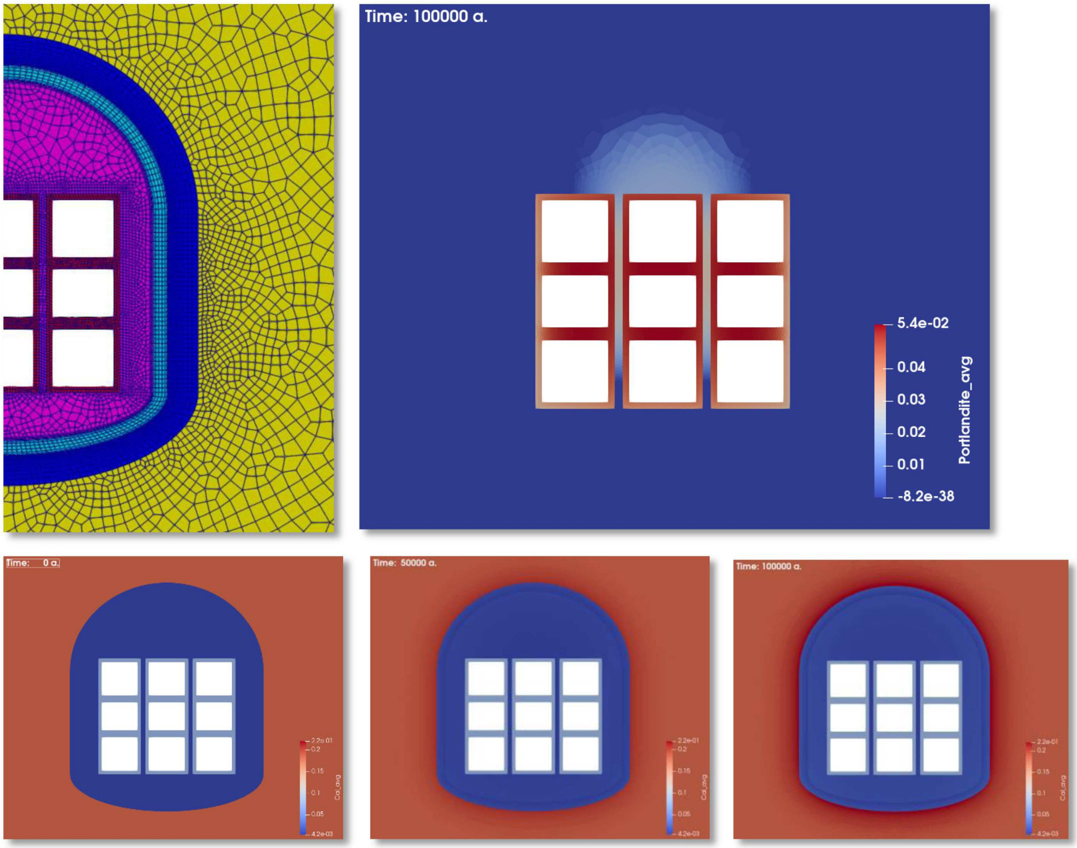


Fig. 5. (Top left) Two-dimensional axis-symmetric simulation domain intermediate level waste in clay. Dark blue area is the excavation damaged zone, yellow is the clay host rock, other colors different types of cementitious materials, the height of the disposal cell is about 13 m. (Top right) Portlandite distribution after 100 000 y. (Bottom) Evolution (50 000 yr, and 100 000 y) of calcite precipitation in the host rock.

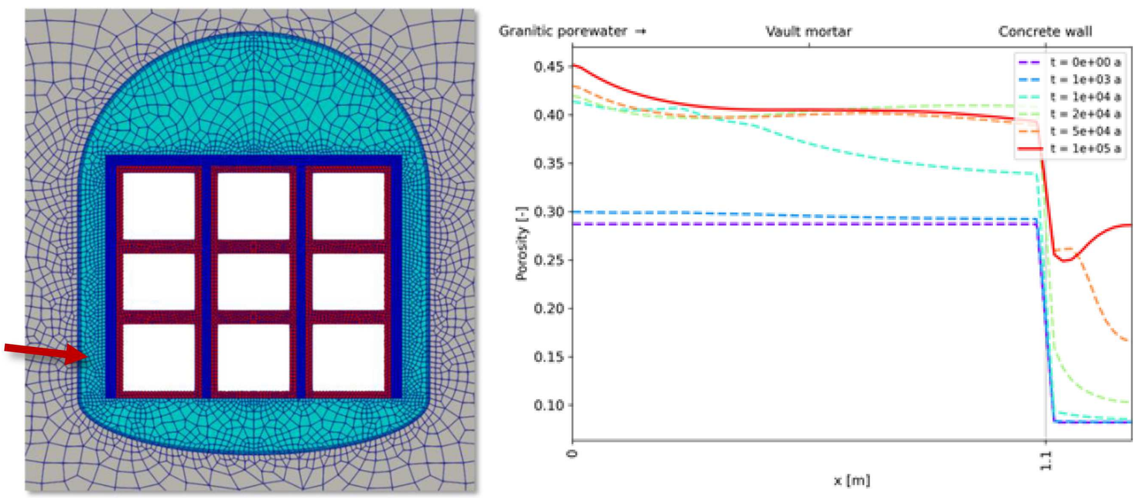
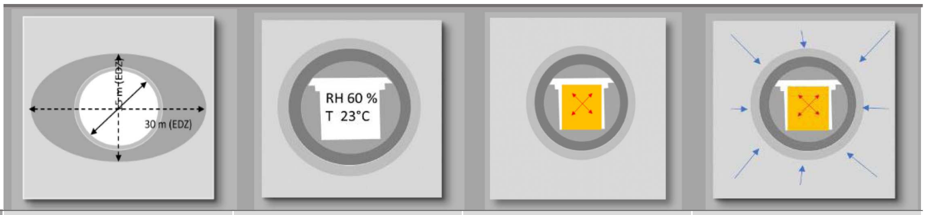


Fig. 6. (Left) Disposal cell representation and indication of the water flow (Darcy velocity $(q) = 1.03 \times 10^{-11}$ m/s) direction (red arrow). (Right) Porosity changes as a function of disposal time in the different cemented barriers.

software, and scientific communities have evolved in different directions (i.e., reactive transport and T-H-M modeling). As a result, chemo-mechanical coupling in concrete degradation studies is often neglected despite its importance, not for scientific reasons but due to a lack of technical capabilities and interaction/collaboration between experts in the relevant distinct fields.



Loading	Construction	Operating phase	Waste disposal	Post-closure
Thermal (T)	Initial conditions and properties of the damaged zone (EDZ) of the rock	Ventilation	Waste heat	T. stabilization
Hydraulic (H)		Humidity effects	Unsaturated media	Saturated media
Mechanical (M)		Rock convergence	Rock convergence	Rock convergence
Chemical (C)		Atmospheric carbonation	Porewater Interaction	Porewater Interaction

Fig. 7. Scenario of T-H-M-C loading in repository systems.

Within MAGIC, a multidisciplinary team of material scientists, chemists, and engineers is developing the coupling of different reactive transport and mechanical codes (finite element codes). For example, this is the case of chemo-mechanical coupling expansion between the HYTEC reactive transport code [32] and the Finite Element code CASTEM [33] or OpenGeoSys [34]. This later development is also connected to the EURAD DONUT WP. An interface for transferring material parameters from pore scale Lattice Boltzmann simulations into the T-H-M-codes is also under development [22,35]. Regarding the upscaling methods from nano to the representative elementary volume, Reduced Order Models (ROM) and an analytical multi-scale model framework for the aggregate-scale HMC models is being built. The integration between the micro- and large-scale processes and the multi-scale algorithm is being tested against available experimental data at the laboratory scale.

Interdisciplinarity between chemistry, physics, and mechanics can be illustrated on one of the structures that receive the greatest mechanical loading and chemical degradation to know the vault/liner of the low and intermediate-level waste emplacement gallery. Indeed, the liner is exposed to (i) the mechanical loading induced by the surrounding rock, (ii) concrete aging during the long term of disposal, and (iii) chemical disturbance due to the contact with the rock. All these processes increase the risk of fracturing, affecting the integrity of this disposal component [36]. Previous structural chemo-mechanical models decoupled the macroscopic modeling from the mesoscopic phenomena [37]; however, in order to compare concrete made of the different matrices, a non-linear analytical homogenization model for the chemical-mechanical behavior of concrete will be implemented. This model is able to manage the cement paste versus the chemical state of the concrete and will be reflected in the mechanical properties (Young's modulus, compressive and tensile strength, creep rate of concrete, and anchorage of steels). Furthermore, during the chemical damage processes (leaching, carbonation, or chloride ingress in the hydrated cement paste), the model also considers the amount and nature of aggregates on the macroscopic residual mechanical properties. In the case of reinforced concrete, which is the material considered in this structural component, until now, the phenomenon of reinforcement corrosion was decoupled from the chemical state of the concrete [38]; hence the lock to be lifted in this chemo-mechanical model consists in predicting the steel corrosion progress as a function of the concrete chemical state at the interface and in localized cracks; and deducing its effect in term of steel anchorage and their contribution on reinforced concrete mechanical performances [39].

The model implementation is done in a Thermo-Hydro-Chemo-Mechanical finite element code, able to compute the evolution of a tunnel over several thousand years [40]. Once implemented, it shall allow a more accurate prediction of the lifetime of radioactive waste disposal structures, but also the simulation of their very long-term behavior under mechanical loading (induced by rock convergence) and physicochemical degradation caused by porewater (carbonation, leaching, corrosion of the reinforcement bars...). Different cement binders (low pH or ordinary Portland cement based) are under consideration to perform comparative studies of envisioned solutions.

4 From individual contribution to complementary added value

While every project by itself will bring novelty and scientific excellence by answering the research questions defined in the project and will integrate knowledge from different scientific communities, they complement each other with the final goal of having a holistic understanding and description of the evolution and performance of the EBS leading to a scientific basis for integrated multiphysic-multiscale modeling of that system, bringing an even bigger added value.

The added value of each individual project should, of course, not be neglected. For example, the BEACON project has made a significant contribution by improving knowledge of bentonite behavior and the simulation of bentonite-based components for the radioactive waste underground repository. While a big part of the project was devoted to modeling and model development, implementing experimental tests using novel techniques such as imaging provided important data to calibrate and feed the models, especially to describe the coupling between micro and macro scales. The modeling teams participating in BEACON have significantly improved the capabilities of their models through the test cases proposed and simulated along the project. As a result of these developments and improvements, 10 teams are now equipped with coupled THM models that reasonably represent the behavior of bentonite-based components in the context of an underground radioactive waste repository. Thanks to this, they were able to model test cases representative of the engineered barrier and sealing concepts proposed by SKB, Nagra, and Andra in the final modeling stage. Teams are generally able to reproduce and predict the mechanical evolution of bentonite in small-scale and large in-situ experiments, particularly the final swelling pressures, dry densities, and degrees of saturation of the bentonite. These are key safety indicators for bentonite used as a buffer or seal in geological disposal facilities for radioactive waste. The progress made throughout the project is illustrated by the improved agreement between models and experiments. This is a consequence of model updates with the inclusion of friction, improved formulations of water retention curves, inclusion of thermal effects, and the development of numerical solvers.

For ACED, DONUT, and MAGIC, it is too early to have a similarly comprehensive and outstanding review of the conducted work. Scientific publications (e.g. [28,41–43]) in a wide scope of journals already exist or are foreseen. Reports generated in these work packages and related scientific publications demonstrate for DONUT a better representation of multi-physical, multi-scale processes of radioactive waste disposal, for ACED a better representation of chemical interaction inside the EBS, for MAGIC integration of multi-scale phenomena in long-term chemo-mechanical models, and all cross-fertilization.

Beyond a better capability to integrate complex interacting processes in a relevant model to decipher the behavior of EBS on a long-term perspective and gain confidence in model abstraction and simplification made either for performance assessment or safety case calculation (see Sect. 5), all four projects actively contribute to knowledge management. Indeed, at the beginning of each project, the state-of-the-art has been gathered and published either as a report for ACED [44], MAGIC, and DONUT [45] or for BEACON as a database integrating a description of experimental tests and the relevant information on the THM models used to represent the behavior of bentonites. As mentioned in the introduction, the different projects respond to a strategic research agenda that meet the priorities of research entities, TSOs, and WMOs. Updated state-of-the-art reports resulting from the research, activities, and joint work in these projects form an important input to adjust the future strategic research agenda. Moreover, documented and archived project data (including computer models) and results are crucial for knowledge transfer across generations and to early-stage national programs.

5 Model abstraction and simplification

As detailed by Govaerts et al. [31], performance and safety assessment and supporting models often need to be relatively simple and/or fast to allow computations for large scales and extremely long time scales or to execute it many times with different parameters for sensitivity and uncertainty analysis. Within the above-described projects or work packages, complex (in terms of couplings, concepts, geometries, etc.) and computationally intensive models were developed. To be operational, in the context of a performance and safety assessment, it implies model abstraction as to said, a methodology for reducing the complexity or the computational burden of a simulation model while maintaining the validity of the simulation results with respect to the question that the simulation is being used to address [46].

Within EURAD, a comprehensive review has been carried out for model abstraction [31]. Even though it was oriented towards reactive transport, the principles and guidelines given in the review can be applied to all the models developed in the above-mentioned projects. Firstly, the need for model abstraction should be justified in terms of the saved computational cost. Secondly, the context of the modeling problem has to be reviewed to ensure the objectiveness and comprehensiveness of the model abstraction. Thirdly, model abstraction techniques (e.g. surrogate models) have to be selected to simplify the model. Fourthly, it is necessary to carry out verification calculations to ensure the abstracted model performs sufficiently accurately. Fifthly, the justification, abstraction process, and verification have to be reported in a traceable and transparent way. And last but not least, the benefits of abstraction have to be reaped, for example, in a local or global sensitivity analysis.

6 Conclusion

Three work packages (ACED, DONUT and MAGIC) of the EURAD joint programming initiative and an H2020 project named BEACON contribute to improving understanding of and capabilities for assessing the long-term evolution of engineered barrier systems. And last but not least, they support knowledge management and encourage collaboration between scientific communities.

Conflict of interests

The authors declare that they have no competing interests to report.

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Data availability statement

This article has no associated data generated.

Author contribution statement

F. Claret, A. Dauzères, D. Jacques, and P. Sellin discussed and designed the architecture of the papers, checked the consistency of the manuscript, and wrote the paper. B. Cochepin, L. De Windt, J. Garibay-Rodriguez, A. Mon Lopez, L. Montenegro, V. Montoya, J. Samper contributed to the writing of the part dealing with the ACED WP, N. Prasianakis contributed to the writing of the part dealing with the DONUT WP, V. Montoya contributed to the writing of the MAGIC WP and O. Leupin and J. Talendier contributed to the writing of the BEACON project. J. Govaerts wrote the part dealing with model abstraction.

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