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ABSTRACTS

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For

PRESENTATIONS

HM and THM Interactions in Bentonite Engineered Barriers

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Abstract

The contribution summarizes Task D of the DECOVAEX 2019 project that addresses the hydromechanical (HM) and thermo-hydro-mechanical (THM) interactions in bentonite engineered barriers. The Task is based on the modelling by different teams of two large scale in-situ experiments: the EB test performed at the Mont Terri URL (Figure 1) and the FEBEX test carried out at the Grimsel Test Site (Figure 2).

The engineered barriers for the two tests use the same material: FEBEX bentonite whose THM behaviour that has been comprehensively characterized. The barrier in the FEBEX tests was composed of compacted bentonite blocks whereas the barrier of the EB test was largely made up of bentonite pellets except for a pedestal of bentonite blocks on which a dummy canister rests. Both experiments have been operational for very long periods: 10.5 years for the EB test and 18 years for the FEBEX test. The EB test has been performed under isothermal conditions whereas the FEBEX tests incorporates two heaters that maintain a constant maximum temperature of 100ºC of the bentonite. The FEBEX bentonite barrier was hydrated naturally form the host rock (granite) while artificial hydration was used in the EB test. Both barriers were largely saturated at the end of the experiments. It is apparent, therefore, that the two tests, while sharing the same material, they provide a wide range of conditions making the modelling exercise more valuable.

The two tests have been carefully dismantled providing direct information on the state of the barrier at the end of experiments. The FEBEX test has undergone two episodes of dismantling thus providing data on the state of the barrier at two different stages of its evolution. The dismantling data together with the observations gathered from the different sensors during the performance of the tests provide an extensive database to assess current modelling capabilities. The contribution discusses the modelling results of the two tests highlighting present capabilities and current shortcomings. Special attention is paid to two aspects: i) the final degree of homogenization of the barrier when reaching saturation and ii) the evolution of the state of the barrier, in terms of dry density and degree of saturation, during the transient stage.

Figure 1: The EB test

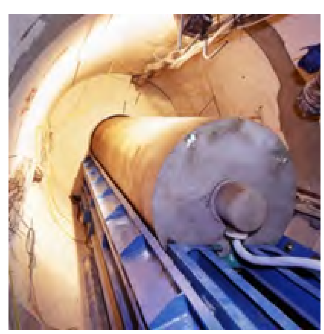

Figure 2: The FEBEX test

Homogenisation in Bentonite: Lessons Learned from Laboratory Testing

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Design concepts for the geological disposal of radioactive waste frequently incorporate an engineered barrier material, which is commonly chosen to be bentonite. Understanding the long-term behaviour and performance of bentonite is therefore critical for establishing the safety case to enable its use in a repository setting. As bentonite expands into the engineering voids in the repository, the non-uniform development of swelling pressure may result in material heterogeneity in terms of density, permeability and mechanical property variations, which could adversely affect the performance of the bentonite as a mechanical and flow barrier. To address this knowledge gap, the BGS have performed a series of laboratory experiments examining the swelling capacity of pre-compacted bentonite as a function of sample size, orientation and clay-composition.

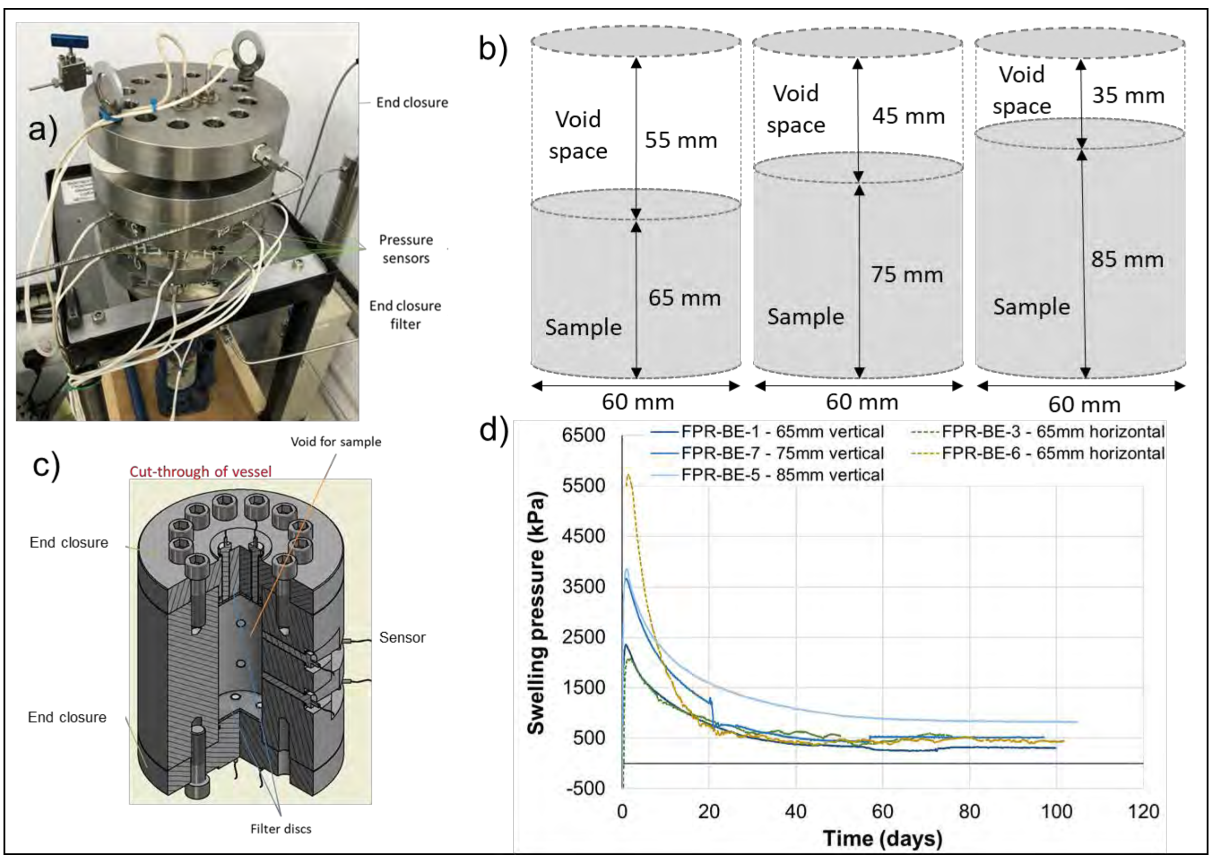

Figure 1: a) The custom-built experimental apparatus showing the arrangement of pressure sensors. b) Schematic of the starting sample dimensions and void space. c) Cut-through schematic of the testing vessel design. d) Swelling pressure versus time for each of the experiments.

In each test, a pre-compacted sample of bentonite with a specified length (ranging from 65 to 85mm) was sited in the base of a custom-built 316-stainless steel, constant volume testing vessel with two end closures (and internal length 120 mm) and the remaining void was filled with deionised water (Figure 1). High precision Teledyne ISCO D-Series 260D syringe pumps connected to the apparatus at each end of the sample were used to apply a uniform pore-pressure of 4.5MPa to the sample. The sample was left to hydrate and swell into the cavity initially occupied by deionised water and the swelling stress and pore-pressure were continuously logged using FieldPoint^{TM} and cRIO logging hardware and a bespoke software programme written in LabView^{TM}. The data from 5 experiments shows that bentonite under zero hydraulic gradient is able to swell and completely fill an engineering void with dimensions nearly as large as the start volume of the sample. However, the development of the full swelling pressure in each sample was spatially complex and time-consuming. Even after 100 days of testing, significant spatial variance in the measured swelling pressures across all sensors still existed (Figure 1d). At the end of each test, a small but measurable swelling pressure was observed at the top of the void above the clay and the analysis of flow into and out of the vessel below and above the clay indicated differential swelling. Large differences in the measured moisture contents and the estimated dry density along the length of the post-test samples support this (Figure 2); the smallest post-test moisture contents were measured in the sample end furthest away from the original void space (Figure 2b). The post-test samples from the tests performed in the horizontal orientation also show evidence of gravity segregation. Although persistent differential stresses were observed in all tests, the longevity of these features remains unclear based on the length of these experiments. To address this issue, longer-term experiments are required.

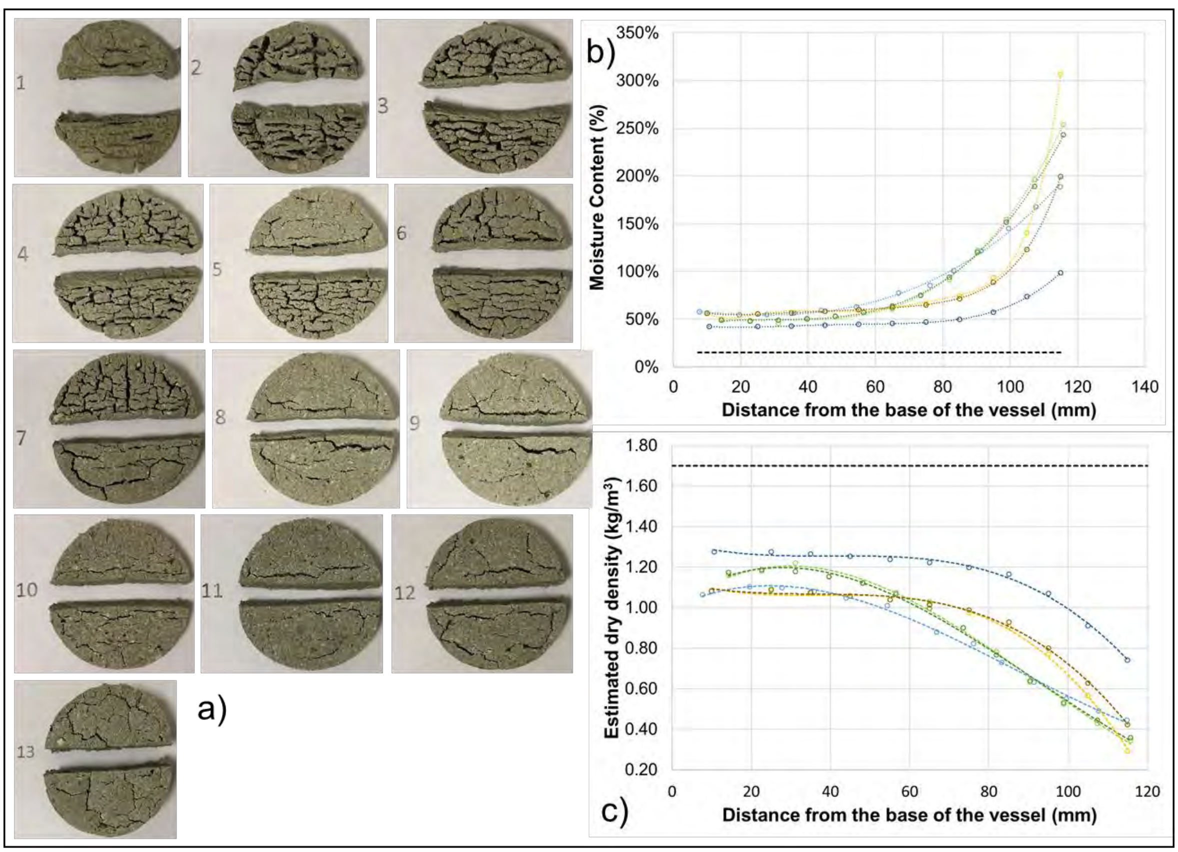

Figure 2: a) Images of each post-test slice along the length of the FPR-BE-3 test sample; b and c) the measured moisture contents and estimated bulk densities of each sample along its length at the end of the test.

Hydro-Mechanical Behaviour of a Bentonite Pellet/Powder Mixture. Experimental and Modelling Results.

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Abstract

Most European concepts for deep geological disposal of high and intermediate level-long lived radioactive waste involve bentonite-based materials as buffers, backfills and seals of disposal galleries and access shafts/ramps to ensure isolation and containment of the waste from the biosphere. Swelling pressures of buffers, backfills and seals are requirements for these components to achieve their safety. It is well documented that the swelling pressure depends principally on the dry density of material. Accordingly, a relatively small change in density can induce significant changes in swelling pressure. That is why most of laboratory and large scale tests have focused on achieving the required average dry density. However, very few experiments have focused on the dry density heterogeneities at initial state and in the course of hydration and their influence on swelling pressure. For long-term safety assessment of the repository, it is essential to predict the evolution and the final state of the initially heterogeneous seal and to evaluate the effects of remaining density gradients and swelling pressure differences on its long term performance. To this end, an appropriate constitutive Hydro-Mechanical (HM) model that accounts for spatial and temporal distributions of the relevant properties of the bentonite pellet/powder is fundamental.

In this paper, the hydro-mechanical behavior of a pellet/powder MX80 bentonite mixtures were investigated by means of Microfocus X-ray Computed Tomography (μ-CT) observations and laboratory small scale infiltration tests. This material, consisting of a mixture of low-density bentonite powder and highly compacted bentonite pellets, is obviously highly heterogeneous in its initial state. The degree and distribution of heterogeneities will vary during hydration and the average dry density might be not sufficient to characterize its final state and containment performance. A HM model which takes into account the initial heterogeneous distribution and transient microstructural features characterizing the high density bentonite pellets (damage upon wetting) is developed. The formulation is applied to the modelling of the small scale infiltration tests. The model allows the anisotropic swelling behaviour of the mixture to be satisfactorily reproduced when accounting for the spatial variation of the material initial porosity. Detailed analysis of the modelling results demonstrates the existence of dry density gradients at long term and their influence on swelling pressure anisotropy.

Modeling of THM Processes in Bentonite Sealing Barriers

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Abstract

The contribution summarizes experience with the analysis of thermo-hydro-mechanical (THM) processes in engineered barriers based on bentonite material. A model is described, which couples flow in an unsaturated barrier driven by the Richards equation with isothermal or non-isothermal vapour flow, mechanical deformation described by nonlinear elasticity with moduli dependent on the deformation state and saturation, swelling and heat transfer.

The described and implemented THM model includes a lot of couplings of the individual processes: saturated permeability depends on deformation, retention function, as the relation between the suction and either effective saturation or mass water contents, is enriched by dependency on the deformation and in the non-isothermal case also on the temperature change. The formula for swelling stress is a linear function of saturation determined by maximal swelling stress depending on dry density. The thermal expansion coefficient of all materials is included. Heat conduction coefficient is a function of saturation. The coupling of the processes is mainly due to mutual influences in the model parameters as mentioned above, the Biot coupling terms (effective stress and shrinking or opening of the pore space) do not play the main role. Moreover, the implemented model works with a specific phenomenon, - bentonite can store more water inside its volume than is indicated by its pore space.

The present model is validated against laboratory experiments and mainly against long term in-situ experiments. Within the Decovalex project, such validation was done with SEALEX, EB and FEBEX experiments. Both 2D and 3D simulations were done with the (T)HM model implemented with the aid of the COMSOL Multiphysics software. Each application requires to incorporate specific features as parameters for bentonite blocks or pellets, bentonite/sand mixture, modelling of technological gaps between host rock and bentonite barrier, inner-blocks gaps modelled as lower dimensional objects etc. The modelling clarified sensitivity to various parameters and terms including in the model description.

Modelling of Reactive Transport in Bentonite Considering Chemomechanical Coupling

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Abstract

Bentonite is the key component in the engineered buffer system of many radioactive waste repository concepts. Two of the crucial properties for the performance of bentonite, swelling pressure and porosity distribution, vary with the chemical environment. Therefore, also bentonite saturation and equilibration, as well as its transport properties depend on the chemical environment. This can change due to repository-induced processes (e.g., interaction with cement leachates), or external influences (e.g., melt water infiltration). Evaluation of literature data shows that swelling pressure drops by 75% when increasing ionic strength of the equilibrated NaCl electrolyte from 0 to 3 M for an effective montmorillonite dry density corresponding to 1500 kg/m^3 MX-80 bentonite. Swelling pressure of $CaCl_2$-equilibrated montmorillonite drops only by 40% for the same ionic strength increase (Jenni & Mäder, 2018).
In contrast to the well-known swelling pressure dependence on water composition, the chemical influence on the pore size distribution in confined systems has been poorly investigated. Experimental data indicates different average montmorillonite interlayer distances at different ionic strengths at constant dry density. Assuming a constant volume for solids and electrolyte, interlayer volume changes must be compensated by a corresponding change in some other type of porosity. Such an ionic strength-porosity coupling can explain differences in advective and diffusive transport commonly observed in clays tested with different background electrolyte concentrations, but at the same density (Jenni & Mäder, 2018).
Direct observations of porosity distributions at different chemical environments provide the basis for modelling this chemomechanical (CM) coupling. Such data is necessary to formulate or validate continuum models describing the CM behaviour of montmorillonite stacks ("microstructure"). Their changes in volume and swelling pressure (in confined systems) interact with the bentonite's coarser "macrostructure". This mechanical interaction is also modelled with the continuum approach, resulting in the prediction of discretised porosity distributions, bulk transport properties, and bulk swelling pressures. Chemical processes such as kinetic mineral reactions, speciation, and cation exchange are also considered and interact with the mechanical processes. The present project is based on three approaches:

- Processing of various experimental data from literature leads to estimates of interlayer distances and forces between basal sheets of montmorillonite at different ionic strength outside the interlayer and cation occupancy inside. The resulting data is used to either validate existing models, or to formulate CM dependencies, which are then implemented in the overall reactive transport model.
- Implementation of chemical processes into an existing approach based on the conceptual framework of the Barcelona Expansive Model.

- Extension of pioneering dual porosity reactive transport models (electrostatic controlled Donnan porosity close to clay sheets, and free water porosity): porosity distribution and swelling pressure are calculated considering the porewater chemistry.

So far, these models are focussed on fully saturated systems. First simplified CM simulations predict significantly different swelling pressures and diffusive transport at different ionic strength porewaters (Yustres et al., 2017), in line with experimental observations.

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Coupled Processes Across a Claystone-Concrete Interface: Results of a Combined X-ray CT and PET Transport Experiment

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Abstract

Interfaces between dense clay materials and cementitious materials are studied in the context of deep disposal of radioactive waste for one main reason: mineral reactions due to contrasting chemistries will modify the pore network and affect transport of water, solutes and gas. Substantial research efforts were directed towards mineralogical and physical characterisation of interface regions (e.g. Mäder et al. 2018) but little evidence exists on direct observations of transport behaviour across such skins. This study aims at providing evidence on how mineralogical-physical changes at such an interface affect transport of water and solutes, and linking mineralogical-physical characterisation, X-ray computed tomography and positron emission tomography (PET).

We developed an X-ray transparent core infiltration apparatus whereby a sample core subject to a hydraulic confining pressure can be tested with a hydraulic gradient (Mäder, 2018, for details of method and design in steel and titanium). This compact apparatus uses a carbon fibre tube as pressure vessel and various polymer plastics for other components. Several small pressure tanks integrated into the apparatus allow for self-contained operation for several days, and switching of the percolating fluid. A further extension in form of an integrated lead-shielded pressure container allows also for using radioactive tracers such that the equipment can be used for positron-emission tomography (PET). PET is a superb method to directly image the mobile phase in 3D, and its time evolution (Kuhlenkampff et al., 2017).

A 14 year-old sample core was recovered by stabilized drilling from a long term in situ experiment (CI) at the Mont Terri rock laboratory (Mäder et al., 2018), containing a physically preserved interface between Opalinus Clay and OPC concrete. This larger sample (101 mm DM) was sub-sampled and a 50x50 mm core was stabilised and cored from it. The clay part shows pre-existing bedding-parallel weak jointing that can also be seen in high resolution X-ray CT. The aged interface shows mineral transformations at the mm scale with complex mineral alteration patterns in both clay and cement matrix at a sub-mm scale, including porosity re-distribution and net reduction. The OPC concrete contains aggregate and gas pores. The compound sample may represent a repository situation of a claystone somewhat disturbed by excavation, in contact with a concrete liner, with pore water transport from clay across concrete.

A long-term transport experiment was set up by injecting a synthetic claystone pore water into the core sample on the clay-side, and force advection/diffusion across the interface and out of the cement-side. The fluid is traced with deuterium as water tracer, and periodically sampled for chemical and isotopic analysis. The sample was monitored frequently by high resolution X-ray CT during the first few days, and then regularly for the first 4 months. The running experiment was then transported to Leipzig and prepared for PET. ^{124}I was used as PET tracer, and the chosen dose allowed for continuous PET scanning during two

weeks, initially every 3 hrs.

A very large data set of 2D interface characterisation (SEM/EDX mapping, etc.) and time-resolved 3D CT and PET is presently being evaluated, enhanced, imaged and interpreted. Preliminary results document an initial self-sealing effect of the joint system in the Opalinus Clay, permeation into the diffusion-controlled pore network in claystone and cement matrix, and partial filling of gas pores. PET captures some preferential flow across claystone along some remaining joints, a spreading of the tracer plume at the clay/cement interface, and some moderate preferential flow across OPC.

This approach provides much more detailed information of coupled processes in complex porous media by imaging both the stationary and the mobile phase. Compared to summation parameters, such as tracer breakthrough, there is infinitely more information obtained about the localisation of flow and the nature of the pore network and its temporal evolution.

The research leading to these results has also received funding from the European Union's European Atomic Energy Community's (Euratom) Horizon 2020 Programme (NFRP-2014/2015) under grant agreement, 662147 – Cebama. Uni Bern acknowledges funding contributions by Nagra and the Mont Terri Consortium (CI Experiment).

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Lessons Learnt from THMC Modeling of a System

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Abstract

The most common buffer material for engineered barrier system (EBS) is compacted bentonite, which features low permeability and high retardation of radionuclide transport. The safety functions of EBS bentonite include limiting transport in the near field; damping the shear movement of the host rock; preventing the sinking of canisters, limiting pressure on the canister and rock, and reducing microbial activity. To assess whether EBS bentonite can maintain these favorable features when undergoing heating from the waste package and hydration from the host rock, we need a thorough understanding of the thermal, hydrological, mechanical, and chemical (THMC) evolution of bentonite under disposal conditions. In 2015, an *in situ* test conducted at the Grimsel Test Site in Switzerland was dismantled after 18 years of heating and hydration. The comprehensive THMC data obtained during the heating phase as well as from the dismantling sample analysis provide a unique opportunity to validate coupled THMC models and deepen our understanding of the THMC evolution in bentonite. In this presentation, we describe coupled THMC models developed for the *in situ* test. Water content data obtained after dismantling and relative humidity data measured during the experiment showed that the hydration of bentonite is slower than predicted by the typical Darcy flow model. THMC models that consider the porosity and permeability changes due to mechanical processes match reasonably well all the THM data. However, they did not provide a desirable fit of the measured Cl concentration profile. Further calibration of porosity/permeability changes over the course of hydration and swelling and considering thermal osmosis eventually lead to a model that sufficiently explain all the THMC data. Over the course of modelling the FEBEX data, we learned that (1) chemical data provide an important additional piece of information for calibrating a THM model; (2) key processes needed to reproduce the THM data include vapor diffusion, as well as porosity and permeability changes due to swelling and thermal osmosis; (3) Ion concentration in the aqueous phase are predominantly relied on for constraining model and understanding the geochemical change in the bentonite; (4) The concentration profiles of cations (calcium, potassium, magnesium and sodium) were largely shaped by transport processes despite their concentration levels being affected by mineral dissolution/precipitation and cation exchange. The concentration profile of pH, bicarbonate and sulphate were largely determined by chemical reactions; (5) The model results showed a small amount of illite precipitation and montmorillonite dissolution in the vicinity of the heater, which is neither proved nor disapproved by measured mass fractions of illite in the illite/smectite mixed layer because the data were scatter and indistinguishable from the reference bentonite. These findings enable more reliable calculation of the time frame and condition of early unsaturated phase in bentonite, the porosity and permeability after the bentonite becomes fully saturated, and how transport processes interact with reactions, which affects the long term mechanical and chemical evolution of bentonite and is important to evaluate whether bentonite barrier can function sufficiently.

Gas Transport in Bentonite – A Model Validation Exercise in the Context of SKB's EBS Task Force

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Abstract

Bentonite is a preferred sealing material for the Engineered Barrier System (EBS) of deep geological repositories for radioactive waste. After repository closure, gases may be generated by the corrosion of metals or by the degradation of organic waste components, giving rise to the accumulation of a free gas phase in the backfilled underground structures. The percolation of such a free gas phase through the saturated bentonite may impair the safety functions of the EBS.

The complexity of the coupled thermo-hydro-mechanical (THM) processes associated with gas transport in bentonite buffers gives rise to a multitude of phenomena, which seem hardly predictable by the means of existing numerical modelling tools. For this reason, a comprehensive experimental programme has been accomplished to characterise the phenomena and processes, associated with gas percolation through bentonite samples at the laboratory scale. The laboratory programme comprised the geo-mechanical characterisation of unsaturated bentonite samples (index tests, compaction and retention behaviour), bentonite hydration (swelling pressure, saturated permeability) and gas injection tests in oedometric configurations. Complementary microstructural investigations of the as-compacted and the hydrated material were carried out to get insight in the evolution of porosity during hydration. Further studies were dedicated to the evolution of microstructure before and after gas percolation.

The acquired data bases were made available to a benchmark exercise as part of the "SKB Task Force on Engineered Barriers", aimed at modelling gas transport in compacted bentonite. Three modelling teams participated in this modelling task, drawing on different THM codes and applying different process models for the simulation of the gas percolation phenomena for a range of test configurations and gas injection scenarios. A common feature of all modelling approaches was the use of composite models (bi-modal property distributions, double structure and embedded fracture concepts) to account for a distinct breakthrough behaviour and localisation of gas flow. The benchmark exercise comprised the back-analysis of existing test data and predictive modelling of new gas injection tests. The evaluations of the modelling results reveal that the as-compacted state of the test sample and the hydration procedure have a major impact on the gas percolation through the specimen. Furthermore, the importance of a rigorous uncertainty assessment was highlighted as an indispensable step in the model validation process.

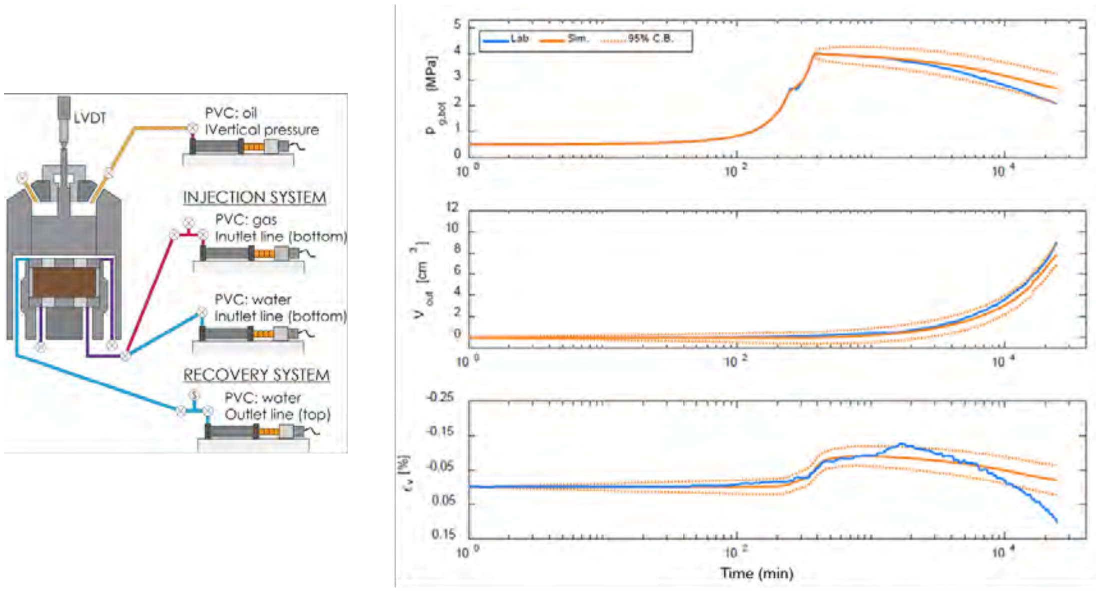

Figure 1: Back analysis of a gas injection experiment in oedometric configuration (left): gas injection pressure (upper), volumetric outflow (middle) and vertical extension of the bentonite sample (lower)

Modelling Advective Gas Flow in Compact Bentonite: Lessons Learnt From Different Numerical Approaches

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Abstract

In a repository for radioactive waste a substantial volume of gas will be generated through corrosion of metals, degradation of the waste and radiolysis of water. If gas generation exceeds the diffusive capacity of the host rock/engineered barrier, a free gas phase may form. In clay based systems the movement of this gas is often accompanied by dilation of the fabric and the development of localised pathways. Historically, conventional two-phase flow models have been highly employed to represent these systems, however, they are not able to describe the full complexity of gas migration processes and therefore, new and novel numerical representations for the quantitative description of advective gas flow are required. This paper presents a summary of work performed in Task A of the current phase of DECOVALEX (D-2019) in which 8 teams have attempted to model the movement of gas in 1D and 3D experiments (Figures 1a and 1b) performed under controlled laboratory conditions. Five types of modelling approaches have been developed: (i) standard two-phase flow models incorporating a range of different mechanical deformation behaviours, (ii) an enhanced two-phase flow models in which fractures are embedded within a plastic material, (iii) discrete fracture approaches using a rigid-body-spring network to represent fracture growth and flow, (iv) a single-phase model incorporating a creep damage function in which only gas flow is considered, and (v) a conceptual approach used to examine the chaotic nature of gas flow. Application of these models show that some continuous strategies (Figure 1(c)) are capable of obtaining a good fitting with respect to experimental stress measurement results. However, these models require substantial calibration of fitting parameters and do not reproduce all of the stochastic behaviour observed in the experiments.

Continuous approaches with preferential pathways have less constraints within the models and while they fail in fitting some experimental details, the phenomenological processes presented are more robust. Similarly, discrete models, whose basis reflects the underlying physics of gas flow, also struggle to capture some the key experimental features of the data. Varying results are also observed in the prediction of bulk flow, see Figure 1(d), with different models performing well. While basic continuous strategies can provide some good fits to the data, it again reflects the higher level of prescription within these codes. This may limit their use as a general predictive tool but they are a necessary step towards building understanding of the important experimental phenomena. Thus, in the application of these approaches prescription, constraints and parameterisation of the codes emerge as key considerations in the modelling of advective gas.

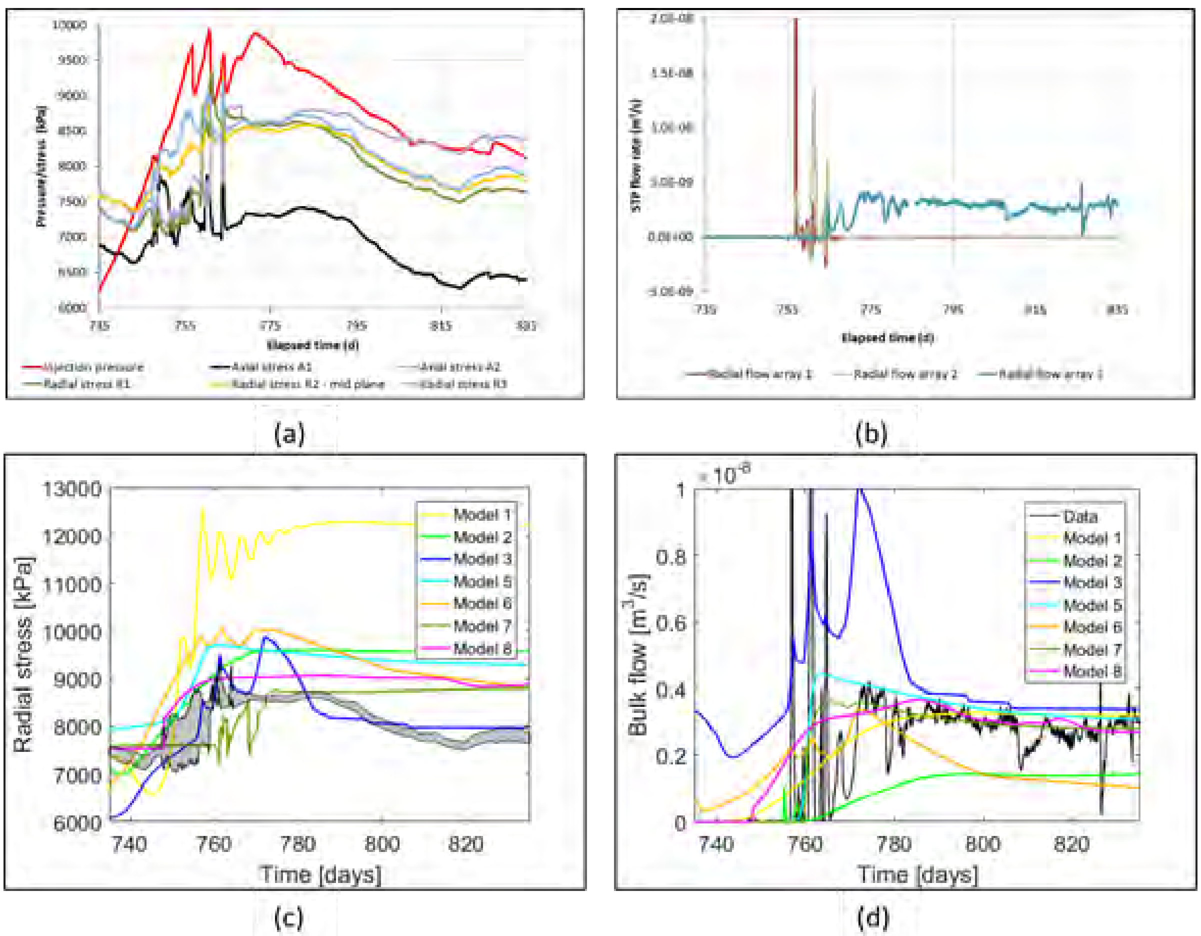

Figure 1: Experimental results from a 3D test: (a) evolution in gas pressure, stress and outflow during multiple gas breakthrough events; (b) outflow of gas to radial arrays. Modelled versus observed results: (c) radial stress (at load cell 1) and (d) bulk flow. Similar results are obtained for radial stresses monitored at different load cells.

Development of an Upscaled HM Model for Representing Advective Gas Migration Through Saturated Bentonite

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Abstract

Understanding gas transport through engineered and natural clays is important for its use in buffers and seals in a range of Geological Disposal Facility (GDF) concepts. Gas migration via processes of multi-phase flow of water and bulk gas and transport of dissolved gases has been widely studied and is well understood for traditional porous media. However, models using only these processes are unable to represent the complex behaviour of gas flow in water-saturated clays, where gas migrates through the creation of additional flow paths (via dilatant pathways / tensile fractures). In order to further understanding of these processes and how best to model them, Task A of the DECOVALEX-2019 (D-2019) project considers small-scale laboratory gas testing experiments in which gas is injected both at the end of (one-dimensional flow test) and into the centre (three-dimensional flow test) of saturated MX-80 bentonite samples (Harrington et al., 2019).

The D-2019 Task A experiments have been used to develop a bespoke fully-coupled hydro-mechanical (HM) model representing gas flow through dilating capillaries, to make it easier to conceptualise and understand the experimental data. In the model, gas is considered to have a separate permeability to water within the saturated bentonite. Modelling gas as a single phase was found to be sufficient to represent key features of gas migration in the experiment and is consistent with experimental observations of negligible water being displaced by gas and minimal water movement. A continuum modelling approach has been adopted to allow for future upscaling (over space and/or time), which may be required if the model is going to be applied in a performance assessment (PA) or GDF safety case context.

Good agreement of the model results to the experimental data can be obtained (see Figure 1 and Figure 2) after calibration of a few key parameters. Both experiments feature a gas breakthrough event followed by a period of sustained gas outflow but, since the experiments employ different gas testing regimes, there remain uncertainties over other processes such as the development of residual gas permeability or post-breakthrough gas permeability evolution. Further confidence is gained by applying the model to a historical dataset with a similar experimental design (Harrington and Horseman, 2003).

The model appears to provide a useful foundation for representing gas flow through saturated bentonite and understanding the key phenomena from the experiments. As part of this work, useful experience has been gained in the interpretation of the experimental configuration and how to model these gas tests. The calibration differences between models of the separate experiments likely arise from the differences in experimental setup / flow geometry. Any future work should seek to reconcile some of the key calibration

parameters with measurable properties of the bentonite as well as examining a wider range of experiments so that multiple, independent examples of key processes can be represented using this approach.

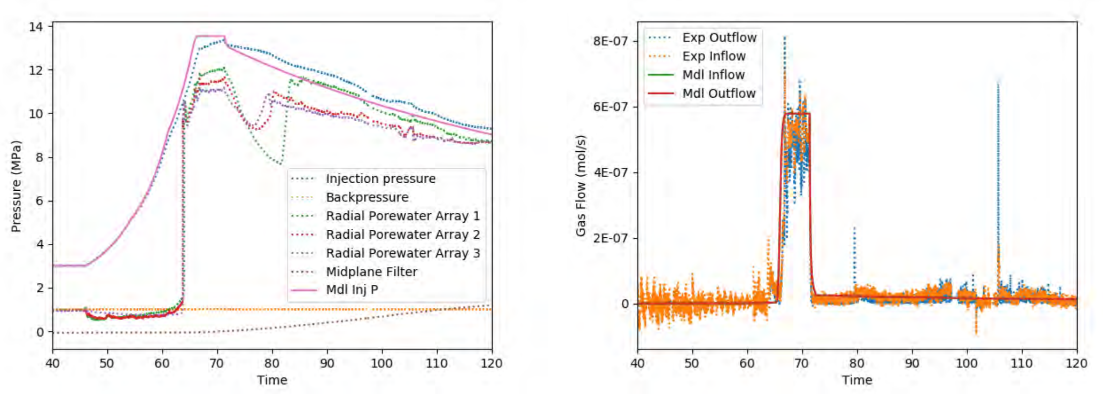

Figure 1: Comparison of modelled injection pressure (left) and gas flow rate (right) with data from the Stage 1A experiment

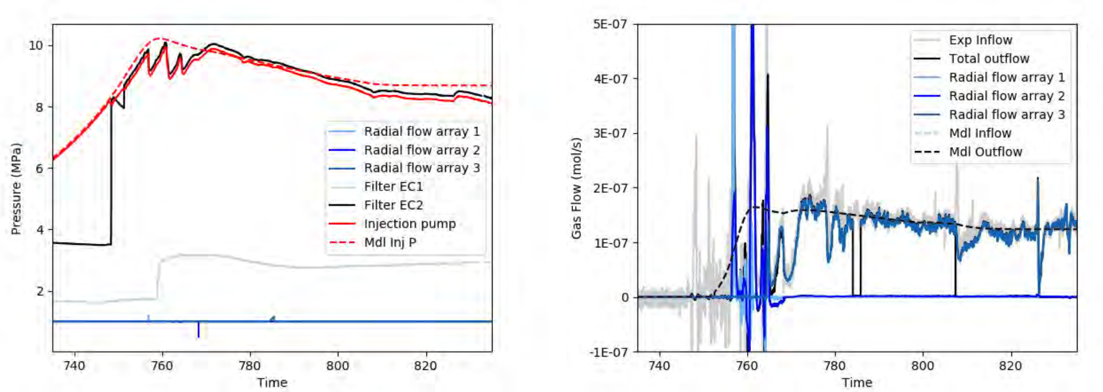

Figure 2: Comparison of modelled injection pressure (left) and gas flow rate (right) with data from the Stage 2A experiment

Acknowledgements: This work was funded by Radioactive Waste Management Limited (RWM; https://www.gov.uk/government/organisations/radioactive-waste-management) as part of participation in the international DECOVALEX project (https://decovalex.org/).

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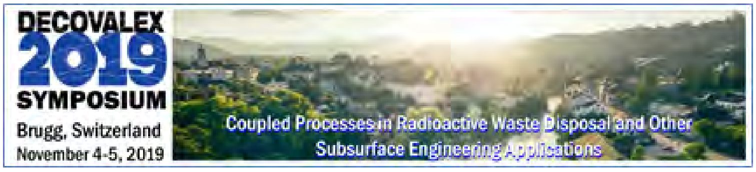

Simulating hydraulic tests in an Excavation Damage Zone

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Abstract

Researchers for Task G of Decovalex 2019 (Seoul National University/SNU, Technical University of Liberec/TUL, geomecon GmbH/GMC) worked for four years aiming to increase the understanding of how the development and evolution of the excavation damage zone (EDZ) changes the bedrock permeability throughout the life cycle of a spent nuclear fuel repository. An increased understanding regarding hydrogeological evolution of the bedrock close to the spent nuclear fuel in a repository system is important in order to better constrain the consequences of possible radionuclide releases after closure.

Hydraulic tests performed in the TAS04 tunnel in Forsmark (Sweden) were chosen to calibrate independent numerical models. The TAS04 tunnel was excavated by the drill and blast method in a fine-grained crystalline host rock. Several holes, 1-2 m in length, were drilled into the tunnel floor. Each drill hole was sealed off into 10 cm to 20 cm long intervals and used as for injection while changes in pore pressure were recorded in the neighboring drill holes. These interference tests were used to determine the transmissivity of the rock mass. For numerical calibration, only tests, which a) were performed in the same rock type, b) lack indications of irregularities due to leakage either around packers or through sealing of borehole extension, and c) showing observations of connections of varying magnitude were chosen.

Because fluid flow in the rock mass is governed by fractures, several fracture networks have been deployed to simulate the interference tests. Fracture networks consist of fractures: a) extracted from tunnel and drill core mapping; b) interpretation of ground penetrating radar measurements; c) discrete fracture modelling.

The researchers used independent codes (*3DEC* and *COMSOL Multiphysics)* and techniques to simulate the interference tests. SNU used 3DEC, which is based on the Discrete Element Method (DEM) where the fracture planes divide the rock into discrete blocks and the mechanical behaviour between blocks follows the constitutive models of rocks and fractures. Based on the relationship between fracture apertures and transmissivities, according to the cubic law, fracture transmissivities are derived from the fracture apertures. Based on the fracture transmissivities, the hydraulic constitutive model determines the hydraulic parameters.

TUL and GMC used *COMSOL Multiphysics*, which is a numerical package based on the Finite Element Method (FEM). TUL performed parametric sweeps to determine the best fit of hydraulic parameters for the implemented fractures and EDZ while GMC studied if fractures subjected to pore pressure increase can be represented by failed rock volumes.

Throughout the various codes and techniques involved, the pore pressure responses in the observation holes could only partly be matched. This is mainly because the codes cannot handle high numbers of discrete or irregularly shaped fractures, either due to too high computational cost or discretization problems. These limitations result in a representation of the EDZ that is probably not fully correct and hence cannot fully represent the interference tests.

Planned Coupled Thermo-Mechanical Experiments in Nizhnekansk Underground research facility

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Abstract

Construction of the underground research facility in the Nizhnekansk Granite-Gneiss Massif will open opportunities to study the processes related to the deep geological repository functioning under the realistic conditions. One of the key aspects of the repository integrity is the host rock and engineered barriers behavior under combined thermal and mechanical loading. In particular, two experiments are planned to study the thermo-mechanical processes relevant to deep geological disposal of high-level radioactive waste.

The first experiment aims on the study of large-scale thermo-mechanical properties of the host rock and the evolution of 3D stress-strain field induced by temperature gradients. The experimental setup (Figure 1) will consist of two boreholes with heaters. The experiment will include two stages. During Stage I (1-2 years) thermo-mechanical properties of the rock will be obtained. One heater will be used giving relatively simple temperature field. Stage II (3-5 years) with both heaters in use aims on the study of the rock stress-strain state evolution under non-uniform heating.

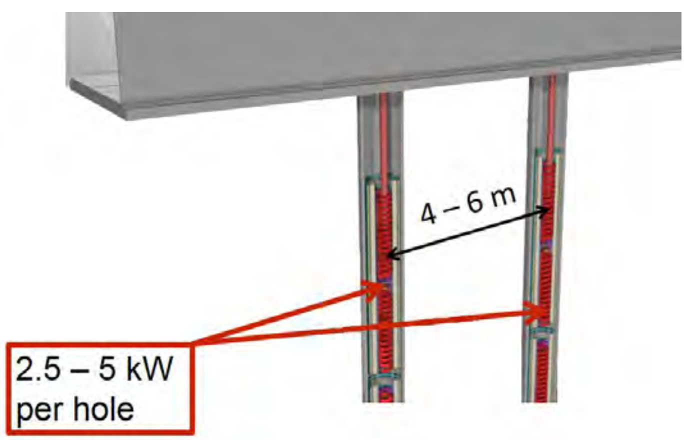

Figure 1: Schematic view of the host rock study experiment

This experiment is related to those held in Äspö (APSE) and ONKALO (POSE). However, since the rock structure and properties in the Nizhnekansk massif differ from ones at Äspö and Olkiluoto, it is essential for the repository safety assessment. There are concerns that thermal conductivity of dry host rock can be 1 W/(m·°C) or less. That will affect heat removal from the waste and lead to temperature increase in the engineered barriers. Water content in the rock and its correlation with temperature and estimated rock thermal conductivity will be measured to address this issue.

Test planning simulations were performed with the finite-element coupled thermo-mechanical code FENIA. Von Mises stress due to thermal expansion reaches 10-15 MPa between the boreholes and 20 MPa near the tunnel wall (Figure 2). The simulations show that the experimental setup provides temperature conditions close to those expected in the HLW repository. Expected temperature gradients and stresses are high enough to be measured, while will not result in rock damage.

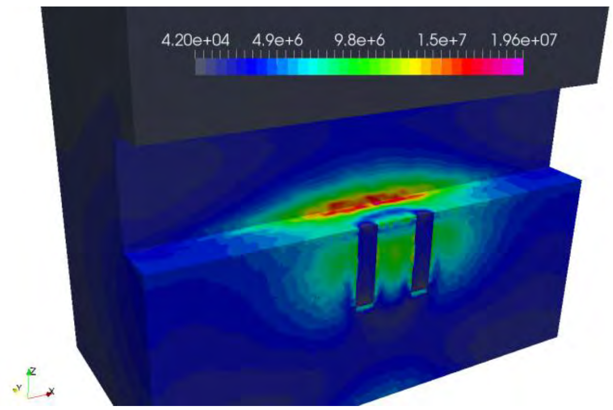

Figure 2: Spatial von Mises stress distribution

Another experiment aims on the study of shotcreted tunnel walls and ceilings under heating. The excavation damaged zone (EDZ) with shotcrete-filled cavities and cracks can be highly inhomogeneous, especially for drilling and blasting method. Preliminary simulations show that even small temperature gradient (several ^{0}C) combined with difference in thermo-mechanical properties yields considerable stress. Since it will exceed above-mentioned values for homogeneous rock, this can lead to shotcrete spalling or crack propagation.

The setup (Figure 3) consists of two perpendicular tunnels with heaters located at the wall bottom, top and on the ceiling. The configuration is preliminary and will be adjusted after the numerical simulations. Since the crack pattern in the EDZ depends on tunnel orientation to the principal stresses, such setup will provide the comprehensive information on horizontal tunnels. In conjunction with ONKALO In-Situ Concrete Spalling Experiment in the vertical hole, it will cover main drift orientations. Naturally, the EDZ will depend on the rock properties and on the tunnel construction method. Still, these experiments will form a solid base for study of shotcreted EDZ behavior.

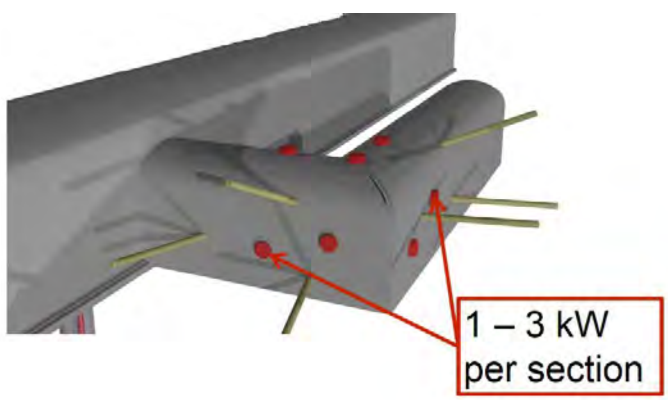

Figure 3: Schematic view of the EDZ study experiment

Methodology Development for Modelling and Simulation of the Environmental Recovery Process After the Tunnel Closure. - Overview of DECOVALEX-2019 Task C: GREET -

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Abstract

The construction of underground facilities for the geological disposal of radioactive waste will change the environmental conditions which are identified in the surface survey prior to the construction of the facility. However, knowledge of whether or not the disturbed environment will recover after the closure of the facility is still insufficient. An experiment known as GREET (Groundwater REcovery Experiment in Tunnel) is being conducted at the Mizunami Underground Research Laboratory of the Japan Atomic Energy Agency (JAEA) to evaluate the environmental recovery process around underground galleries in fractured crystalline rock. The experiment has been planned to observe any environmental changes following water-filling in Closure Test Drift (CTD). The baseline hydro-mechanical- chemical (H-M-C) condition was identified prior to the excavation of CTD. Then excavation of CTD and isolation by the water-tight plug, and subsequent flooding with groundwater were conducted. Environmental disturbance and recovery were observed for more than 6 years. The collected data was used for the DECOVALEX-2019 Task C, which aimed to develop a modeling and simulation methodology for the environmental recovery process.

In Task C, three research teams, JAEA, Sandia National Laboratory in the United States (SNL), and Technical University of Liberec in the Czech Republic (TUL) challenged to simulate the observed environmental changes. The simulation targets are the water pressure drawdown/recovery and variation of water chemistry during the tunnel excavation and closure observed in the monitoring boreholes and in the CTD. In these simulation trials, a stochastic approach using a discrete fracture network (DFN) model and an equivalent continuum porous media (ECPM) model, and deterministic approach based on mixed-hybrid finite element methods were applied by each team to reproduce the hydraulic change and chlorine concentration in groundwater around the CTD. Furthermore, the reactive transport modelling and basic thermodynamic analysis by PHREEQC were examined to capture the chemical evolution of isolated groundwater in the CTD.

As a result of endeavoring by each team, the methodology for modelling and simulation achieved following technical level. The combination of stochastic and deterministic approach with an iterative calibration considering high permeability fracture is available to present the range of groundwater inflow rate into the tunnel, hydraulic drawdown and the recovery. By the ECPM model converted from the DFN model, the variation of chlorine concentration around the tunnel can be roughly reproduced. However, the precise chemical variations of groundwater in the fractures around the tunnel can only be reproduced qualitatively. It is possible to identify water-mineral interactions that will affect the future chemistry of isolated groundwater in the tunnel by the thermodynamic analysis. Further check of the applicability of reactive transport modelling methodology is required to estimate the chemical variation of groundwater around the tunnel in the future.

Direct In Situ Probing Of Fracture Deformation Coupled To Fluid Pressure At Relevant Nuclear Waste Repository Depths – The COSC-1 Deep Borehole Experiments (Sweden)

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Abstract

A unique field test was recently conducted (June 2019) by a joint LBNL (USA) -Uppsala University (Sweden) team, at the COSC-1 deep borehole in Sweden, to study in real-time the coupled hydro-mechanical process in deep fractures in granitic rock. The COSC-1 borehole is well characterized in previous investigations in terms of the presence and locations of conductive and non-conductive fractures as well as the intact, non-fractured rock. This information was used to choose the intervals to be tested. A number of field problems arose from the fact that such experiments have not been previously carried out at great depths. These were resolved on site and good data were obtained.

Detailed gamma log mapping of the borehole permitted precise location of selected intervals. At depth intervals bracketed by packers in the borehole, we simultaneously measured the time evolution of 3D rock deformation, the injection flow rate and water pressure in a step up and step down procedure, including large pressures that can open up fracture aperture and even crack the rock. Seismic response was measured simultaneously. Data was obtained for (1) an interval with a hydraulically conducting fracture at 504.5 m depth, previously identified as conductive by FFEC logging, (2) an interval with a non-conducting fracture at 515.1 m depth, not too far away from the conducting fracture, and (3) an interval of intact rock at 485.2 m without pre-existing fractures, at which injection pressure was raised to cause hydraulic fracturing.

This presentation will present the experimental procedures, as well as first results and preliminary interpretations of the data in terms of coupled hydro-mechanical behaviour of fractures in deep rock systems in situ.

Brine Availability Test in Salt (BATS): Coupled Processes

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Abstract

The US Department of Energy (DOE) Office of Nuclear Energy is conducting a brine availability test in bedded geologic salt at the DOE Office of Environmental Management's Waste Isolation Pilot Plan (WIPP), near Carlsbad New Mexico. While several large-scale tests related to disposal of transuranic and heat-generating radioactive waste were conducted at WIPP in the 1980s and 1990s, this new test is unique in its use of brine availability to gather data on coupled processes in a disposal environment. Brine availability to a borehole or excavation is impacted both by the distribution of water in the salt (i.e., intergranular brine, fluid inclusions, and hydrous minerals) and characterization of the pathways allowing the brine to flow to the excavation. The porosity and permeability of the salt in the far-field is almost unmeasurably low. The mechanical damage imparted to the near-field by the access drift excavation process is responsible for creating the pathways for liquid and gas to migrate to the heat source. The porosity, permeability, tortuosity, and pore-size distribution of the salt around the excavation and boreholes impacts transport of brine and gas. Two parallel tests will compare the response of heated (120 °C) and unheated salt. Observations of borehole closure and brine migration will be supplemented by geophysical surveys (electrical resistivity tomography, fiber-optic strain and temperature sensing, ultrasonic travel time tomography, and acoustic emissions) sensitive to changes in porosity and saturation with time. Brine and gas composition and stable-water isotopic makeup will be analysed at a high frequency to estimate the contribution of observed brine from each of the three types of water found in geologic salt deposits under both heated and unheated conditions.

While previous field tests for characterization of coupled processes relevant to radioactive waste disposal in salt have focused on the thermal-mechanical interactions, we are focusing on the hydrological and geochemical response. Brine availability is sensitive to a host of thermal, hydrological, mechanical, and chemical processes in the salt. We present a summary of the test and some preliminary data. The tests are a modular design and located in horizontal boreholes (i.e., avoiding mapped horizontal anhydrite and clay layers), which can be modified to understand different effects in possible follow-on tests.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. SAND2019-6537A

Investigation of THMC-coupled processes on sealing systems in rock salt

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Abstract

For the safe disposal of high-level and heat emitting radioactive waste in Germany the disposal in deep geological formations is foreseen. Corresponding to the safety requirements of the Federal Ministry for the Environment, Nature Conservation, Building and Nuclear Safety (BMUB), the disposal must ensure that radionuclides are confined in the containment providing rock zone and are isolated from the biosphere as long as possible [1]. During mining activities, the host rock is penetrated by shafts and drifts which presents potential pathways for intrusion of solution or release of radionuclides. Hence, shafts and drifts need to be sealed with plugs from adequate construction material. A sealing system consists of the sealing material itself, the excavation damaged zone (EDZ) and the contact seam between sealing material and EDZ (*Figure 1*).

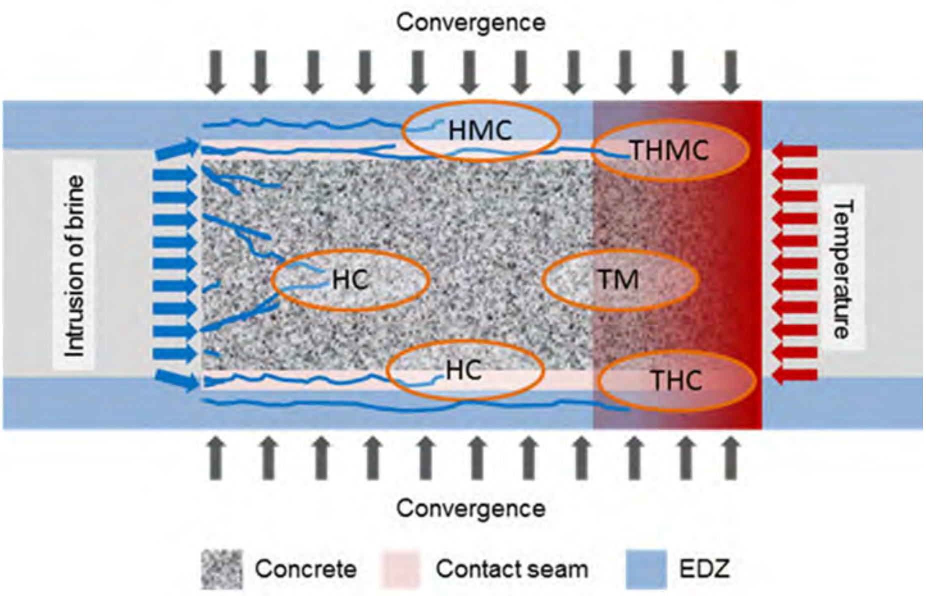

Figure 1: Impacts of a sealing system in rock salt

Within the scope of the ThyMeCZ_Project (FKZ: 02E11698), GRS is currently investigating sealing and backfilling materials planned to be applied in a nuclear repository in a salt formation. The program aims at providing experimental data needed for the theoretical analysis of the long-term sealing capacity of the sealing system, including the closing of the contact seam and the recovery of the excavation damaged zone (EDZ) under load and dry or wet conditions and with or without increased temperatures. The interaction with sealing materials is simulated in laboratory experiments by using hollow cylinders of rock salt equipped with a central concrete seal (*Figure 2*).

Figure 2: Combined samples of salt concrete and rock salt for lab tests in GRS

The influence of thermal (T), hydraulic (H), mechanical (M) and chemical (C) impacts to the sealing capacity of a sealing system is investigated systematically by lab experiments:

HC-Test: Combined samples are percolated by saline solutions and the change in fluid permeability and in phase composition with time due to corrosion mechanisms are investigated.

HMC-Test: Combined samples will be exposed to various stress states with and without percolation of saline solutions. Development of fluid permeability and changes in solution composition will be determined.

THC-Test: Extension of the HC-Test by temperature. The influence of temperature to the development of fluid permeability and phase composition is investigated. Caused by the increased temperature, an acceleration of the processes is expected.

TM-Test: First, samples will be loaded by a stepwise increasing isotropic stress. In the second step, the stress state will be kept constant and the temperature will be increased. The aim is the investigation of the stress and temperature dependent long-term deformation behaviour.

The workshop contribution will present current results of the above-mentioned lab experiments.

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Quantification of hydrocarbon release due to underground excavation in rock salt

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Abstract

The underground will be excavated for the final disposal of radioactive waste in deep geological formations. Due to stress redistribution after excavation, an Ed/DZ (excavation disturbed/damaged zone) will be generated in the near field of an opening. The hydraulic and mechanical properties of the rock mass may be significantly changed in that zone. Hydrocarbons found along grain boundaries in rock salt, which are quasi-randomly distributed in rock and sometimes can only be observed with ultraviolet light, can even be mobilised and migrate at potentially significant speed towards the excavation.

Within the international cooperative project DECOVALEX-2019, the migration mechanism of such fluid inclusions in rock salt is being studied intensively under two conditions: a) altered hydro-mechanical conditions as a consequence of tunnel excavation or borehole drilling and b) coupled thermo-hydro-mechanical-chemical conditions during the heating period in the post-closure phase of a repository. A multi-scale modelling strategy has been developed (Shao et al., 2019). A macroscale coupled hydro-mechanical modelling of an underground excavation was performed to determine hydraulic and time-dependent deviatoric stress conditions, taking into account the rock salt creep behaviour. Under these constraints, microscale modelling of a pathway dilation along the halite grain boundary was performed with a coupled two-phase flow and elastoplastic model taking into account permeability changes. The increase in permeability resulting from the pathway dilation can be estimated at two orders of magnitude. Based on the permeability determined, a series of pressure build-ups measured from a borehole with a high release rate of gaseous hydrocarbons, a total of 430 build-ups within a monitoring time of 938 days (Paul et al., 2015), can be simulated quite well with a macroscale compressible flow model taking account of different zones around the opening (Figure 1).

As a conclusion, the locally distributed hydrocarbon with high pressure can flow with an increased permeability of approx. 1E-20 m² resulting from the change in the surrounding stress state due to excavation. The evaluated permeability is two orders of magnitude higher than the intrinsic one of the rock salt.

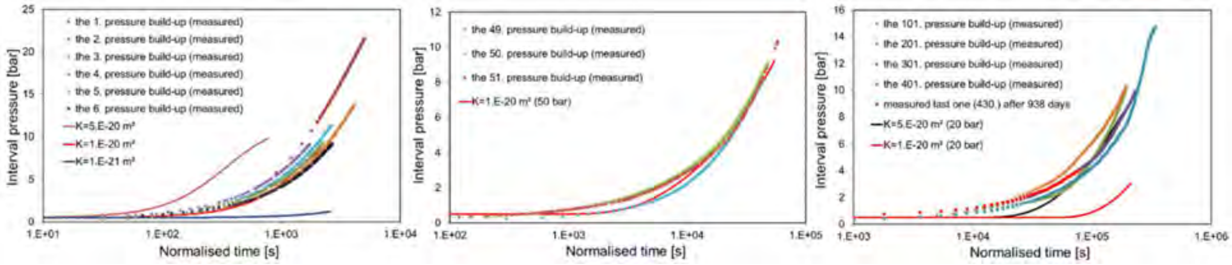

Figure 1: Simulated with the FE code OpenGeoSys (Kolditz et al., 2012) and measured pressure build-ups from a borehole with a high release rate: fluid inclusions located in the EDZ (l), in the EdZ (m) and in the undisturbed zone (r) with a later increased permeability in the Ed/DZ around the borehole

Keywords: Fluid inclusion, rock salt, microscale pathway dilation, multiscale modelling, hydromechanical coupling, OpenGeoSys

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The Full-scale Emplacement (FE) Experiment Modelling Task Force

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Abstract

The Full-scale Emplacement (FE) Experiment at the Mont Terri Underground Rock Laboratory imitates the construction, waste emplacement, backfilling and early-stage evolution of a spent fuel / high-level waste (SF / HLW) repository tunnel in a clay-rich formation (Opalinus Clay), using heaters instead of SF / HLW canisters. The different project phases (e.g., tunnel construction, heating, etc.) have been/are monitored using several hundred sensors distributed in the tunnel and in the surrounding Opalinus Clay. This large data set is the basis for all subsequent modelling efforts, coordinated by a Task Force set by Nagra. The mission of the Task Force is (1) to confirm the completeness and technical readiness of the conceptual thermo-hydro-mechanical (THM) framework needed to assess the impact of Repository Induced Effects (RIE) on the long-term performance of the HLW near field, covering the full spectrum of relevant phenomena and processes, (2) to calibrate THM models, i.e., to derive best-fit parameters as input for phenomenological system analyses in support of the assessment of the RIE, (3) to validate the applied THM models for the intended use, comprising the safety-relevant impacts of RIE on the Engineered Barrier System (EBS) and on the host rock, and (4) to provide modelling capabilities for the decision-making of the future heating strategy and layout optimizations.

A structured approach involving modelling Tasks with increasing degree of sophistication has been proposed by the Task Force. Task 1 "Validation of thermally induced THM effects in the rock around the FE-tunnel" involves (1) a THM code and calculation verification, (2) the back-analyses of THM observations in the host rock, and (3) the validation of THM models in the context of a prediction-evaluation exercise. To that end, two different models have been set-up by the École polytechnique fédérale de Lausanne (EPFL) and by the Universitat Politècnica de Catalunya-BarcelonaTech (UPC). Models are three-dimensional and include the actual geometry of the FE set-up (e.g., concrete lining, EDZ, Opalinus Clay, heaters, etc.; Figure 1), all project phases and all relevant THM phenomena and processes. In the context of subtask 1.1 "Code and Calculation Verification", a simplified -although realistic- model set-up with given parameters is used. The set-up of models (e.g., geometry, zonation, etc.) to be used in subsequent subtasks on back-analyses and validation will be refined in view of the results of the first subtask, and the parameters will be calibrated.

In this presentation, the results of the comparison between THM codes Code_Aster (used by EPFL) and Code_Bright (UPC) will be summarized. The comparison is carried out both in space and time by analysing the differences between THM code outputs at (1) selected observation sensors vs time, and (2) spatially, at selected control times.

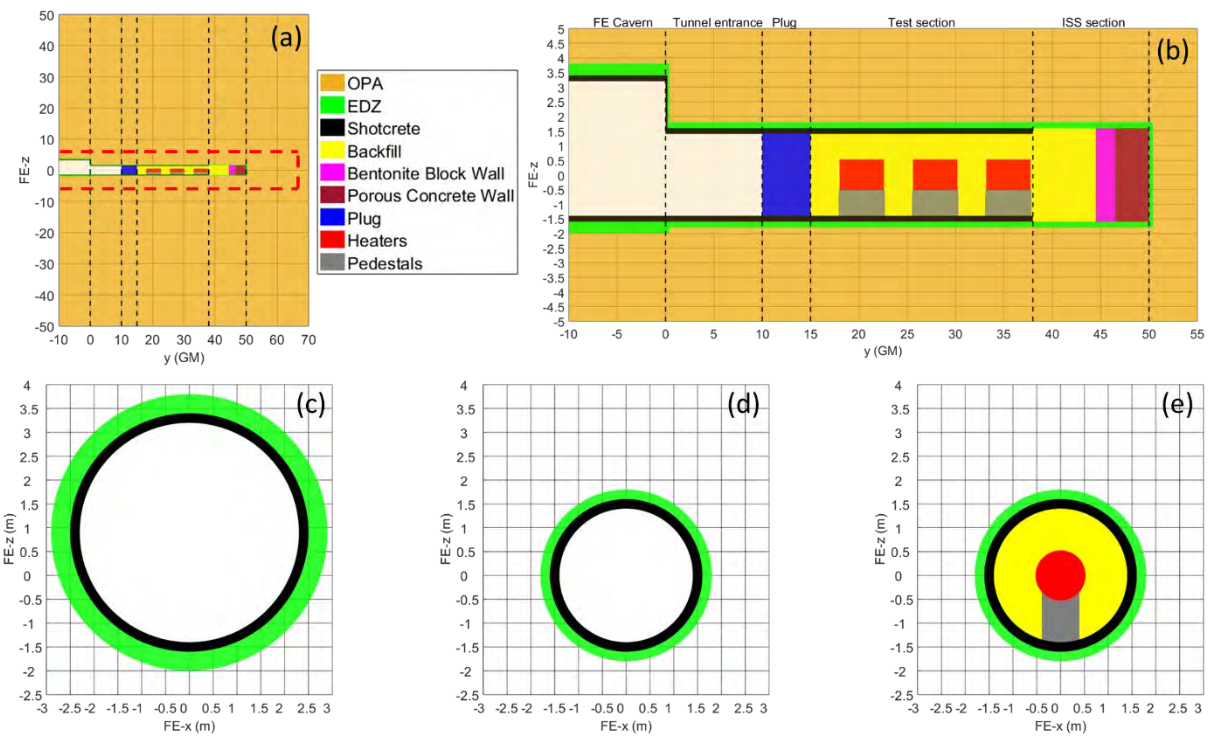

Figure 1: Specified geometry for subtask 1.1 ("Code and Calculation Verification"): (a) Longitudinal cross section along tunnel axis; (b) zoom to model components (not to scale). (c) cross section orthogonal to tunnel axis at y=0 (interface FE cavern-tunnel entrance); (d) cross section orthogonal to tunnel axis the tunnel entrance; (e) generic cross section orthogonal to tunnel axis at a heater.

A Reliable Numerical Analysis for Large-Scale Modelling of a High-Level Radioactive Waste Repository in the Callovo-Oxfordian Claystone

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Abstract

The study and design of deep geological repositories for high-level radioactive waste by means of numerical tools requires not only an extensive study of the host rock parameters and the different multiphysics couplings of its constituents but also a good understanding of the different assumptions regarding numerical issues. Defining proper initial and boundary conditions as well as the use of efficient numerical strategies to save computational resources are of great importance. Evaluations of different approaches is required to understand the reliability of results.

Within the framework of the DECOVALEX 2019 project, a task is devoted to upscaling modelling from small scale to one-to-one scale, and finally to the repository scale. Five research teams have approached these subjects using different numerical methods and codes. The first part of this work consists in upscaling THM modeling from small-size experiments (some cubic meters) to real-scale cell experiments (some ten cubic meters) in order to characterize the host rock and to study its THM response under thermal loadings. These two experiments were conducted in the Meuse/Haute-Marne Underground Research Laboratory by the French national radioactive waste management agency (Andra) in a Callovo-Oxfordian (COx) claystone formation. In most of the cases, the results based on the thermo-poro-elastic approach obtained by the research teams successfully captured the main features of the measured temperature and pore pressure evolution.

In the second part, the research teams performed an illustrative case study of a large-scale high-level radioactive repository including access tunnels and up to 168 cells for comparison and validation of their numerical approaches (see Figure 1). Followed by the analysis of several assumptions: a) different boundary conditions at the far field as well as the cell walls, b) plane-strain assumption, c) domain simplifications taking into account symmetry planes, d) parameter sensitivity analysis, e) variability of parameters in the COx layers, and f) numerical strategies to reduce the computational time. Finally, this paper highlights the conclusions obtained from these analyses and provide some preliminary guidelines/best practice for modelling large-scale deep geological repositories.

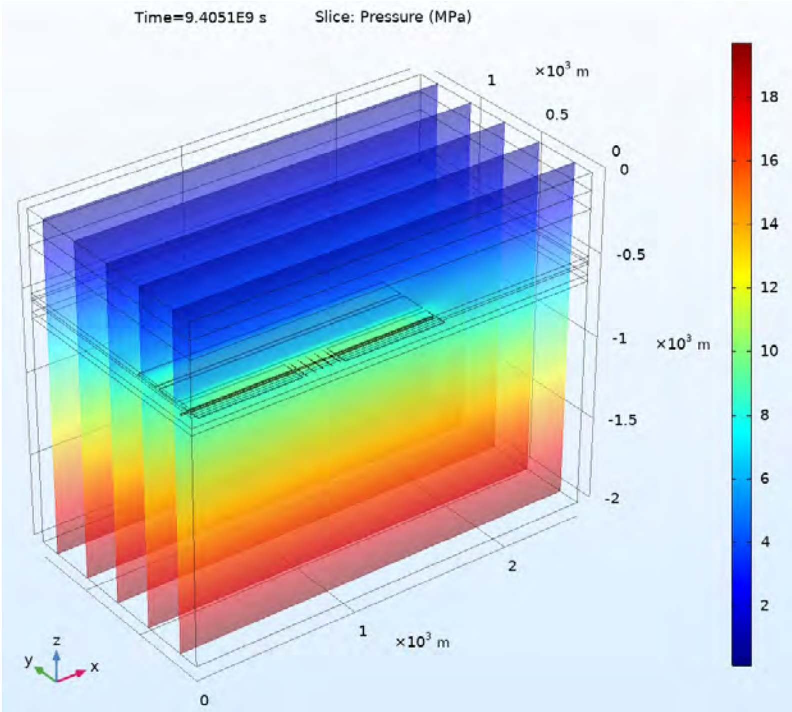

Figure 1 : Pore pressure from 3D model at 300 years (NWMO)

Coupling Clay Swelling Properties to Hydro-Geochemical Conditions: A Reactive Transport Modeling Approach

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Abstract

The mineralogical and chemical properties of clays have been the subject of longstanding study for the long-term disposal of nuclear wastes in geological repositories. The low permeability of clay materials, including shales, provides at least part of the safety functions for radionuclide contaminants confinement. From a geochemical and mineralogical point of view, the high adsorption capacity of clay minerals adds to the effect of low hydraulic conductivities by greatly increasing the retardation of radionuclides and other contaminants, making clays ideal where isolation from the biosphere is desired. While their low permeability and high adsorption capacity are widely acknowledged, it is clear nonetheless that there is a need for an improved understanding of how the chemical and mineralogical properties of shales impact their macroscopic properties. It is at the pore-scale that the chemical properties of clay minerals become important since their electrostatic properties can play a large role. The negative electrostatic potential field at the clay mineral surfaces results in the presence of porosity domains where electroneutrality is not achieved: cations are attracted by the surfaces while anions are repulsed from them, resulting in the presence of a diffuse ion swarm – or diffuse layer. Numerical methods for modeling macroscopic properties of clay media with the consideration of the presence of a diffuse ion swarm have met a growing interest in diverse communities in the past years. In this presentation we will highlight the complex interplays of mineralogical, chemical and microstructural characteristics of clay materials that are ultimately responsible for a remarkable array of coupled macro-scale properties, including swelling. A coupling scheme for predicting swelling pressure as a function of chemical conditions will be presented in the framework of a reactive transport modeling approach.

Complexity of Fault Rupture and Fluid Leakage in Shale: Insights from a Controlled Fault

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Abstract

Faults of various sizes may be reactivated by thermal, hydraulic and mechanical disturbances during operational or post-closure periods. The Fault Slip experiment (FS) has been designed to study the creation of permeable flow paths for contaminant transport by reactivating faults in otherwise low permeability argillaceous rocks. Several fluid injections have been conducted at 340 m depth within a mature fault zone in the low permeability Opalinus Clay formation in the Mont Terri Underground Research Laboratory (Switzerland). Here we describe the rupture mechanisms that were evaluated using data from continuous measurements of the three-component borehole wall displacements and fluid pressure in two sections hydraulically isolating the fault zone, one used for stepwise fluid injection and the other for monitoring. Because of the very low permeability of the fault zone, fluid injection initially causes a strong pressure increase in the injection well, followed by an overall normal (i.e., 'opening') activation of the mechanically weak fault planes connected to the injection source. As the rupture patch of large excess pressure around the injection well increases in size, fluid sudden discharge into the principal shear zone of the fault and generates further fault rupture instability characterized by a large slip event and an associated seven-order-of-magnitude permeability increase. This event appears to be favored by the small difference between principal stresses, by co-rupture stress rotations, and by the geometrical complexity of the fault. Our analysis highlights the importance of considering the detailed fault architecture and

heterogeneous hydromechanical behavior of fault compartments when evaluating fault activation and associated leakage at the crustal scale. Thus, a single plane model for fault activation might not be sufficient and may underestimate leakage potential. The FS experiment was modeled in the Task B of the DECOVALEX-2019 project where different numerical models for activation of minor and major faults, including mechanical responses and associated changes in fault permeability were compared.

Results from an International Simulation Study of a Controlled Fault Activation Experiment at Mont Terri Laboratory

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Abstract

We present results from a modeling study of a controlled fault activation experiment with the objective to develop, compare and validate models for fault hydromechanical behavior in Argillite formations. The study is part of the international DECOVALEX-2019 project and focuses on modeling of two fluid injection tests conducted at two different locations within the main fault crossing the Mont Terri Laboratory, Switzerland (Figure 1). Seven modeling teams participate in analyzing the test data using different modeling approaches that could be categorized into models representing a fault by an interface as opposed to models representing a fault by finite thickness solid elements. In addition to the field tests, a set of benchmark problems were modeled for code-to-code verification and were also used for identifying differences in the model and reasons for any disagreements in the modeling results between different modeling teams. For example, it was found that it is important to have a consistent representation of the borehole and its intersection area with the simulated fault plane in order to be able to make useful model comparisons. The benchmark simulations also clarified differences between the interface and solid element representations of a single fault plane and how to properly determine elasto-plastic parameters for the solid elements. The modeling teams first modeled hydromechanical responses associated with an injection test in the damage zone of the Mont Terri main fault (injection in BFS2 at 38 m, Figure 1). This test could be modeling using a conceptual model involving propagation of shear and/or tensile failure along an initially impermeable minor fault plane. In general, pressure and flow responses could be matched quite well, while the calculated mechanical fracture opening was overestimated by most modeling teams. The teams then modeled another injection test in the damage zone of the main fault (injection in BFS2 at 40.6 m), with monitoring of pressure and displacement responses 3 m away, at the interface between the fault core and the fault damage zone (monitored in BFS1 at 37.65 m). The conceptual model used by the modeling teams for this injection test was more complex, including a few intersecting fractures or minor faults. Overall, this DECOVALEX-

2019 task has resulted in significant model developments and adaptations of existing numerical models to model fault activation and also resulted in increased understanding of the hydromechanical behavior of faults and fractures in low permeability Argillite.

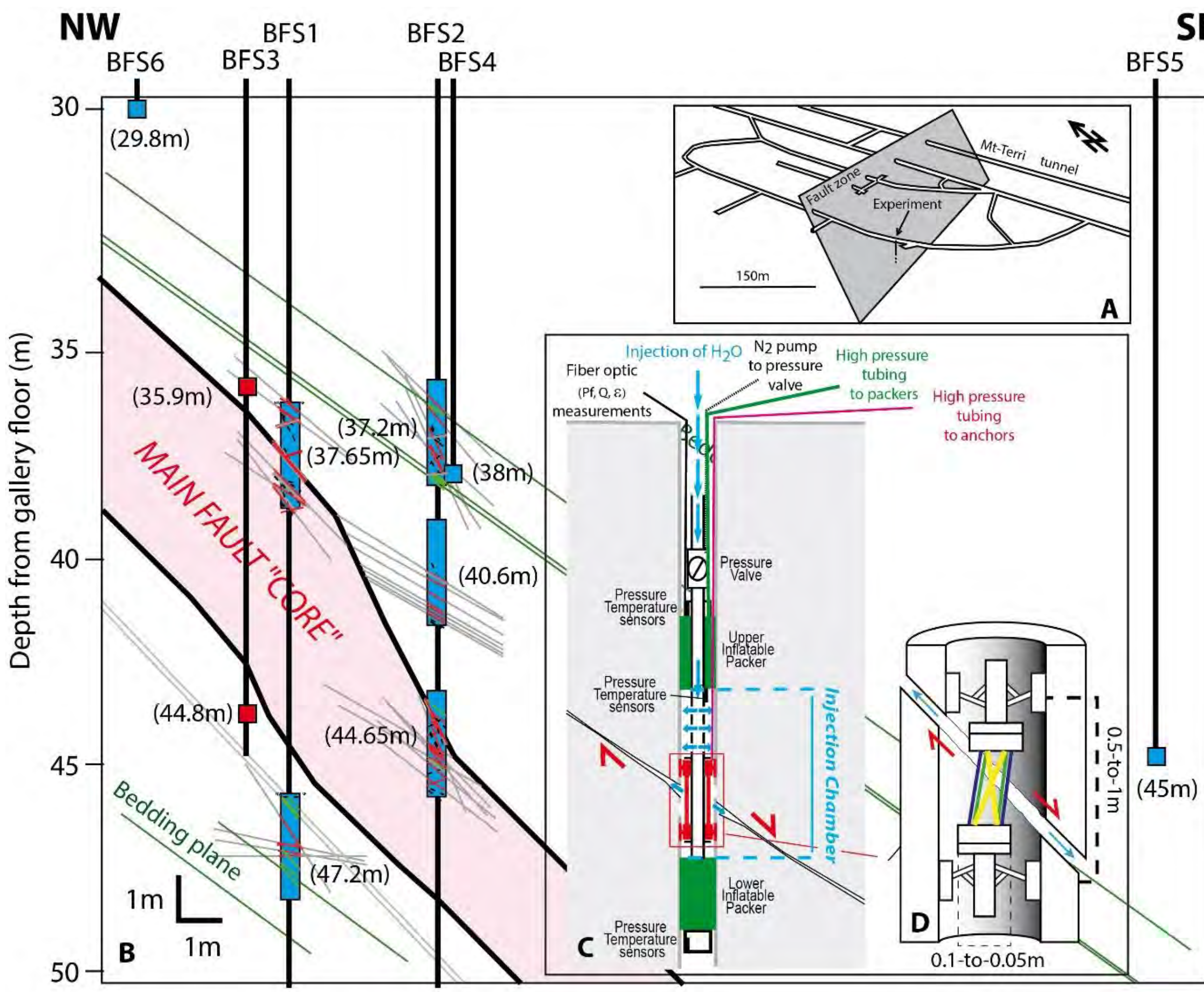

Figure 1: Mt Terri fault activation experiment setting (courtesy Yves Gulielmi). (A)Three-dimensional view of the Main Fault plane with the location of the FS experiment; (B) Simplified cross section of the Main Fault with the blue rectangles indicating the location of the packed-off sections (test intervals) inboreholes BFS - 1and BFS-2.(C) Set-up of the SIMFIP test equipment; (D) Schematic view of the three – dimensional deformation unit.

Coupled Processes in Clay: Preliminary Results from Mont Terri CS-D and FS-B Experiments

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Abstract

The joint effort of two experiments (CS-D lead by ETH Zurich – Zappone et al., 2019– and FS-B lead by LBNL – Guglielmi et al., 2018) allows for a detailed characterization of the poroelastic response of the rock mass and the Mont Terri Main Fault Zone. Geophysical, geomechanical, and hydrogeological monitoring include: (1) pressure as well as geochemical monitoring in several boreholes intervals; (2) deformation at a chain extensometer, fiber optics grouted in boreholes (normal to bedding and parallel to fault zone), as well as detailed 3D displacement at the SIMFIP probe (Guglielmi et al., 2013); (3) continuous recording of passive seismic signal through borehole geophones and acoustic emission borehole and surface sensor.

Injection activities started in December 2018, with multiple step up tests at pressures up to 6 MPa, in order to define the hydraulic response of the fault. Tests where interrupted in May 2019, due to tunnel excavations for the extension of the Mont Terri Underground Rock Laboratory and the final breakthrough in proximity of the CS-D/FS-B experiment site. The excavation was recorded by our monitoring system, and constitutes an extremely valuable calibration for our instrumentation. A prolonged injection of CO2 saturated brine at constant head pressure will start in June 2019 and will continue for the next months.

At the symposium, we will summarize the observations and will combine numerical modelling and observed trend. The results of the analysis could help shading light on the poroelastic behaviour of clay, providing interesting hints for the DECOVALEX community and helping in planning of future CO_2 storage or nuclear waste repositories.

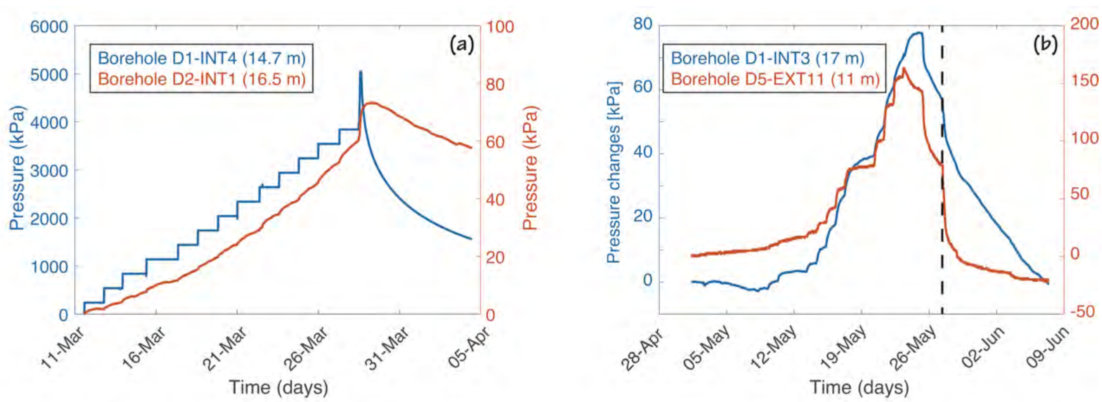

Figure 1: (a) A Prolonged Step Test (constant head with step of 1 day). The blue line is pressure changes at injection point, while the red curve is the response at the monitoring point. (b) Recording of pressure changes (blue) and deformation (red) in two boreholes located next to the excavation front. The dashed line represents the time of breaktrough (May 27th)

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Development of EPCA^{3D} and its applications in coupled THMC processes in geological media

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Abstract

The study presents the development and applications of a self-developed 3D elasto-plastic cellular automaton (EPCA^{3D}), a simulator for the analysis of rock mechanics and rock engineering under thermo-hydro-mechanical-chemical (THMC) coupling conditions. The theory, basic idea and associated components of EPCA^{3D}, including the definition of cellular automaton, the heterogeneous material model, constitutive relations, failure criteria, the post-yield softening scheme, CA updating rules for coupled THMC process, parallel CA updating rule, etc. are introduced. The simulator is validated against in lab tests and experiments conducted in several URLs. The applications of this simulator are presented to show the ability of EPCA^{3D}, including rock fracturing process under complex stress conditions, stability analysis of rock tunnel after excavation. The emphasis is placed on coupled THMC processes in geological system within the framework of DECOVALEX project.

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The role of coupled processes in managing the risk of induced seismicity in GeoEnery applications

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Abstract

Induced seismicity is one of the major risks that deep underground GeoEnergy projects are faced with. The list of projects that have been delayed or abandoned is ever increasing, with economical losses amounting to Billions of Euros. At the same time, public acceptance of this risk is steadily decreasing. The most recent illustrative example of such a failure is the Enhanced Geothermal System project in Pohang (South Korea), which induced in Nov. 2017 a Mw5.4 earthquake, causing more than 80 injuries and losses exceeding $300 million. Existing approaches to risk mitigation, such as traffic light systems, are therefore clearly insufficient. We postulate that in order to make progress, risk assessment and risk mitigation must be based on an improved understanding and modelling capability of the underlying processes, and on truly risk-based, probabilistic methods that are updated in near-real time as new relevant data arrives. ETH together with a number of partners are tackling the challenge of induced seismicity primarily through two closely related groups of activities:

1) In underground lab experiments, we are conducting hydro-shearing, hydro-fracturing and fault re-activation experiments, monitoring in great detail a range of geophysical, chemical and hydraulic parameters through multi-parameter sensor arrays. Experiments are currently conducted in Mont Terri (CS-D, focus on fluid leakage and fault reactivation potential related to CO_2 injection) as well as in the Grimsel and Bedretto Labs (www.bedrettolab.ethz.ch, focus on enabling deep geothermal energy by permeability enhancement, while controlling induced seismicity).

2) Developing and validating adaptive, data driven approaches to risk assessment and mitigation. These Advanced Traffic Light Systems (ATLS) couple a) real-time observations (seismicity, deformation, hydraulics); b) statistical or hybrid (coupled) forecasting models that allow to balance and optimize reservoir development and induced seismicity; c) Ground-motion prediction models, exposure and vulnerability of assets at risk. A first real-time deployment of ATLS is planned for the summer of 2019 in Iceland.

In this presentation, we will overview how progress in understanding coupled processed can be used for enhancing induced seismicity risk assessment and mitigation throughout all stages of GeoEnergy projects. We will also explore how benchmarking exercises such as DECOVALEX can be highly synergistic with our efforts to manage induced seismicity.

Coseismic Secondary Failure in Fractured Crystalline Rocks Triggered by Large Earthquake Events

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Abstract

Crystalline rock formations have been tested and/or selected by many countries worldwide for developing underground nuclear waste repositories at a depth of around 500 m in order to achieve safe geological disposal of high-level, long-lived radioactive waste. A multi-barrier concept is often designed such that spent fuel is stored in copper-shelled iron canisters which are emplaced in deposition holes and isolated from the geosphere by high-density bentonite clay buffers. During the repository assessment period of up to one million years, the occurrence of large earthquakes with a moment magnitude ≥5 within a 5 km radius around the repository may not be excluded. Such massive seismic events, possibly triggered by intraplate activities and/or glacial processes, may significantly alter the state of stress in the Earth's crust and cause strong ground vibrations in the near-field. The superimposed permanent and transient stress perturbations may induce coseismic slip along secondary fractures (especially if they are critically stressed and preferentially oriented/located), resulting in shear failure of waste canisters. Thus, it is of great importance to understand and quantify the seismo-mechanical response of the repository site during large earthquake events in order to better predict its long-term performance. To investigate this problem, we develop and apply an advanced seismo-mechanical model to simulate the evolution of earthquake-induced seismic waves and coseismic processes in the fractured crystalline rocks. The numerical model is able to capture seismic wave propagation, scattering and attenuation in fractured media together with rock damage and fracture slip under mutually-imposed static and dynamic loadings. We elucidate how the distribution and properties of discrete fracture networks affect seismic wavefields and what mechanisms govern coseismic secondary failure in fractured rocks. The research findings have important implications for the long-term safety assessment of planned radioactive waste repository in crystalline rocks.

Far-From-Equilibrium Thermo-Hydro-Mechanical Multiphase Gas Transport in Hierarchical Porous Media

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Abstract

Gas transport in heterogeneous fractured porous media has relevancy to such subsurface engineering endeavors as geologic carbon storage, unconventional hydrocarbon recovery, and long-term underground storage of nuclear waste. We compare experimental results with numerical techniques applicable to far-from-capillary-equilibrium multiphase transport in porous media with capillary heterogeneity, focusing on transitions from capillary-dominated to viscous forces dominated flow under far-from-capillary equilibrium conditions, and viscous fingering to localized fracturing in visco-plastic media. Experimental results injecting gas into porous media with varying degrees and spatial distributions of capillary heterogeneity show transition from steady to oscillatory flow with an increase in capillary number. Modeling results show that dynamic models for two-phase transport depend on physical constraints such as capillary number, and gas compressibility, but also on topological factors relating to distributions of microporosity. Under far-from-equilibrium conditions, two-phase gas flow coupled with thermal and mechanical behaviour experiences localization which can be challenging for standard numerical approaches. The phase-field approach is proving useful in describing migration and stability of drying fronts, localization of damage, and fracturing associated with high velocity gas injection. We apply models to advancing understanding of CO2-brine transport near and far from injection wellbores, gas migration in gaps in engineered bentonite barriers, dry-out and capillary hysteresis in wetted bentonite, and localization of methane migration in so-called seismic chimneys in sedimentary basins.

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Lessons Learned in the Development of Source Term Surrogate Models for Repository Performance Assessment

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Abstract

Surrogate modelling is useful in repository performance assessment (PA) for rapidly emulating source term process models. For the Fuel Matrix Degradation (FMD) process model involved in this study (Jerden et al. 2015), each time step requires significant computational time to simulate the coupled thermal-hydrological-chemical (THC) processes. With thousands of waste packages, PA simulations involving source term process models can be prohibitively expensive.

Three types of surrogate models are under development to simulate the effects of the FMD process model in *GDSA Framework* (*GDSA Framework*, a geologic repository PA software based on PFLOTRAN. See pa.sandia.gov.): a polynomial regression surrogate, a neural network surrogate, and a k-Nearest Neighbours regressor (kNNr) surrogate. These surrogates are operational and are undergoing optimization. During development, several general lessons were learned or reinforced:

- Understand the process model.
    - For a process model that runs its own time loop, the set of inputs used at each time step can be much larger than the set of initializing inputs used by the process model.
    - The set of inputs used at each time step by the process model may be quite different from the optimal predictors chosen by the surrogate.
    - In addition to target outputs, the surrogate model may need to calculate values for predictors (e.g., corrosion layer thickness) and store these values for use in the following time step.
- Generate training and testing data for the realm of interest. For example, if the PA model will never call the surrogate model until simulated time is high, then including process model results at low simulated time in the training data can be counterproductive or wasteful, depending on the type of surrogate model.
- Ensure that the accuracy of the surrogate model is not limited by the training and testing data. Before generating training and testing data with the process model, perform a spatial and temporal discretization convergence study on the process model.
- Include in the surrogate model explicit process model calculations. For example, if the process model explicitly calculates an important predictor variable (e.g., dose rate) for the current time step, make this quantity available as a predictor.
- Consider how the surrogate model will be applied to the performance assessment model. In this case, the FMD process model starts at time zero. In the PA model, fuel dissolution starts only after

waste package breach. This delay, along with time steps that are not synchronized between the PA and process (or surrogate) model, complicates PA integration.

The performance of each of the three surrogate models will be compared against the performance of the FMD process model, both as standalone models and after integrating with PFLOTRAN. A common model problem will be used to provide a measure of relative computational cost and relative accuracy of quantities of interest. Preliminary results indicate that each of the surrogate models will enable *GDSA Framework* to rapidly and accurately simulate spent fuel dissolution for each individual breached spent fuel waste package in a probabilistic repository simulation.

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Acknowledgments

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Laboratory Study on the Volumetric Response of Gas Shale Samples with Controlled Pore Fluid Pressures

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Abstract

Gas shales are partially saturated due to hydrocarbon generation and often encountered with fairly low in-situ degree of saturation less than 50 %. This, combined with nano-scale pore sizes and high salinity, leads to extremely high suction values up to dozens of MPa inducing substantial fluid imbibition into the formation during field operation. As it shed lights on the impact of such conditions on the mechanical behavior of the shale, recent research showed that suction change can significantly alter the elastic properties and the volumetric behavior. However, the experimental methodologies were based on total suction change with relative humidity control and did not provide a direct correlation with the pore fluid pressures. The average pore pressure in partially saturated gas shales is therefore still poorly understood. We introduce a laboratory study on the volumetric response of gas shale samples with direct control of the pore water and air pressures. Observations are provided on how the two pore fluid pressures, matric suction, and saturation sum up to constitute the average pore pressure. We further discuss how these observations point to the effective stress framework of partially saturated gas shales.

Keywords: Gas shales, volumetric response, matric suction, average pore pressure

Insights into Hydro-Mechanical Responses of a Crystalline Rock Mass during Hydraulic Stimulation Experiments

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Abstract

Hydraulic stimulations are a common procedure to enhance the reservoir permeability in the context of oil/shale gas extraction and exploitation of deep geothermal energy. The major difficulties of this technique, e.g. in the framework of deep geothermal energy are a) the risk of inducing seismicity strong enough to be felt at earth's surface, and b) creating an effective and sustainable heat exchanger. Both issues strongly depend on hydro-mechanical rock mass responses and the interaction of brittle discontinuities within the rock mass. Predictive modeling on stimulations require experimental insights into these responses for validation. Due to the strong non-linearities in the upscaling of the hydro-mechanical parameters, intermediate scale experiments provide valuable input for the theoretical understanding of hydraulic stimulation processes and the possible validation of numerical models.

In February 2017, six decameter scale hydraulic shearing (HS) experiments were conducted in the context of the In-situ Stimulation and Circulation (ISC) project in crystalline rocks at the Grimsel Test Site, Switzerland. During these experiments, four ductile and two brittle-ductile shear zones were the target for high-pressure fluid injections. A fluid volume of ~1 m³ per experiment was injected using standardized injection protocol. The experimental volume has an overburden of ~480 m and the maximum principal stress is dipping 40° towards East with a magnitude of 13 MPa. Here, we present observations and first interpretations of the hydro-mechanical responses of the target shear zones and the host rock during the six stimulation experiments

The hydro-mechanical responses within the test volume were captured along six boreholes. Three of them are dedicated to monitor fluid pressure perturbations within the different shear zones, using a total of seven packed-off intervals. In the other three boreholes, a total of sixty longitudinal Fiber-Bragg Grating strain sensors were installed. These sensors have a base length of one meter and are installed across intact rock, fractures or shear zones.

During most of the HS experiments, the near-wellbore injectivity and transmissivity were successfully increased. It was observed that the injection pressure value at which the hydraulic response at the injection well turned into a hydro-mechanical response reduced during most experiments. The induced slip dislocation at the injection point was in the range of 0.5 - 1.5 mm. Away from the injection well, we detected pressure perturbations up to a radial distance of ~16 m. These perturbations were rarely induced by steep pressure fronts that would expected from non-linear pressure propagation. Outside of the target shear zone, the pressure data suggest poro-elastic pressure responses. The strain data revealed two different deformation zones: a) close to the injection location transient deformations were variable (i.e., a mix of compression and extension), and b) further away from the injection location only

compressional deformation was captured. During the experiments, a meter scale Poisson effect was directly measured in the rock mass. Additionally, the formation of wing cracks was detected.

Our data indicate the superposition of shear-induced stress redistribution and poro-elastic stress transfer during the hydraulic stimulations. Both deformation mechanisms should be included in full-scale hydraulic stimulation models.

Coupled Thermo-Hydro-Mechanical Simulations of A Supercritical Geothermal System

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Abstract

Understanding coupled processes is essential to properly assess the performance and risks of supercritical geothermal systems. These systems are found in especially hot reservoirs, at the deep root of volcanic areas, in which water is encountered in supercritical conditions because the pressure (p) and temperature (T) are above their critical values, i.e., $p > 22.06$ MPa and $T > 373.95$ ºC. Thus, supercritical geothermal systems experience strong induced deformations and stress redistributions induced by pore pressure variations and cooling during cold water re-injection performed to balance fluid depletion. While pressure changes are balanced in the injection and production well doublet, strong cooling occurs asymmetrically around the injection well, which significantly contracts the rock and causes a thermal stress reduction. The effective stress changes may lead to fault reactivation and induced seismicity. In order to investigate the potential of seismicity induced by cold water injection in deep supercritical geothermal reservoirs, we have performed coupled thermo-hydro-mechanical (THM) simulations of a doublet system with a steeply dipping conductive fault between the two wells. The fault is modeled as a continuum with higher permeability and compliance than the surrounding rock. We have performed THM finite element analyses with the object-oriented, C++ based and open-source finite element solver OpenGeoSys. We have implemented advanced features such as: i) porosity-dependent permeability, ii) full poro-mechanical coupling and iii) IAPWS-97 equations of state for water present in various phases. The porosity-dependent permeability evolves along with porosity changes, which in turn are a function of the changes of temperature, pore pressure and stress.

The injected cold water absorbs heat from the rock mass on its way toward the production well, crossing the fault. Under conditions relevant for supercritical reservoirs, deformation is mainly controlled the cooling front and is less affected by pressure changes, which reach a pseudo-steady state shortly after the beginning of fluid circulation. Fluid velocity is highest in the fault, whereas major mechanical effects are a consequence of thermal deformation. We compare cold water re-injection with a case of isothermal injection, showing that the rate of seismicity production strongly decreases when thermal effects are neglected. This difference highlights the importance of controlling injection conditions not only in terms of

pore pressure, but temperature as well. Possible risk mitigation strategies could include limiting cold-water injection by either increasing inflow temperature or by decreasing the flow rate.

Experimental and Analytical Assessment of Draupne Shale Seal Integrity for CO_2 Storage Sites

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Introduction

Carbon dioxide (CO_2) capture and storage is one of the most important measures to reduce the atmospheric concentration of CO_2. To ensure safe storage, operations must be conducted in way that respects operational limitations. Furthermore, the operational limitations should be based on models appropriately accounting for relevant material properties and in-situ stress conditions. In this study, we combine various experimental approaches on the Draupne shale to get a more complete picture of the properties of intact and naturally fractured samples and to evaluate the feasibility of using passive seismic to monitor this North Sea caprock. The measured properties combined with in-situ stresses are used to calculate stresses acting on arbitrarily oriented fractures and associated stabilities using an in-house developed software.

Material and methods

The material used in this is the Upper Jurassic Draupne Formation from the Ling Depression in the North Sea. It is described as a low-permeable, homogeneously anisotropic black shale. All samples are sub-cored from 133 mm diameter cores retrieved from a depth of approximately 2580 meters below sea level. The 9-meter core section of high-quality shale provides a rare opportunity to comprehensively study both the intact and naturally fractured properties of an important North Sea caprock.

The intact strength and anisotropy of the core has been extensively studied through isotropically consolidated undrained (CIU) triaxial tests on samples sub-cored at different angles relative to layering (Skurtveit et al. 2015). Strength and frictional properties of a slickensided natural mode II fracture are investigated in the direct shear box. The fracture is characterized both before and after testing using, among other techniques, photogrammetry and Scanning Electron Microscopy (Smith et al. 2019). An elaborate test program is designed to examine the relationship between shear stress and increasing normal load, and to examine the shear stress response to increasing shear displacement rates. The latter can indicate whether the rock is expected to behave aseismically or not during slip. The expected aseismic behaviour is finally compared to triaxial test data on an undrained, isotopically consolidated sample, using simultaneous monitoring of acoustic emissions during shearing of the material. During this triaxial test, the failure plane is exposed to several re-activations at different effective horizontal stresses, relevant to different depths of this formation in the North Sea.

Main results and Conclusions

The experimental program performed enables an in-depth understanding of the mechanical properties of intact and fractured Draupne shale. The analytical software allows for calculation of stresses and stabilities acting on fractures with random orientations in a 3D stress field, informing on the stability of fractures in the sub-surface. In the current project, the input parameters from laboratory testing indicates that critically oriented fractures are already close to activation under the present stress conditions at Ling Depression. Hence, the main consequence of this study for CO2 storage is the increased precision in operational limitations, to avoid unwanted inelastic deformation. state.

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The Importance of Natural Rock Heterogeneity in Governing Transport During CO_2 Storage

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Abstract

A system of CO_2 and brine flowing through permeable rock, relevant to CO_2 storage underground, includes a wide range of physical and chemical processes. These are conventionally modeled using continuum rock properties – permeability, dispersion, mineral surface area. The foundational assumption that within the rocks there exists a scale where the properties are homogenous is a significant source of uncertainty and inaccuracy. Improving on this, however, presents challenges for both modeling and observation. How can we derive information from laboratory observations that is both practical to obtain and practical to use for more rigorous modeling efforts?

I will present the results of investigations into many of the physico-chemical processes relevant to CO_2 storage across the scales that can be observed in the laboratory (*Boon et al., 2017; Jackson et al., 2018; Lai et al., 2015; Lin et al., 2015; Reynolds et al., 2017*). Within the pores of the rocks synchrotron and laboratory X-ray micro tomography has been used to observe dynamic and equilibrium fluid displacement. It has also been used to characterize the distribution of reactive mineral surface area. At the centimeter scale conventional X-ray imaging has been used to characterize solute transport in 3D and to evaluate the impact of rock heterogeneity on multiphase flow and trapping. Combined the results show the pervasive role of heterogeneity on macroscopic flow and reactive processes. They also provide insight into viable paths for incorporating this information into more rigorous models of multiphase flow and reactive transport in the subsurface.

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DECOVALEX 2019 SYMPOSIUM
Brugg, Switzerland
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ABSTRACTS

For

POSTER SESSION

Modelling Volume Change Behaviour of Compacted Bentonite Using a Hydro – Mechanical Coupled Framework

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Abstract

Long term assessment of deep geological repositories for nuclear waste involving compacted bentonite in their design require realistic constitutive models for the volumetric response of the bentonite. Many models for unsaturated low activity clays benefit from the use of a generalized effective stress, meaning that a single stress variable is conjugated to elastic strains. By including the degree of saturation in its expression, such effective stress results in several hydro – mechanical coupling mechanisms. However, such effective stress approach has not found the same degree of success in modelling expansive soils. One of the possible reasons is the complex water retention behaviour of these materials, which requires careful consideration of not only fluid pressures but also of the volume change response of the material. Here a hydro-mechanical coupled approach to simulate the stress – strain behaviour of compacted bentonites is suggested. An explicit distinction between interlayer adsorbed water and capillary water is used to simulate the water retention behaviour. A Bishop – type effective stress is used for the stress – strain response with the degree of saturation as the averaging variable between air and water pressures. Additional coupling mechanisms are introduced in the mechanical formulation by using the degree of saturation as the variable that quantifies capillary hardening. Some interesting results derived from such a framework include the shrinkage limit, the increase in stiffness of the elastic regime and the use of a single elastic coefficient for both wetting – swelling and reloading stress paths.

Unconfined Compressive Strength for Unsaturated-Saturated Bentonite

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Abstract

High dense compacted bentonite or bentonite-sand mixture contribute to safety as manmade buffer at deeply underground. They performed to ensure the stability of the repository and to completely prevent interaction corrosion due to seepage of natural water from bed rock. During the construction operation of a deep geological repository, with the variations of relative humidity changing, water permeability, volume changes of whole bentonite barrier cause instability, stress redistributions and developing of stiffness which lead to changes of stress state of bentonite barrier system. In addition, heating affects produced from waste disposal that influence on swelling, conductivity hydration, strength and deformation of bentonite. Also, clay components interaction with salt concentrations in ground water indicate difference properties comparison to swelled bentonite by distilled water used in laboratory. It is essential that profusion of experimental working is much importance with effective scrutiny of simulation parameters in mathematical frameworks. Therefore, it is particularly necessary to investigate stiffness, strength, deformation and stress-strain relationship on both unsaturated-saturated bentonite including several efforts factors in thermos-hydro-mechanical properties. Regard unsaturated bentonite, the peak strength, volume change and stress-strain relationship could be indicated with the framework of critical state theory with addition suction loading. Under the framework, Alonso et al. (1990) employed the critical state relationship for unsaturated soil in the BBM model using matric suction. On developing coupled thermos-hydro-mechanical (THM) processes, correct evaluations of strengths in mechanical properties is significantly that almost of experimental investigations in laboratory accepted triaxial compression test with long time consuming. The triaxial test results contribute to establish constitutive models that many literatures were published, and applied to practice problems regard to radioactive disposal buffer system. Instead of triaxial compression test, unconfined compression test is so convenience and it has accepted as one objective obtaining interpretation previously for shear resistance.

In this study, unconfined compression tests were carried out on unsaturated-saturated bentonite and bentonite-sand mixture. The bentonite used in this study was Na-type Kunigel V1 and Iitoyo sand in named had a high uniformity in grain distribution. Several conditions were prepared to specimens in order to dwell on assessing to couple thermos-hydro-mechanical (THC) framework

that high agree of elaboration lead exact determination of bentonite properties in THC. They are mentioned as follow; difference between unsaturated condition and saturated condition. Influence of decreasing suction on shear resistance. Unconfined compressive strength at later swelled in salt water from chemical interactions perspective. Estimating of substantial thermal effort on macro structures from stress-strain curve. In manifold parameters, compression speed was controlled to be more systematic analysis in mechanism. With the results of unconfined compressive strength measured using thermal compression apparatus, limited efforts used in this study proved that were extremely importance evidence and raise multiple modifications to mathematical simulation models. In this abstract, modified thermal triaxial compression apparatus, influence of compression speed, decreasing of unconfined compressive strength due to suction reduction and producing reduction by thermal heating were described.

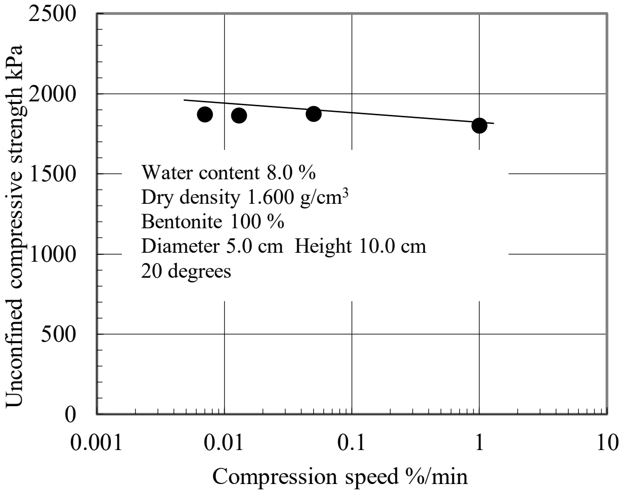

Figure 1. Influence of compression speed.

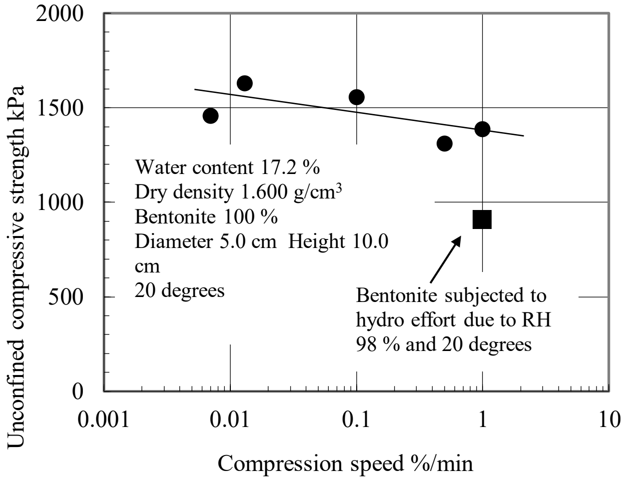

Figure 2. Reduction due to suction decreasing

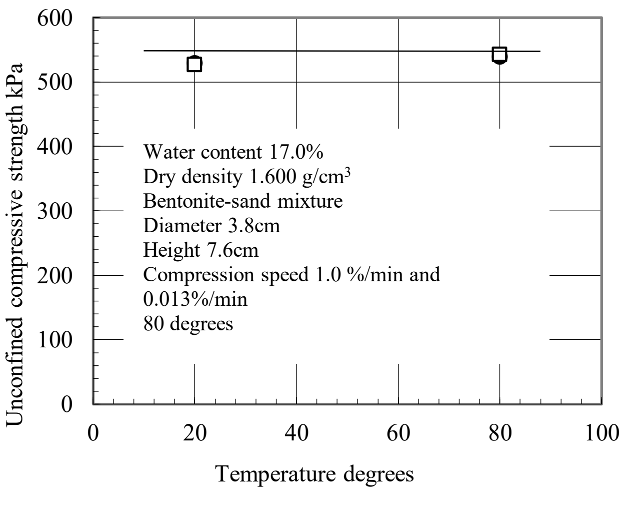

Figure 3. Influence of thermal effort.

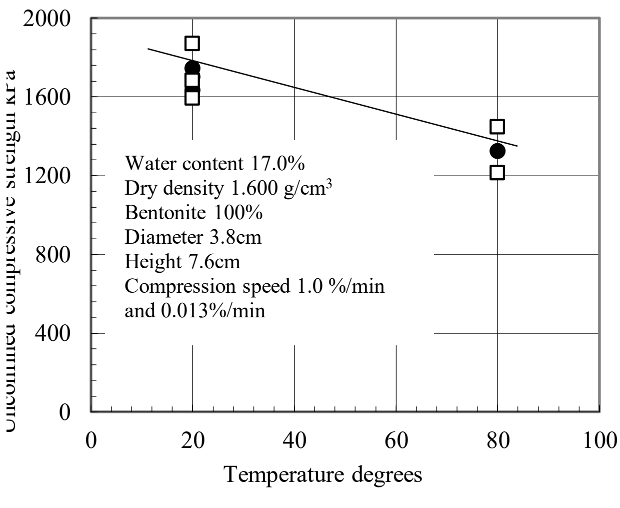

Figure 4. Case of decreasing of soil moisture.

Thermo-Hydro-Mechanical Coupled Simulation of FEBEX In Situ Test

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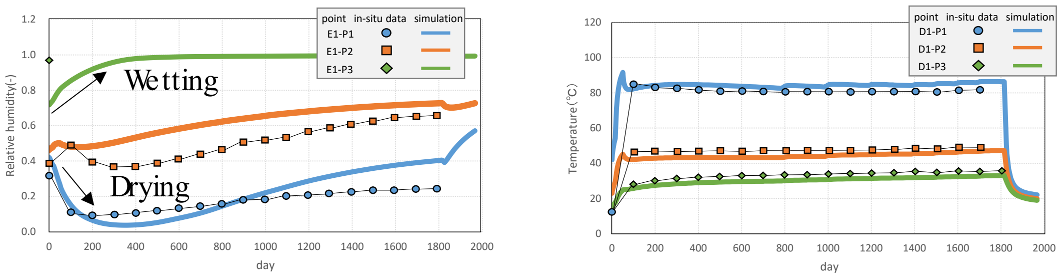
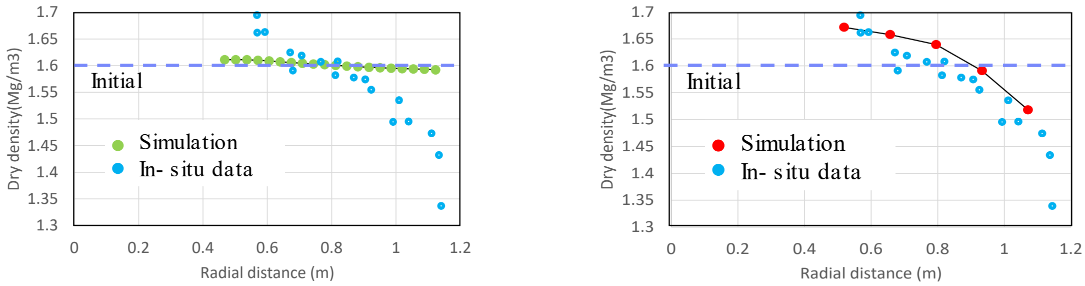
Abstract

The real scale coupled thermal, hydraulic and mechanical experiment (FEBEX in situ test) has been performed at Grimsel test site in Switzerland in order to evaluate the coupling processes on high high-level radioactive waste disposal. The heaters as waste canisters were put horizontally based on the Spanish disposal strategy. In this study, the existing coupling model which has been validated with in-situ test such as the coupled experiment at Kamaishi mine was applied to FEBEX in situ test and the validity of the coupled model was examined. This coupling model was developed by Ohnishi et al. 1985, and has been extended to take into account of the behaviours in the bentonite materials such as the water movement due to thermal gradient and the swelling phenomena. A linear elastic constitutive model with the addition of a swelling term was applied to bentonite material in this coupling model. Simulation results of FEBEX in situ test show that this coupling model can reproduce the hydraulic and thermal behavior of bentonite as shown in figure 1. It is also confirmed that the changes in total stress can be roughly reproduced by this mechanical model. However, as shown in the figure 2 (a), it is difficult to reproduce the dry density distribution after dismantling. Therefore, as another approach, analysis was conducted using unsaturated elasto-plastic constitutive model proposed by Ohno et al. 2007 in which the effective degree of saturation is used as a parameter relating to stiffness. The parameters of this constitutive model were identified by the simulation of the suction controlled oedometer test and the swelling pressure test (ENRESA,2000) typically carried out to examine the swelling behavior of bentonite. It is confirmed that this constitutive model can describe the typical mechanical behavior of FEBEX bentonite as shown in the figure 3. Using the identified parameters, simulation of FEBEX in situ tests was conducted. Not only the change in total stress but also the dry density distribution showed good agreement with the measured values as shown in Figure 2 (b).



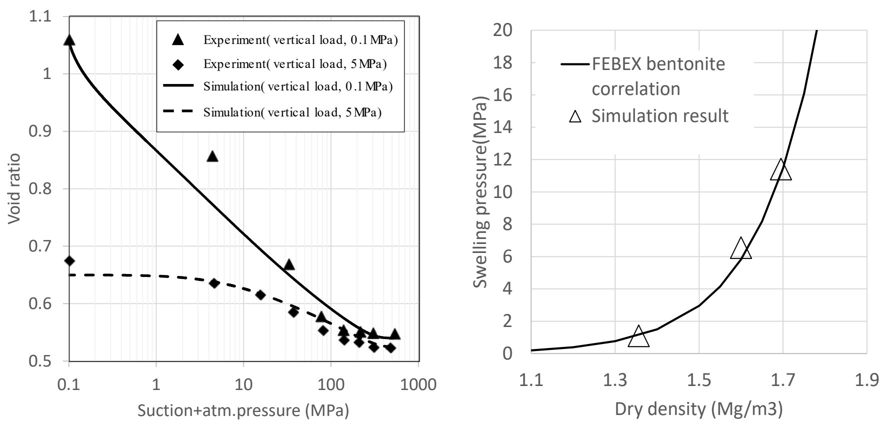
(a) Relative humidity (b) Temperature

Figure 1: simulation results of thermal and hydraulic behavior



(a) A linear elastic constitutive model (b) Unsaturated elasto-plastic constitutive model

Figure 2: Distribution of dry density after dismantling



(a) Suction controlled oedmeter test (b) Swelling pressure test

Figure 3: Simulation of suction controlled oedmeter test and swelling pressure test

Influence of Pore Water Vaporization on Saturation Process in the Buffer Material Coupled Thermo–Hydro–Mechanical Analysis

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Abstract

Objective

The saturation process in the buffer material is affected by the heat generated by the vitrified waste in the high-level radioactive waste geological disposal. Especially, the phase changes occurred in the pore water, such as water vaporization and dissolution of the pore air in to the liquid phase affects the water movement in the buffer material. Hence, it is important to evaluate the coupled thermo-hydro-mechanical (THM) behavior considering phase transformation of pore water in the buffer material.

Therefore, we carried out the coupled THM analysis to investigate the generation of water vaporization during the saturation process. Additionally, we discussed the influence of relative permeability as one of the gas phase advection properties.

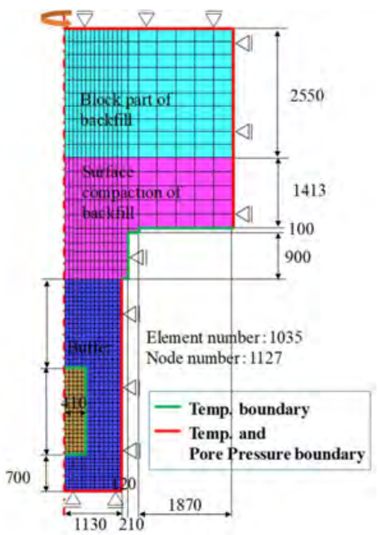

Fig. 1 Analytical model

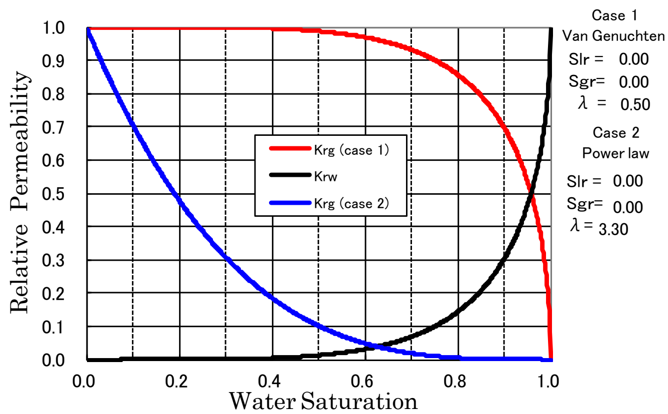

Fig.2 Relative permeability used in the analysis

Methodology

The coupled THM analysis code is CODE_BRIGHT. The analytical model is shown in Fig.1. The full scale in-situ engineered barrier system (EBS) experiment has been performed at the Horonobe Underground Research Laboratory (URL) consists of the simulated overpack, the buffer material and the backfill material.

This analytical model is two-dimensional axisymmetric model which simplified the EBS experiment. In this analysis, the buffer material is modeled by the Barcelona Basic model which is an elastoplastic constitutive model, and other materials are by linear elasticity. Material parameters were set based on the data obtained from laboratory tests. The temperature of the surface of the overpack was set at 100 degrees centigrade. Two cases of analyses were performed by varying the relative permeability, which is one of the two-phase flow parameters affecting the gas phase advection. The parameters used in the analyses for the relative permeability are shown in Fig.2.

Result & Discussion

Evolution of porosity in the buffer material obtained by the analysis is shown in Fig.3. An increase in the porosity around the heater was observed due to the water vaporization and resulted in a heterogenous distribution of the dry density. In addition, buffer material stress state has changed with the change in the relative permeability. This change in the parameter has also affected the amount of swelling of the buffer material, which resulted in an increase in the vertical displacement (Fig.4). As a result, the importance of considering the water vaporization in the analysis was demonstrated in order to more accurately assess the long-term behavior of the buffer material. Additionally, it was found that the evaluation of the relative permeability is also important for an accurate prediction.

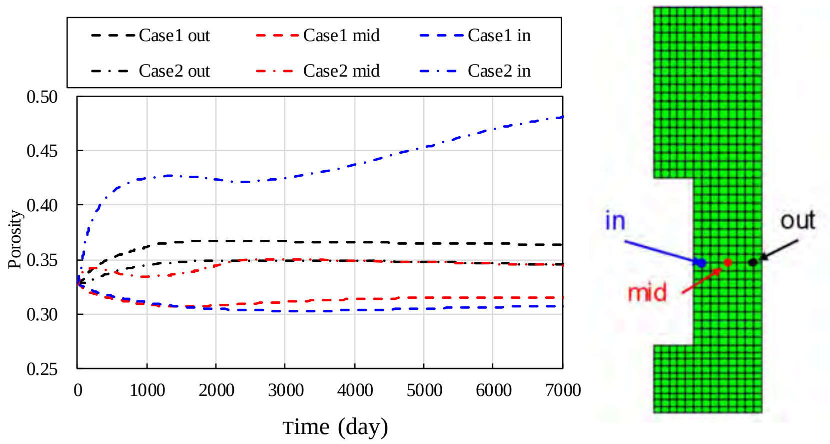

Fig.3 Evolution of porosity in buffer

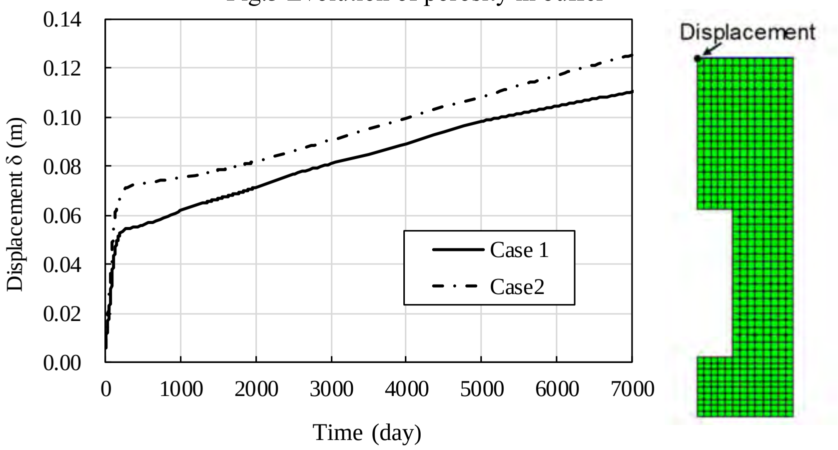

Fig.4 Vertical displacement of top of buffer material

Numerical Analysis of Coupled Hydro-Mechanical and Thermo-Hydro-Mechanical Behavior of Buffer Materials

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Abstract

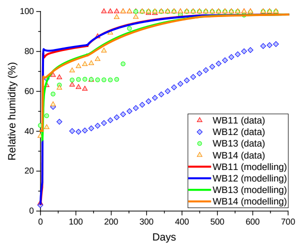
Numerical simulations of engineered barrier emplacement (EB) experiment at Mont Terri URL and full-scale engineered barriers experiment (FEBEX) at Grimsel test site have been carried out to analyze the HM and THM interactions in the bentonite barriers and to predict the change of the dry density which has great influence on the thermal, hydraulic and mechanical properties within the framework of Task D of the DECOVALEX-2019 project. A numerical approach of linking two existing codes, TOUGH2-MP which is a parallel version of TOUGH2 and FLAC3D was used to simulate the coupled HM and THM behavior of the buffer materials. TOUGH2-MP/FLAC3D can't calculate the coupled THM behavior simultaneously. The coupled problems should be solved sequentially and coupling parameters are transferred to each equation at specific intervals.

In this study, Barcelona Basic Model was used to simulate the mechanical behavior and to calculate the dry density changes in the buffer materials. Before the numerical simulations, BBM was implemented into TOUGH2-MP/FLAC3D by extension of an existing Modified Cam Clay (MCC) module in FLA3D. The MCC module was modified to BBM module by User Defined Model (UDM) capability and FISH function in FLAC3D for suction-dependent strains and net stress in unsaturated soils.

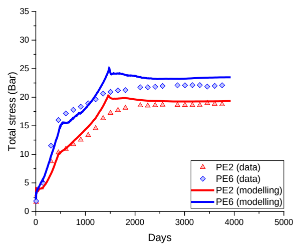
Figure 1 shows the results of EB simulations. The calculated Rh was sharply increased at the early stage and Rh was slowly increased after 2nd artificial hydration phase. In the EB simulations, the volume of water injected to buffer materials is unreliable information, because some leaks were observed at the experiment. Therefore, the Rh evolutions are not well captured during the early stage of hydration process, but Rh is approached to 100 % after several hundred Days. The calculated total pressure and upward displacement evolutions show good agreement with measured data. Calculated maximum upward displacement is similar to measured data, but the mechanical response is slightly late, because saturation response is late in the modeling. Measured dry density is significantly changed near the tunnel wall, however, these observation is not satisfactorily reproduced by the numerical simulations.

Figure 2 shows the results of FEBEX simulations. Temperature evolution shows good agreement with measured data at section D2. However, the calculated power is slightly underestimated before the heater #1 switched off, on the other hand, after the heater #1 switched off, the calculated power is slightly

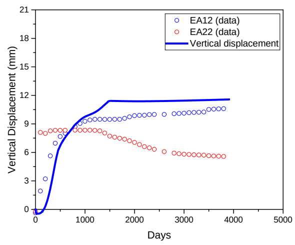
overestimated. The modeling results at SHP2 and SHP3 show similar Rh evolutions, but the calculated Rh near the liner is lower than measured Rh. The calculated dry density is underestimated near the heater, but the distribution of dry density shows good agreement with in-situ data in general.



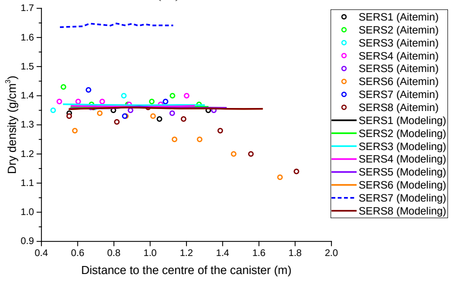
(a) Rh



(b) Total stress

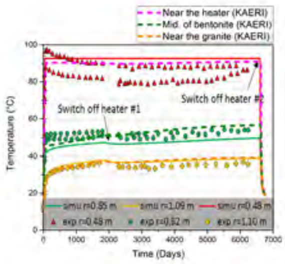


(c) Displacement

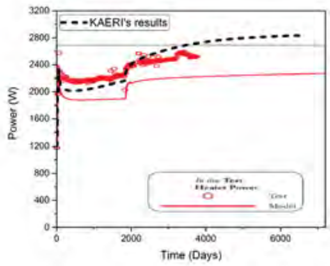


(d) Dry density

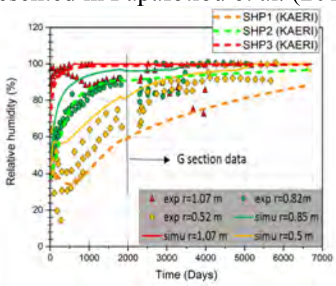
Figure 1: Simulation results of the EB experiment with measured data.



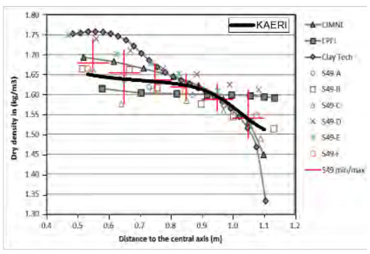
(a) Calculated temperature with modeling results presented in Papafotiou et al. (2017)



(b) Calculated power with modeling results presented in Sanchez et al. (2012)



(c) Calculated Rh on section H with modeling results presented in Papafotiou et al. (2017)



(d) Calculated dry density with simulation results presented in Papafotiou et al. (2017).

Figure 2: Simulation results of the FEBEX with modeling results presented in the previous studies.

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Modelling of Reactive Transport in Bentonite Considering Chemomechanical Coupling

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Abstract

Bentonite is the key component in the engineered buffer system of many radioactive waste repository concepts. Two of the crucial properties for the performance of bentonite, swelling pressure and porosity distribution, vary with the chemical environment. Therefore, also bentonite saturation and equilibration, as well as its transport properties depend on the chemical environment. This can change due to repository-induced processes (e.g., interaction with cement leachates), or external influences (e.g., melt water infiltration). Evaluation of literature data shows that swelling pressure drops by 75% when increasing ionic strength of the equilibrated NaCl electrolyte from 0 to 3 M for an effective montmorillonite dry density corresponding to 1500 kg/m^3 MX-80 bentonite. Swelling pressure of $CaCl_2$-equilibrated montmorillonite drops only by 40% for the same ionic strength increase (Jenni & Mäder, 2018).

In contrast to the well-known swelling pressure dependence on water composition, the chemical influence on the pore size distribution in confined systems has been poorly investigated. Experimental data indicates different average montmorillonite interlayer distances at different ionic strengths at constant dry density. Assuming a constant volume for solids and electrolyte, interlayer volume changes must be compensated by a corresponding change in some other type of porosity. Such an ionic strength-porosity coupling can explain differences in advective and diffusive transport commonly observed in clays tested with different background electrolyte concentrations, but at the same density (Jenni & Mäder, 2018).

Direct observations of porosity distributions at different chemical environments provide the basis for modelling this chemomechanical (CM) coupling. Such data is necessary to formulate or validate continuum models describing the CM behaviour of montmorillonite stacks ("microstructure"). Their changes in volume and swelling pressure (in confined systems) interact with the bentonite's coarser "macrostructure". This mechanical interaction is also modelled with the continuum approach, resulting in the prediction of discretised porosity distributions, bulk transport properties, and bulk swelling pressures. Chemical processes such as kinetic mineral reactions, speciation, and cation exchange are also considered and interact with the mechanical processes. The present project is based on three approaches:

- Processing of various experimental data from literature leads to estimates of interlayer distances and forces between basal sheets of montmorillonite at different ionic strength outside the interlayer and cation occupancy inside. The resulting data is used to either validate existing models, or to formulate CM dependencies, which are then implemented in the overall reactive transport model.
- Implementation of chemical processes into an existing approach based on the conceptual framework of the Barcelona Expansive Model.

- Extension of pioneering dual porosity reactive transport models (electrostatic controlled Donnan porosity close to clay sheets, and free water porosity): porosity distribution and swelling pressure are calculated considering the porewater chemistry.

So far, these models are focussed on fully saturated systems. First simplified CM simulations predict significantly different swelling pressures and diffusive transport at different ionic strength porewaters (Yustres et al., 2017), in line with experimental observations.

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Shaft Sealing Elements Made of Bitumen – Numerical Analysis of the Construction Process and Long-Term Behaviour

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Abstract

Within the R&D project ELSA 2, BGE TECHNOLOGY GmbH in collaboration with Technical University Bergakademie Freiberg has been developing shaft sealing concepts for repositories in salt and claystone formations. However, the minor knowledge about the in situ conditions of a (possibly) suitable German claystone formation complicates the design development of such shaft sealing concepts. Hence, open questions like the technical need of a partly removal of the Excavation Damaged Zone (EDZ) at shaft contour or the risk of an additional damage related to the hot installation of bitumen cannot be answered satisfactorily, today. Therefore, BGE TECHNOLOGY GmbH performed different numerical modelling of a generic, 800 m deep and 10 m wide shaft and shaft contour in a claystone formation. Main goals were the estimation of the depth of the EDZ, a quantitative analysis of the permeability changes inside the EDZ especially in combination with the thermal impact of hot installed bitumen as well as the prediction of the long-term flow behaviour of the bitumen. In Germany bitumen is considered as an additional sealing material inside shafts.

The analysis of the permeability of the shaft closure shows that the shaft sinking changes significantly the main characteristics of the permeation. As initial condition, a permeability parallel to bedding at least one magnitude higher than perpendicular to the bedding is assumed. Due to the shaft sinking permeability within the first 10 cm of the shaft contour increases by four of magnitude. Inside this highly damaged zone the main flow direction changes from parallel to bedding to parallel to shaft contour. Plastic deformation of the rock next to the shaft can be considered as the main reason for a change in permeability. A further analysis of the effects related to thermal impacts based on bitumen installation and a partly removal of the EDZ show that the damages induced by the thermal impact are marginal compared to the removal of additional rock material. The EDZ around the shaft is already characterized by a highly increased permeability due to the shaft sinking. An additional removal of rock is related to an additional reorientation of the stress field. The removal of the first 50 cm of rock from the shaft contour increases the permeability inside the remaining EDZ.

The second part of the investigation focuses on the fluid-like long-term behaviour of bitumen. The long-term behaviour of bitumen, which is characterised by very high and strongly temperature depending viscosity, inside a filled shaft was investigated. The permeability of the EDZ is the main parameter for the flow inside the EDZ, beside viscosity.

The numerical modelling provides additional insight regarding the conditions at shafts in claystone formations and the conditions during sealing of such shafts. Size and quality of the EDZ is mainly influenced by the deformation and the stress conditions due to shaft sinking. Additional thermal impacts have only marginal influence. The lessons learned will help to improve the shaft sealing concepts for a potential German repository in claystone formations.

Parameter Study of Bentonite Based Drift Sealing Concepts in German Repositories in Crystalline

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Abstract

Sealing of access drifts creates an additional barrier between the shaft sealing and the near field sealing systems inside the emplacement areas. Within the framework of the R&D project "Development of a safety and verification concept for a repository for heat-generating radioactive waste in crystalline rock in Germany" (Christa II), BGE TECHNOLOGY GmbH has developed a conceptual design for drift seals. The drift sealing has to provide a sufficient low hydraulic conductivity as well as a long-term stability with regard to the chemical composition of the pore water and a mechanical stability against the rock and pore water pressure. Requirements on the thermal properties of the sealing construction seem to be less important due to the large distance to the heat producing waste packages. The conceptual design includes concrete based abutments and main sealing elements made of bentonite. For the bentonite sealing different design variations are in consideration, see Fig. 1. Bentonite can be installed A) in combination with bitumen as an element with short term sealing function and with a gravel filled chamber to homogenise saturation, B) as a single sealing element.

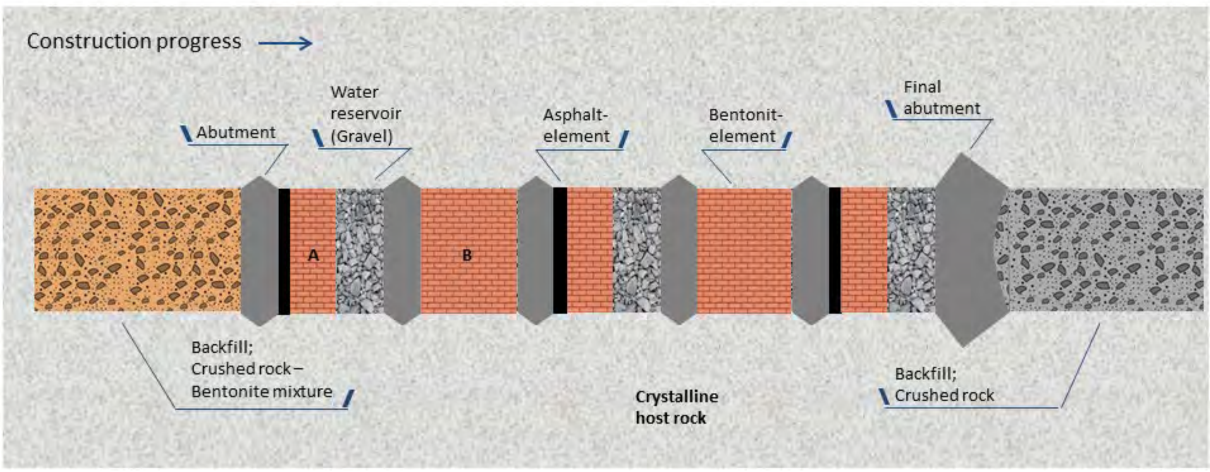

Figure 1: Conceptual design of a main drift seal for German repositories in crystalline host rock with different designs of bentonite based sealing elements, denoted as **A** and **B**

Bentonite possesses such properties as swelling and radionuclide retardation, which are fulfilled under water saturated conditions. Volume expansion of bentonite as a result of swelling process can provide the sealing of the contact zone between seal and host rock. The main goal of this study was to quantify the duration of water saturation of various bentonite sealing plug configurations under isothermal conditions.

Due to different conditions of water inflow to the bentonite element in two sealing design variations, it is essential to investigate the influence of material parameters of bentonite on water saturation evolution. Using the computer code TOUGH2, three-dimensional simulations were performed to simulate the flow of water and air in a simplified drift seal model. Results of modelling will help to understand the importance of material parameters for the flow with special regard to the design of the sealing constructions.

The Hydraulic Performance Evolution of Compacted GMZ Bentonite Corroded by Cement Degradation in a HLW Repository Condition

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Abstract

After the long term operation of a high-level radioactive waste repository, the bentonite as buffer/backfill material will undergo some chemical effects resulting from the chemistry of site water and the alkaline solutions produced by cement degradation. To investigate the hydraulic conductivity of compacted GMZ bentonite under the chemistry conditions of the site water and cement degradation water, constant-volume permeability tests were carried out. Before the tests, three types of pore water were prepared to simulate site groundwater (synthetic Beishan Site Water - BSW) and two cement solutions (Young Cement Water – YCW and Evolved Cement Water – ECW). According to the results, the effect mechanism of chemical solutions on the hydraulic conductivity of GMZ bentonite was demonstrated.

Results show that: 1) The hydraulic conductivity of compacted GMZ bentonite increases with the increase of the concentration of infiltration solution. 2) The hydraulic conductivity of bentonite with the infiltration of cement solutions is higher than that in the case of synthetic site water, which may be due to the dissolution of montmorillonite in the reaction between alkaline solution and bentonite.3) With the extension of reaction time, the hydraulic conductivity of bentonite decreases resulted by the decrease of the porosity, which may be due to that the formation of some colloidal or amorphous secondary minerals coat on the surface of bentonite.

The hydraulic property of compacted GMZ bentonite can be reduced by cement solutions in the long-term operation of repository.

Impact of Earthquakes on Geotechnical Barriers

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Abstract

To prevent the penetration of fluid into an emplacement area in an underground repository, the integrity of the geotechnical barriers under different safety-relevant scenarios, e.g. impact of an earthquake, needs to be considered. Gravel is to be implemented in several sections of the shaft sealing elements to act both as porous reservoir and as abutment for sealing elements installed in top of it. The objective of the present study is to determine to what extent the settling of a gravel column due to an earthquake can be estimated by means of numerical modelling.

In order to realistically simulate the mechanical properties of gravel particles, the general purpose Distinct-Element modelling framework PFC3D was used. Representative particle samples of different sizes were generated based on a grain size distribution of rail ballast. Each particle consists of two spheres of the same size (so called clumps) and a linear contact model simulates the friction and displacement behaviour. Calibration tests were carried out to determine the relevant input parameters of the constitutive model. The validation of the particle model was done by the simulation of the gravitational settling behaviour and the silo effect of a 45-meter-high gravel column and comparing it with the analytical solution. It was shown that the processes that are responsible for the silo effect are simulated realistically. The characteristic stress gradient across the height of the column is comparable with analytical results based on Janssens's equation. In order to reduce the calculation runtime during the following dynamic calculations, it was necessary to decrease the number of particles by using a grain size scaling. Since the size scaling can have an influence on the results, comparative calculations with different scaling factors were carried out. A scaling factor of 6 was found as a good compromise between calculation runtime and accuracy.

In order to enable a realistic simulation of the far field during the dynamic calculations, the PFC3D particle model was coupled with the continuum code FLAC3D. FLAC3D simulates the rock mass (200m x 200m x 50m) around the gravel column in which the gravel column is embedded. FLAC3D transfers the seismic load at the model boundaries to the PFC3D gravel column and additionally allows the setting of realistic dynamic boundary conditions (Far-Field-Boundaries) with the aim of adsorbing waves at the model boundaries. The earthquake impulse with duration of 5s was generated using seismological parameters recorded from earthquake profiles of northern Germany and applied at the lower boundary of the model by a P-wave and time-delayed S-wave stimulation. First results show that the earthquake impulse is too low to cause a critical settlement for the gravel column.

Modelling of Atmospheric Cement Carbonation in Disposal Containers for Low- and Intermediate-Level Nuclear Waste

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Abstract

During the operating phase of a geological repository for low- and intermediate-level nuclear waste, the ventilation of the drifts and shafts will cause the atmospheric carbonation of cementitious materials. This process is particularly relevant to disposal containers made of concrete.

The principal goal of this study is to quantify the extent of carbonation, expressed as the depth of the carbonation front, in cementitious disposal containers during the operating phase of ca. 150 years taking into account both hydraulic (drying, etc.) and chemical processes. Of particular interest are two different types of concrete that are based on either CEM V or low pH cement binders. Beyond the quantification of carbonation of concrete with different cement properties and in different atmospheric conditions, the current study also aims at gaining process understanding, particularly concerning the following aspects:

- Contributions of vapor diffusion and liquid flow in the drying process in different atmospheric conditions and with different concrete hydraulic properties
- Influence of kinetics of mineral reactions and surface complexation reactions on the progress of the carbonation front
- Evolution of the concretes' transport porosity due to carbonation-induced mineral transformations
- Evolution of effective diffusion coefficients due to drying-induced saturation changes and carbonation-induced porosity changes

For the investigation of cement drying and its influence on carbonation we use TOUGH v.3 [Jung et al., 2018b] with EOS4 [Jung et al., 2018a], which includes vapor transport and vapor pressure lowing. The geochemical processes are studied by using the geochemical modelling framework PHREEQC [Parkhurst and Appelo, 2013], the simulations feature a batch reactor, in which increasing amounts of CO_2 react with the cured cement paste. By combining the results and findings from TOUGH and PHREEQC simulations in a reactive transport model we develop a finite element model with simplified geochemical reactions using the PDE solver FlexPDE [PDE Solutions, 2019]. The simplifications are qualified using the finite volume reactive transport code CrunchTope [Steefel et al., 2014]. Variations of crucial model and design parameters are investigated using the MOAT-method [Morris, 1991].

One of the key findings is that the dynamics of the drying process can be decoupled from carbonation due to the much faster progress of the drying front compared to the carbonation front in the investigated concretes and environmental conditions (T+, hygrometry, etc.). With respect to the position of the carbonation front, the simple parabolic carbonation law [Vagelis G. Papadakis, 1991] gives comparable results to the more sophisticated models using FlexPDE and CrunchTope. However, the latter provide the flexibility to integrate additional processes such as detailed mineral kinetics and porosity changes, once reliable experimental data become available.

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Coupled HM and THM Interactions in Bentonite Engineered Barrier Systems

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Abstract

The EB Experiment (Engineered Barrier Emplacement Experiment) and the FEBEX (Full-scale Engineered Barrier Experiment in Crystalline Host Rock) "in situ" test were two different types of full-scale engineered barrier systems in Switzerland. The surrounding rocks of the EB test and the FEBEX test are clay and granite, respectively. The EB experiment only considered the Hydro-Mechanical interactions since the hydration scenario was very complicated due to artificial injection. The FEBEX experiment considered the effect of Thermal-Hydro-Mechanical processes on the evolution of the bentonite blocks. In both experiments, the relative humidity, temperature, and total stress evolutions and their distributions have been measured, and the dry density, saturation and mass water content have also been observed after dismantling.

The goal of this work is to present the EB and the FEBEX simulation results performed by the in-house simulator HYDROGEOCHEM (HGC). The variably saturated flow module, thermal transport module and linear geomechanics module which accounts for bentonite swelling effect were considered in the simulations. Sensitivity studies have been performed to investigate the bentonite properties. We can qualitatively and quantitatively predict the most experimental results. The conservation of solid mass and gas vapour will be included in the future to better address the dry density distribution and relative humidity near the heater.

A Multi-Level Pore Scale Reactive Transport Model for The Investigation of Combined Leaching and Carbonation of Cement Paste

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Abstract

In deep geological disposal interaction of cement with clay pore-water is expected at cement-clay interface. The clay pore water has significantly lower pH compared to cement paste pore water and it might contain dissolved CO2. As a consequence, interaction of cement paste with clay pore-water might lead to the dissolution of portlandite and decalcification of calcium silicate hydrates (C-S-H). These leached calcium ions, would further react with dissolved carbonate ions in the clay pore-water leading to precipitation of calcite which can block transport pathway. Therefore, in order to determine long-term evolution of cement-clay interface it is essential to understand this complex interplay between leaching and carbonation reaction mechanisms.

With aim to improve understanding of cement paste microstructure evolution resulting from competition between carbonation and leaching in this study a three-dimensional multi-level pore-scale reactive transport model has been developed. In the proposed model the capillary pores are explicitly resolved while the C-S-H phase containing nano-scale gel porosity is treated as diffusive porous media. Thus, with the developed model the simultaneous evolution of both of these pore-spaces can be explicitly captured. The governing equations for the mass transport are solved using a lattice Boltzmann method based reactive transport solver, where chemical reactions are accounted assuming thermodynamic equilibrium. With the developed model simulations were carried out to study evolution of virtual 3D cement paste microstructure under combined carbonation and leaching. These simulations show a good quantitative agreement between modelling and the experimental observation at the initial stages. For longer times, the modelling result and experimental observations start to diverge significantly, because the kinetics of C-S-H dissolution and calcite precipitation are not well constraint due to the lack of reliable kinetic parameters.

HM Coupled Modeling of Gas Migration in Buffer Materials of Deep Geologic Repository for Nuclear Waste

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Abstract

In a deep geologic repository for radioactive waste, bentonite is a material of buffer with low hydraulic conductivity, high thermal conductivity and suitable swelling pressure which can efficiently retard the gas propagation from waste canister into the buffer or the host rock. Thus, understanding gas migration in buffer is a key issue in the safety assessment of repository performance. Our simulation study for gas migration in buffer is performed by in-house THMC coupled model in which only the multiphase-flow module and geo-mechanics module for visco-elastic materials are chosen for the presented HM coupled modeling. We design our simulation settings based on the gas-injection experiments performed by British Geological Survey (BGS). BGS provided two laboratory scenarios for gas injecting into a compact and saturated bentonite confined in a pressure vessel. Injected gas (Helium) will accumulate to enter the saturated bentonite when its pressure reach to a criteria and the gas will be detected by gas filters which we call the timing “breakthrough”. They find out the total stress will reach to the maximum value right after breakthrough but not exceed the gas injection pressure. It is shown that our simulation results can catch the lab-testing peak values of total stress and porewater pressure as well as the lab-testing timing of breakthrough. Moreover, our simulation results of both total stress and porewater pressure can well describe the decay trend after breakthrough. From the comparisons of our simulation results with the experimental data, our HM coupled modeling can qualitatively and quantitatively demonstrate gas motion in the buffer and its corresponding mechanical contributions, but the gas outflow is not well reproduced, neither other teams of DECOVALEX-2019. Imbedded fractures will be included in our future geo-mechanical module to better address the outflow of gas migration.

Development of a Poro-Elastoplastic (with Damage) Mathematical Model to Simulate Two-Phase Flow in a Swelling Geomaterial

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For submission to the DECOVALEX-2019 Symposium on Coupled Processes in Radioactive Waste Disposal and Subsurface Engineering Applications Symposium in Brugg, Switzerland (November 4-5, 2019)

Abstract

In a deep geological repository (DGR) for the long-term containment of radioactive waste, gases could be generated through a number of processes. If gas production exceeds the containment capacity of the engineered barriers or host rock, these gases could migrate through these barriers and potentially expose people and the environment to radioactivity. Expansive soils, such as bentonite-based materials, are currently the preferred choice of seal materials. Understanding the long-term performance of these seals as barriers against gas migration is an important component in the design and long-term safety assessment of a DGR.

This study proposes a mathematical hydro-mechanical (HM) model for migration of gas (two-phase flow) through a low-permeable heterogeneous swelling geomaterial. It is based on a theoretical framework of poromechanics, applies Darcy's Law for both the porewater and poregas, and incorporates a modified Bishop's effective stress principle. The study expands upon previous work by the authors, by considering the use of a non-linear poro-elastoplastic model with damage to simulate two-phase flow. Additionally, the model incorporates the Klinkenberg effect, a non-linear swelling stress and the inclusion of heterogeneity. Using the Finite Element Method (FEM), the models were used to simulate 1D and 3D flow through a low-permeable swelling soil. The results were validated against experimental results found in the current literature for a confined cylindrical sample of near-saturated bentonite under a constant volume boundary stress condition. Based on the results, the mathematical model looks promising, and provides insight into mechanisms contributing to multiphase flow.

Applicability of an Empirical Model for Pressure-Induced Permeability Change in Saturated Bentonite Using OpenGeoSys

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Abstract

It is important to understand gas transport processes when considering the geological disposal of radioactive waste (Rodwell 1999). If the rate of gas production, generated by corrosion of the waste/repository containment and the radiolysis of water, exceeds the rate of diffusion, dilatancy-controlled gas flow may occur (Harrington and Horseman 1999) in low tensile strength materials such as clays and bentonite due to high gas pressures.

To understand gas migration processes in saturated material, laboratory and *in-situ* gas injection tests have been conducted. This poster presents numerical model results of several such gas tests with different experimental setups on compacted MX-80 bentonite carried out at the British Geological Survey (BGS) (Harrington et al. 2017, Tamayo-Mas et al. 2018) using finite element code OpenGeoSys (Kolditz 2012, Bilke et al. 2019). The first experiment is a simple homogeneous flow test, performed under a constant volume boundary condition, is comprised of two stages i.e. hydration followed by gas injection using helium as the test permeant. Since the gas entry pressure is difficult to define due to interfering mechanisms such as the displacement of water from the saturated pore, the gas breakthrough pressure was identified when a measurable outflow was observed. After breakthrough, the injection pump was stopped and gas pressure allowed to evolve. During the entire experiment, stress, flow and pore pressure were continuously monitored to provide data for coupled analysis. The second experiment is a spherical gas flow initiated from the center of the bentonite cylinder.

A coupled hydro-mechanical model has been developed to simulate the dilatancy-controlled gas flow in saturated argillaceous rock (Xu et al. 2015). The gas migration in the porous medium is controlled by the gas pressure, the hydro-mechanical states (saturation, stress), and the material properties (permeability, porosity, deformation behavior). The effective stress is defined by using the saturation as weighting functions for the gas and water pressures. The relationship between capillary pressure and water saturation is described by van Genuchten function (van Genuchten 1980) and the relative permeabilities to gas and water by the approach of Mualem (Mualem 1976). Under these assumptions the intrinsic permeability will increase significantly if the injection pressure is higher than the critical pressure, which itself depends on the minimal principal stress (or confining pressure) acting on the sample and gas entry pressure in the pore space. .

Within the project DECOVALEX-2019 the implemented model was used to simulate the abovementioned BGS experiments. The samples are modelled as a continuum porous medium Figure 1. The gas injection

pressure was used as boundary conditions. It could be shown that the models can simulate the measured gas breakthroughs and the subsequent outflow rates.

The results show that concept can be applied to the bentonite MX-80. With regard to the development of the stress and the gas flow rate, the gas breakthroughs could be quantitatively simulated in terms of their timing and their intensity by adapting the concept. This implies that the intrinsic permeability of the compacted bentonite sample increases its original value under the high gas injection pressure. In addition, the shut-in effect with an overall pressure compensation in this two-phase flow system can be observed both in the measurements and in the simulations.

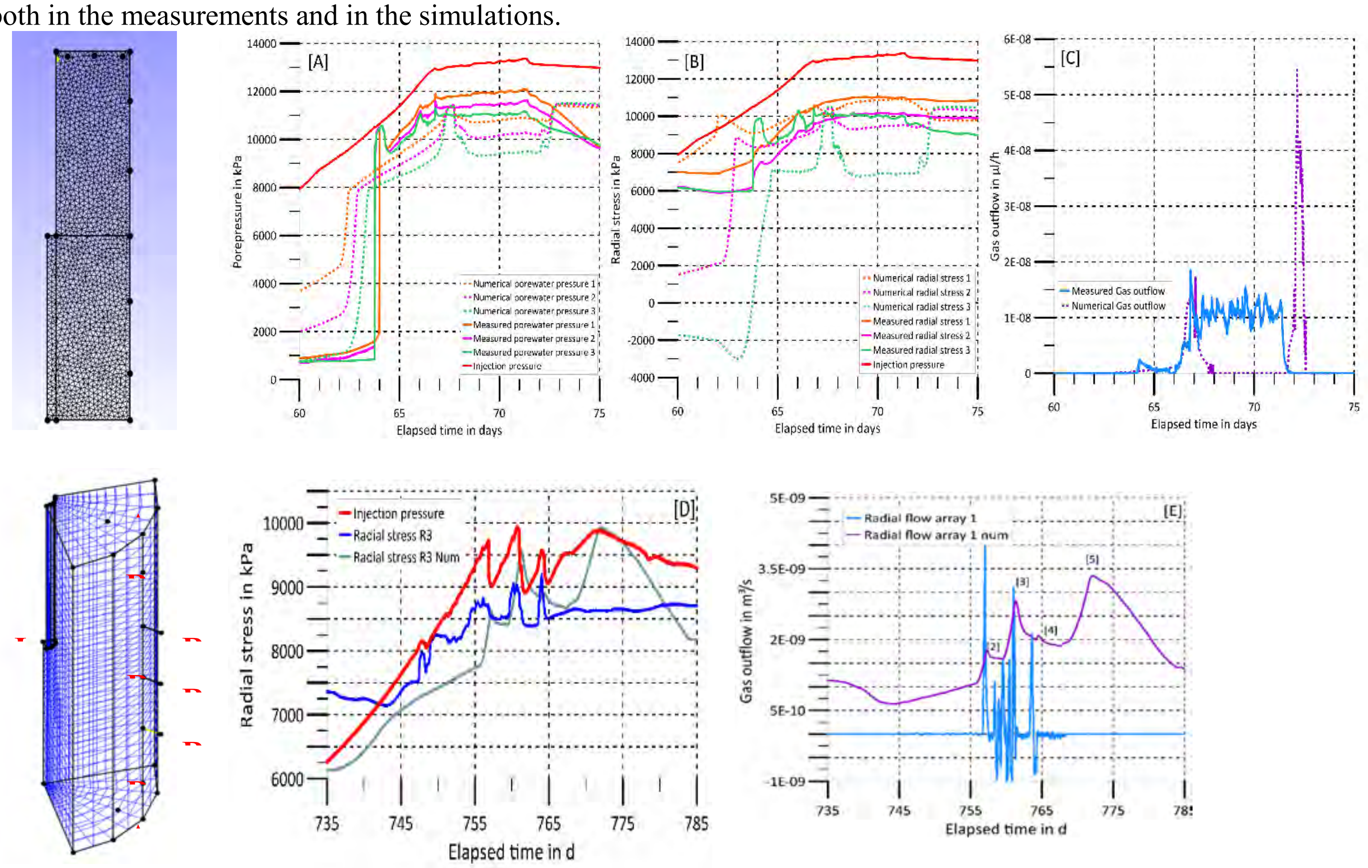

Figure 1: upper model two-dimensional, rotational symmetric conversion of the homogeneous gas flow a) comparison of the pore pressure development, b) comparison of the stress evolution, c) comparison of the outflow development
lower model three-dimensional implementation of the spherical gas flow d) comparison of the stress development, e) comparison of the outflow development

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Nonlinear Dynamics of Gas Migration in Compacted Clay

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Abstract

Bentonite has been proposed as a buffer/barrier material for nuclear waste disposal. Gas generation from metal corrosion and its potential impact on material structural integrity are an important concern in long-term waste isolation. To investigate the underlying mechanism for gas migration in a buffer material, gas injection experiments on bentonite Mx80-D were conducted at the British Geological Survey. The experimental data show that gas migration in a water-saturated compacted clay material exhibits rich nonlinear dynamic behaviors as the injection gas pressure varies: from a constant flow to a periodic flow and eventually to a chaotic behavior (Figure 1). To test if the flow rate variation is truly chaotic, we have performed a time series analysis for gas inflow and outflow measurements. The time series is divided into four segments based on the time variation of injection pressure. We have calculated the embedded dimension using the false nearest neighbor method for each segment. It is found the embedded dimension for the gas migration phenomenon ranges from 3 to 4. We also show that in the embedded space the flow rate seems to possess an internal structure (a chaotic attractor), i.e., not completely random (white noise), indicating a deterministic chaotic behavior. This is further confirmed by the calculation of the spectrum of Lyapunov exponents for gas inflow, which indicates a combination of deterministic and stochastic chaotic components. To explain this dynamic behavior, we have developed a chaotic model based on the concept of delay logistic model. In this model, we show that, given a low permeability of the material, the dominant mechanism for gas migration is first to nucleate a bubble and then push the bubble through the clay matrix through dilation and fracturing. In the wake of bubble movement, matrix compression and fracture healing may also take place. The chaotic model thus provides a new perspective for modeling gas migration in low-permeability materials.

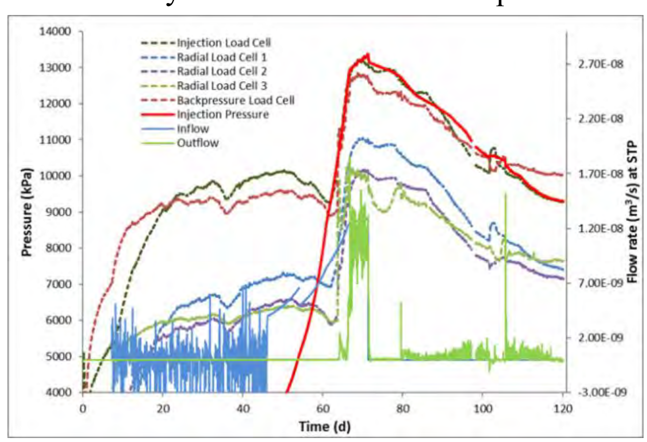

Figure 1. Experimental measurements of gas inflow and outflow rates in water-saturated compacted bentonite Mx80-D.

Advective Gas Flow Modelling Using Mechanical Damage Model

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Abstract

In the case of a repository for radioactive waste, the corrosion of canisters under anoxic conditions generates hydrogen, carbon dioxide, hydrogen sulphide, and methane (Harrington et al., 2017). At this time, if the gas production rate exceeds the gas diffusion rate in the pores of the engineering barrier, the pressure of the gas continuously increases inside the engineering barrier, and a sudden gas flow occurs when the specific pressure is reached. Although classic two-phase flow models are highly extended and employed, they are not able to describe the full complexity of gas migration processes, and therefore, new and novel numerical representations for the quantitative description of advective gas flow in clay-based repository systems are required. Therefore, in this study, we developed a gas migration model using a mechanical damage model, and for a model validation, we have attempted to model the movement of gas in 1D and 3D experiments performed under controlled laboratory conditions.

In order to model the gas migration phenomena, we adopted elastic damage model by Tang et al. (Tang et al., 2002), and in this model, the elastic modulus degrades gradually as damage progresses. Permeability is calculated by the superposition of undamaged permeability and damaged permeability; undamaged permeability is a function of the porosity and damaged permeability is a function of the damage variable. For the gas injection pressure, artificial gas injector is modelled and gas injection pressure is calculated with gas volume in injector, inflow added to the injector, and outflow into the bentonite sample based on the ideal gas law.

Figure 1 shows the results of numerical modelling of 1D and 3D experiments. Figure 1(a) shows pore pressure evolution at injection filter and back pressure filter in 1D experiment. The trend of peak and post-peak pressure is well matched. For the outflow of gas in 1D experiment (Figure 1(b)), we captured the single major peak, however, the flow rate is less than experimental result. Figure 1(c) shows injection pressure evolution in 3D experiment. Trend of injection pressure has a good fitting with respect to experimental results. However, fluctuation due to the damage is not modelled because damage of bentonite is preserved and outflux is continuous in the numerical model (Figure 1(d)).

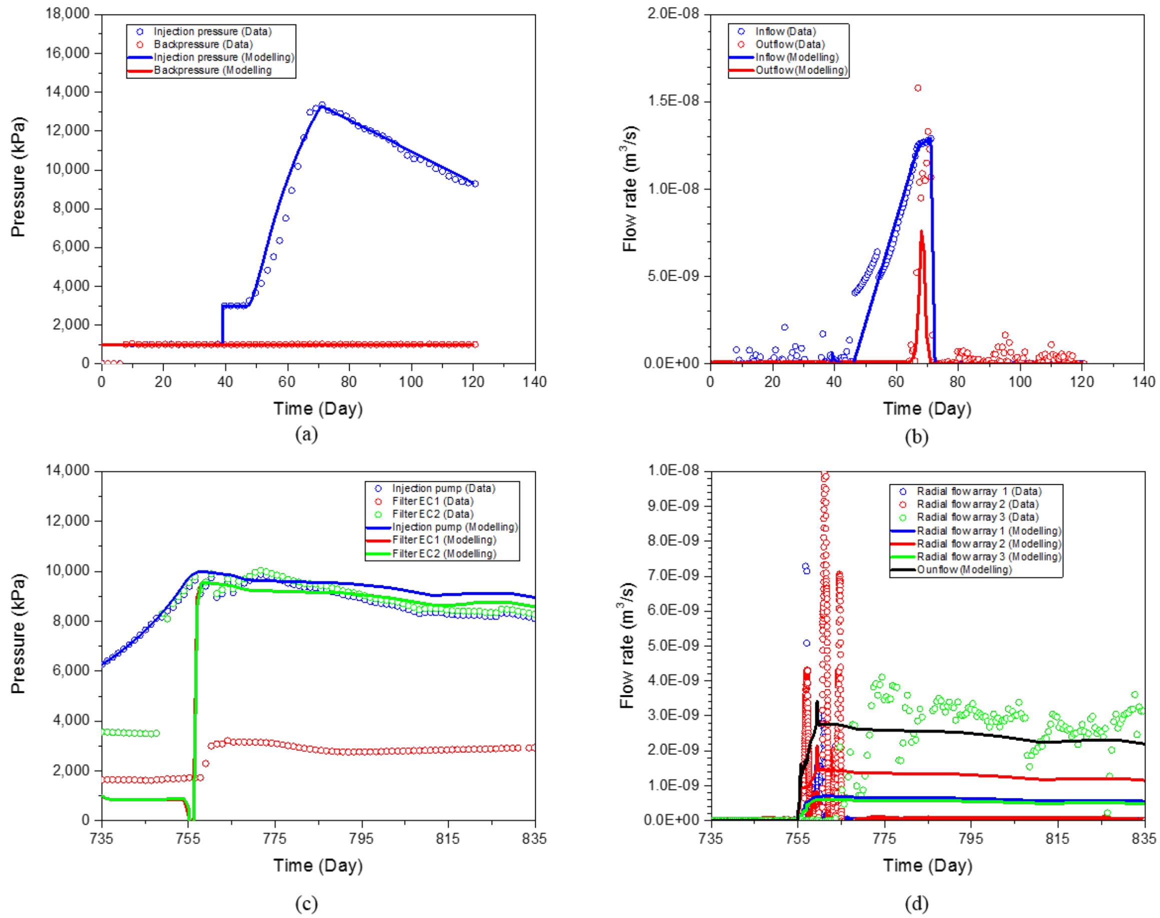

Figure 1: Modelling results from a 1D and 3D gas migration experiment: (a) evolution of injection gas pressure in 1D experiment; (b) inflow and outflow of gas in 1D experiment; (c) evolution of injection gas pressure in 3D experiment and (d) outflow of gas in 3D experiment

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Modelling Gas Flow in Clay Materials: Analysis of Boundary Conditions, Flow Direction, Material Heterogeneity, and Anisotropy

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Abstract

Gas injection tests performed on compact bentonite was carried out at the British Geological Survey. The test is composed of two stages: sample's hydration and gas injection. After gas breakthrough and a period of gas flow through the sample, the injection pump was stopped whilst stresses and pore pressures were continuously monitored. Different tests were performed according to the gas injection system: injecting the gas in one axial side of the sample or in the center with consequent spherical flow generation. A coupled hydro-gas-mechanical 3D numerical model has been developed to simulate the gas injection test and to achieve similar gas pressure responses. Permeability distribution depends on the initial heterogeneity (see Figure 1) and variations induced by gas pressure build up in a deformable system under constant volume conditions. The initial permeability heterogeneity condition assumed along with the proposed model approach including the calculation of permeability variation in space and time let to achieve results with preferential gas flow paths. Sensitivity to parameters and boundary conditions was required in order to obtain the final model calibration with demonstrating the complexity of the problem and followed methodology. In addition, different hypothesis of material anisotropy were considered achieving promising results.

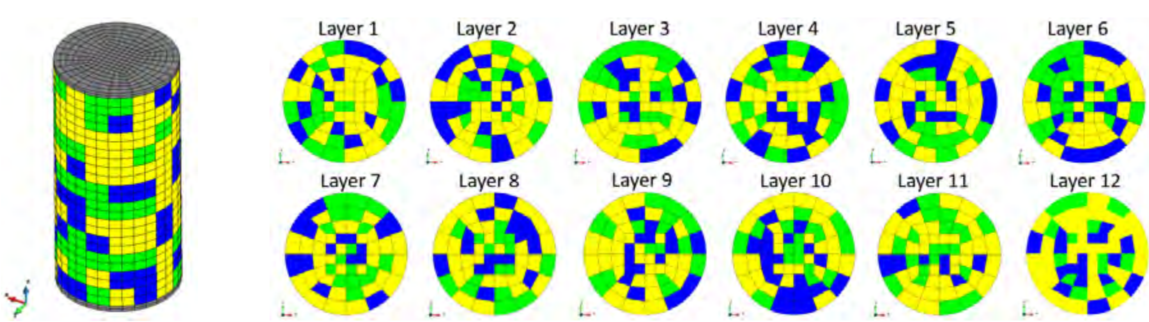

Figure 1: Layer-by-layer random permeability distribution (with different weighting): Green: $k_0 = 1{\times}10^{-19}$ m^2 (1/6 weighting), blue: $k_0 = 1{\times}19^{-20}$ m^2 (1/6 weighting), and yellow: $k_0 = 1{\times}10^{-21}$ m^2 (2/3 weighting).

TOUGH-RBSN Modeling Of Generation Of Discrete Gas Flow Pathways In Bentonite

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Abstract

Gas migration in clay-based buffer materials has been of great interest as a potential factor of safety issues in geological repositories for radioactive waste. A number of relevant experimental studies, for both in-situ and laboratory samples, have been conducted to capture complex mechanisms in the gas migration phenomena. In parallel, various modeling approaches have been proposed for the interpretation of the experimental results and for the analysis of gas release scenarios from the geological repositories in the context of long-term safety assessment. However, the predictive capabilities of the gas transport models are yet limited, and basic mechanisms of gas transport in bentonite are not sufficiently understood to provide the ground for robust conceptual and quantitative models.

As an active participant in Task A of DECOVALEX-2019, we have used the TOUGH-RBSN simulator to model coupled hydro-mechanical (HM) processes of gas pressure-induced fracture and fracture-assisted gas flow. In the numerical framework, sequential two-way coupling procedures between two different modeling codes, the TOUGH2 multi-phase flow model and the Rigid-Body-Spring Network (RBSN) geomechanics model, are established, and a discrete fracture network (DFN) approach is adopted to represent the abrupt permeability enhancement along distinct flow paths created by fracture propagation. In order to address complex mechanisms in the strongly coupled HM processes, we integrated various multi-physical conceptual models, such as poro-elastic strain/porosity changes, moisture swelling/shrinkage effects, multi-phase flow with gas entry threshold, and aperture-dependent permeability change in fractures.

Linear and spherical gas flows in compacted bentonite samples are simulated to validate the TOUGH-RBSN models against laboratory experiments. The simulation results, such as pressure evolutions, gas outflow, and stress responses, are quantitatively compared with the experimental data. The TOUGH-RBSN models demonstrate plausible descriptions of physical phenomena by matching the key observations during gas entry and breakthrough in the experiments. In addition, discrete fracture patterns and pressure distributions are presented for qualitative interpretations. Thus, this study can provide insights into the complex mechanisms of gas migration in bentonite clay.

Modelling Fluid Flow in an Excavation Damage Zone

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Abstract

Hydraulic interference tests, which were conducted between shallow drill holes within the TAS04 experiment (Forsmark, Sweden), are numerically simulated using COMSOL Multiphysics®. These experiments aimed at describing the transmissivity changes induced by excavating a tunnel for spent nuclear fuel in crystalline rock. The modelling has been conducted in the framework of the Decovalex2019 project, Task G (https://decovalex.org/task-g.html).
Two methods have been tested in order to get the best fit between the modelled and measured pressure responses in the interference tests. The first method targets at implementing as much existing fracture data (modelled, observed, and measured fracture sets) as possible into COMSOL Multiphysics®. The second approach targets at replacing these fracture sets by volume elements with higher permeability because importing large amounts of fractures into COMSOL Multiphysics® creates problems in generating the model geometry and later discretisation. Particularly, irregular shaped fracture sets require smoothing, translation and selective deletion of single, isolated fractures to be importable/usable. Efforts have been made to minimise the geometric error resulting from these manipulations. The manipulated fractures have been assigned a stress-dependent aperture value that directly influences the permeability of the fracture given by the cubic law.
Because of the problems with large amounts of fractures, the second approach tries to replace the fractures by finite volumes that get a stress-dependent permeability value. While being superior in model set up, this method comes with a higher computational effort.
Both methods yield a significant difference between modelled and measured pressure responses. Differences in pressure might amount up to 300% in some cases.
While the boundary conditions of the model are well-defined from in-situ measurements, the fracture data might not fully represent the excavation damage zone, or the manipulations might have caused small discrepancies that lead to wrong fluid flows along the fractures. Replacing the fracture data by volumes caused a pore pressure distribution suitable for porous rocks but does probably not represent the fluid flow in fractured crystalline. However, both methods do also show good agreement in some cases. Particularly when low pressures were measured in the field.

Modeling the Groundwater Recovery Experiment in Tunnel with a Discrete Fracture Fetwork

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Abstract

When selecting a geological disposal site for high-level radioactive waste (HLW), the conditions and behavior of the geological environment must be considered. Constructing and operating a large underground facility, such as an HLW repository, will likely influence the geological environment for decades; therefore, the environment's post-closure recovery after backfilling of an underground facility is an important aspect for assessing the safety of geological HLW disposal. Furthermore, the recovery of the environment surrounding the fractured crystalline rock is assumed to be a complex process because the fractures are distributed heterogeneously in the rock mass. Therefore, it is important to understand the rock mass's fracture characteristics to predict the environment's recovery.

The Mizunami Underground Research Laboratory (MIU) was constructed by the Japan Atomic Energy Agency (JAEA) in the Cretaceous Toki granite of the Tono area in Central Japan. The JAEA has conducted the groundwater recovery experiment in tunnel (GREET) at the MIU to investigate the environmental recovery process. GREET was a preliminary test to assess the recovery process at a drift scale, prior to studying it at a facility scale. The closure test drift (CTD) is situated at a depth of 500 m and has a volume of approximately 900 m^3. Prior to the CTD's construction, a pilot borehole, adjacent and parallel to the CTD, was drilled to estimate the baseline hydraulic and hydrochemical conditions. It was then used to monitor both these conditions and any changes caused by the CTD's construction. The gallery's geology was mapped to characterize the fracture distribution, additional monitoring boreholes were drilled, and a watertight plug was installed at the CTD's entrance. We then observed the changes in the geological environment while the CTD was filled with water and subsequently drained.

This study presents the method used to construct a discrete fracture network (DFN) model from the GREET's in-situ data. In particular, we investigate how to determine the DFN model's parameters, such as the fracture density, fracture size distribution, and fracture transmissivity distribution. Results show that this modeling approach can reproduce the statistical fracture distribution around the CTD by focusing on water-conducting fractures. In addition, we conditioned the stochastic fracture parameters based on data acquired from drift wall mapping, BTV surveys, and hydraulic packer tests. We also used a conditional DFN model to simulate the inflow into the drift and groundwater pressure changes around the CTD after drift excavation. These results demonstrate that the conditional DFN model was better able to reproduce the observed data than the previous DFN model. In addition, we have scaled up the

conditional DFN model to create an equivalent continuous porous media model for flow and transport simulations of the CTD being filled by and drained of water. Results obtained herein indicate that DFNs can be a good way to model drift environments.

Thermo-Mechanical Coupled Modelling of a Long-Term Evolution of the Final Repository for Spent Nuclear Fuel at Forsmark, Sweden

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Abstract

In this study, we present a 3D numerical modelling approach applied to the long-term safety assessment of an underground repository for final disposal of spent nuclear fuel. The proposed site is located in a Proterozoic, crystalline basement. The investigation is conducted for the proposed geological repository for spent nuclear fuel in Forsmark, Sweden.

The numerical modelling code used for the analyses is Particle Flow Code 3D (PFC3D), a commercial software developed by Itasca. The code enables modeling of thermo-mechanical (TM) coupled process (conductive heat flow, resulting rock expansion and therefore thermal stress) and dynamic fracturing process (seismic wave generated from a rupturing source propagates and attenuates). Moreover, the code enables implementation of discrete fracture network in a heterogeneously modelled rock mass. Therefore, a discrete fracture embedded in the model is also heterogeneously represented.

Based on the site characterization work performed by SKB, a 3D geological model with the major faults and deformations zones was created, as well as the fracture network model of the rock mass generated from site-specific discrete fracture network data.

Using the TM coupled modelling and applying it to the 3D geological model of the repository at Forsmark site, we investigated the thermal evolution of the repository induced by the long-term heat generated from the spent nuclear fuel. We investigated how the rock temperature increase propagates in the repository rock mass and leads instabilities of the fracture-fault systems in the proposed repository site.

The results demonstrate that the heat induces shear displacements of the fracture system. For the fractures located within the repository panel, a rapid slip increase is observed during 50-100 years after start of heat release. The slip then shows slow decrease after 200 years. The rock fractures that are located within the repository panels show almost no movements in the long term, whereas those outside the panel show steady increase. It was found that the fracture slip is irreversible which attributes to dilatational effect. We discuss how the thermo-mechanically induced irreversible fracture slip can have influence on the hydraulic flow field of the repository rock mass.

In our presentation we also discuss how this modelling approach can be applied to a long-term safety assessment for deep geological disposal of high-level radioactive waste in sedimentary formations.

Flow and Non-Reactive Transport Modeling of Recovery Experiments at the Mizunami Underground Research Laboratory

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Abstract

Characterization of fractured crystalline host rock is of importance to geologic disposal of nuclear waste. The Mizunami Underground Research Laboratory, located in Tono area (Central Japan), provides scientific basis for the research and development of technologies needed for deep geological disposal of radioactive waste in fractured crystalline rocks. Through the Development of Coupled Models and their Validation against Experiments (DECOVALEX-2019) project, a comprehensive set of hydrologic and chemical data were obtained based on experiments in a research tunnel located at 500 m depth. Experimental hydrology data from the Mizunami Underground Research Laboratory in Central Japan have been used to develop a site-scale fracture model and a flow and non-reactive transport model for the study area. The discrete fracture network model was upscaled to a continuum model to be used in flow and transport simulations. In this work development and utilization of the models is presented. The simulations were designed to reproduce hydrology of the modeling area. Modeling results were compared with the project hydrology and chloride concentration data at selected observation locations in a monitoring borehole. This study concentrates on the prediction of pressure recovery and chloride concentration changes following flooding of the Closure Test Drift part of the experimental tunnel. Analysis of simulation results for multiple fracture realizations including history matching is presented.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. SAND2019-6354 A.

Hydraulic and Transport Model of a Drift Excavation and Flooding Using Coupled Fracture-Continuum Approach

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Abstract

The solved topic is a groundwater recovery after the deep geological repository closure, i.e. evaluation of the expected final state of hydraulics and chemistry depending on its original state and on the procedure of excavation and operation of the repository. The presented problem and solution comes from the DECOVALEX-2019 project Task C.

The modelling problem is based on the GREET experiment in the Mizunami URL in Japan. The data has been provided by JAEA and the modelling task has been defined and coordinated by Teruki Iwatsuki from JAEA. The presented work covers the contribution of authors to the common cooperation and comparison.

The experimental drift was excavated in granite in 500 m depth horizontally, with inclined access section. Data of pressures and chemical analyses are available in two long boreholes parallel with the drift and three shorter boreholes perpendicular to the drift (total 24 locations of data series). Chlorides are dominant anions with their concentration rising with depth, thus determining the vertical position of water origin before the human intrusion to the groundwater.

The modelling task has been defined in stages corresponding to stages of the experiment (excavation, drainage, flooding, and equilibration) and additionally split into steps of blind prediction and subsequent calibration. The presentation is limited to the final step of calibration with the all available data, covering all the modelling approaches used in the previous steps.

The near-field of the tunnel, defined as the area covered by the drift and borehole observation (approx.. 10 m), is represented by a set of deterministic discrete fractures coupled to matrix blocks in between (Fig. 1). Total of 14 fracture planes is derived drift wall fracture mapping and pilot borehole logging and packer hydraulic tests; some of them correspond to groups of fractures with similar position and orientation. The far-field of the tunnel is represented as a homogeneous equivalent continuum. The excavation process is represented by quasi-continuous temporal change of boundary condition on the tunnel wall. The plug and flooding is represented by additional elements on the tunnel wall with equivalent physical properties.

The calculation is made in Flow123d software, an in-house code of the authors' department, using mixed-hybrid finite element methods for the flow, coupling the subdomains of different dimensions with

independent discrete unknowns at the contacts, and discontinuous Galerkin method for the transport. The inverse problem is solved by UCODE software, a freeware code of the US Geological Survey, using a gradient method with model input perturbation approximated derivatives (sensitivities).

After calibration, the model was able to capture the main phenomena of the experimental observation, i.e. different pressure response of borehole observation intervals, including some with non-measurable communication. It was not possible to capture the chlorine concentration evolution with the reference model scale and prescribed global vertical gradient on the boundary. Using some of the measured data for model input and larger-scale additional model for introducing the inhomogeneity in the far-field, it is possible to capture the range of concentration and values at some of measured locations.

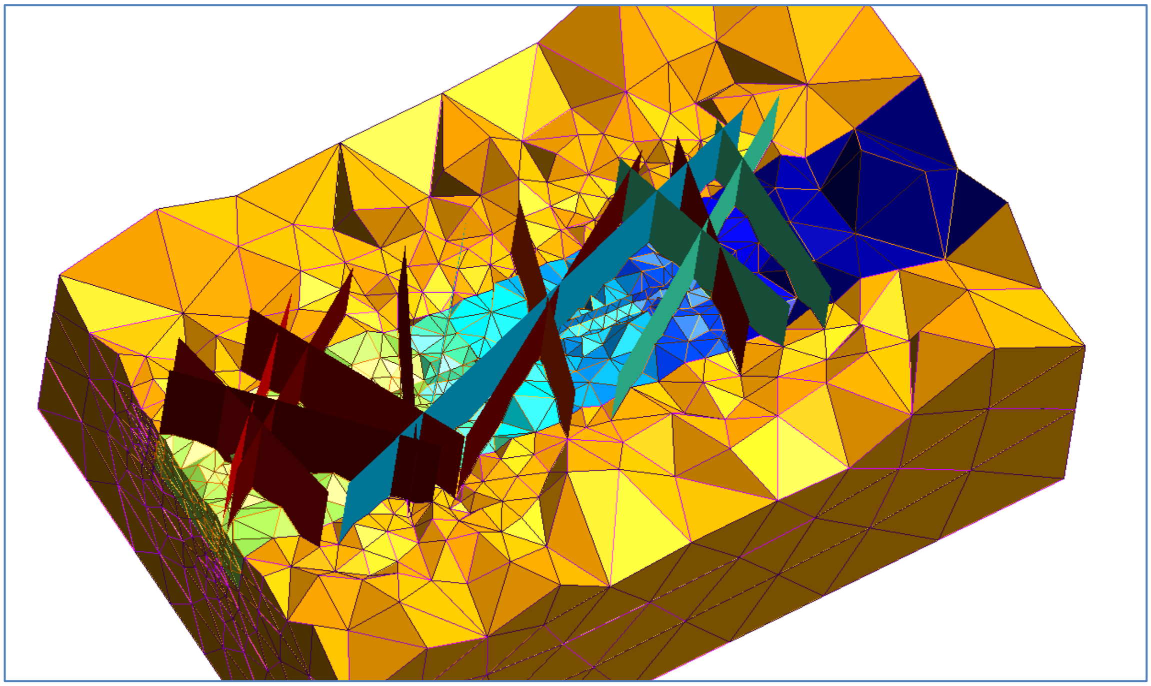

Figure 1: Structure of the model subdomains: fractures and continuum blocks.

Reactive Transport Simulation of Groundwater Recovery Experiment in Tunnel

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Abstract

In subsurface facilities, cement materials are often used to make constructions safer, and high-level radioactive waste repositories are no exception. However, cement materials dissolve when they come in contact with groundwater, making the groundwater's chemistry more alkaline. Such alkaline groundwater can then be diffused by groundwater flows, disturbing the groundwater environment around the repository. Such chemical changes and groundwater distribution processes are important when assessing for the repository's long-term safety and stability.

We conducted the groundwater recovery experiment in tunnel at a depth of 500 m in the granite of the Mizunami Underground Research Laboratory (MIU), Japan, to investigate the post-closure groundwater environment around the tunnel. We constructed a shotcrete-covered closure test drift (CTD) with a volume of 900 m^3 in the fractured granite and filled it with in-situ groundwater for 20 months. During the experiment, we monitored hydrochemical (HC) conditions, such as the water quality and pressure, in and around the CTD to assess the recovery of the geological environment. During this time, the pH in the CTD increased from 8.8 to 10.0 due to shotcrete dissolution and the water pressure recovered in and around the CTD.

Herein, we perform a reactive transport simulation to evaluate the water quality changes in and around the CTD. Specifically, we set the hydrogeological conditions of the CTD, including shotcrete, and input separate set of physical and chemical properties for the part of shotcrete and intact rock around the CTD. Then, we simulate the water quality changes and advection of the chemically affected water. The hydrological simulation results reproduce the observed result that the water pressure was lower in the CTD than in the surrounding rock due to water leaking from the CTD to beyond the water-tight plug. In the chemical-reaction part, the increase of pH in CTD, which was suppressed by the hydrological condition, could be simulated reasonably. Therefore, the proposed simulations demonstrate the HC disturbance caused by shotcrete dissolution in the tunnel. Results suggest that reactive transport simulations can be a useful tool for predicting HC disturbances, even under drainage conditions where convection is dominant.

Thermo-Hydrodynamic Response of Sparse Fracture Systems to Heat Injection

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Abstract

Understanding how heat is stored and transported in tight rocks with sparse fractures is paramount to predict the thermal evolution of spent fuel, high-level nuclear waste repositories. Here we present field results from two controlled heat injection experiments performed through a borehole array deep-seated in crystalline rock at the Grimsel Test Site (GTS), Switzerland. Active heat injection was carried out by heating water using an electrical flow heater up to 45°C for a duration of 10 days (1st test) and 40 days (2nd test). Fluid injection took place across a discrete, 2-m long interval packing off a single flowing fracture. Distributed temperature sensing (DTS) was achieved by deploying optical-fiber through two open boreholes and three grouted boreholes (1st test) or using three packed-off and three fully-grouted boreholes (2nd test). Fluid pressure was monitored at the well head using piezoresistive transducers. We observed multiple thermal breakthroughs, ranging from fast (< 10 hours) to late (>20 days) arrivals, resulting in a temperature increase up to 10°C at 4 to 5 meters from the injection point (Figure 1). The deployment of optical-fiber loops allowed the detection of 3-D thermal fronts (Figure 2). Two responses are identified: (i) a fast, advection-dominated response which developed across a network of well-connected fractures and (ii) a slower, diffusion-dominated response that propagated through low-permeability rock mass primarily by heat conduction. The 3-D thermal response presented herein will be interpreted in the future using a discrete fracture network model.

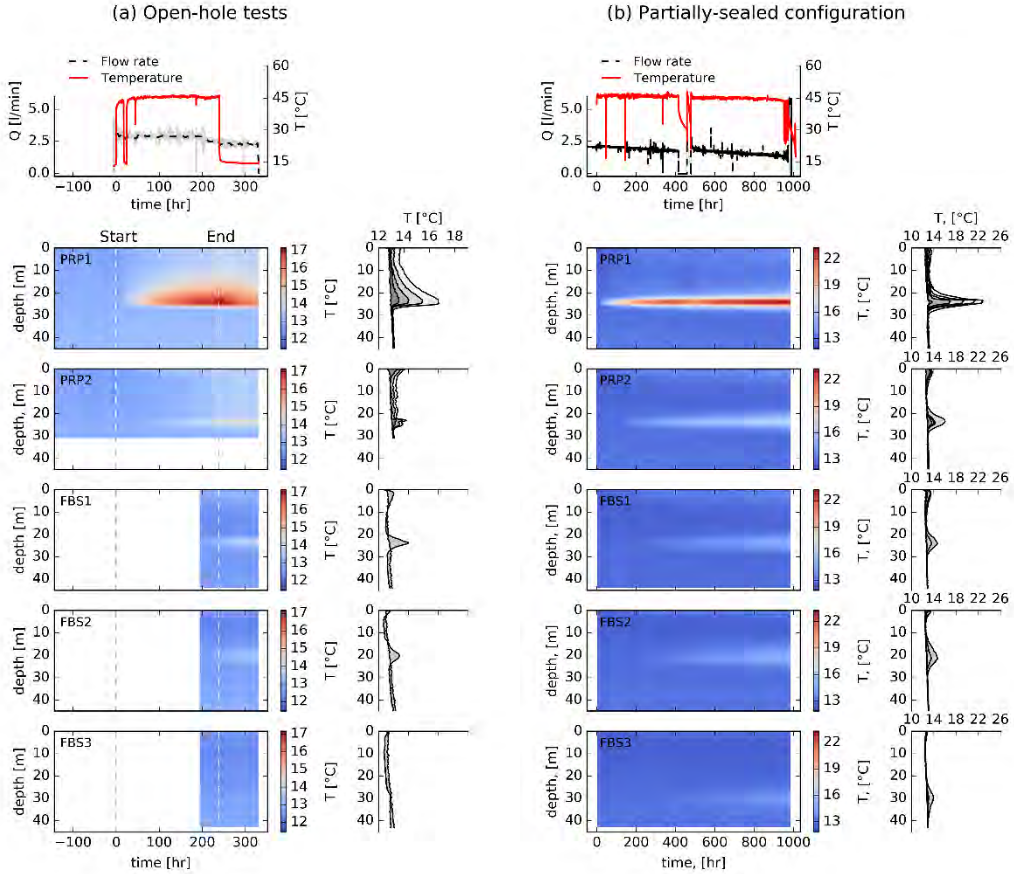

Figure 1: Thermal breakthrough observed during open-hole (A) and partially-sealed heat injection tests (B).

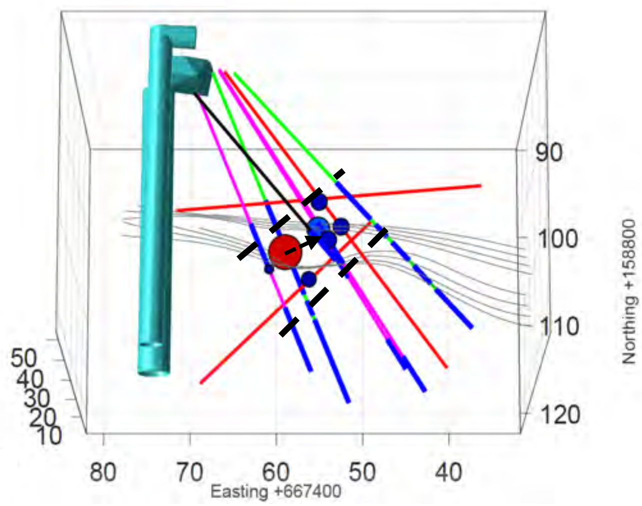

Figure 2: 3D bubble plot showing the location of thermal breakthroughs.

The Numerical Model of the Planned URF Thermo-Mechanical Experiment: Sensitivity Analysis

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Abstract

The implementation of the research, development, and demonstration (RD&D) program is an important aspect of the scientific and technological task concerning the safety case of the repository of high-level radioactive waste. The RD&D program for the deep geological disposal in the Nizhnekansk Granite-Gneiss Massif (Krasnoyarsk Territory) contains over 150 interrelated and linked to the particular part of the safety case research tasks [Svitelman et al., 2018]. Both numerical modelling and experimental activities are envisioned in the RD&D program for key processes.

The construction of the underground research facility (URF) has been approved as a part of this program. The experiments that are planned in the URF should provide reliable data on the repository system properties and evolution. And numerical models development and the analysis of simulation results are very important for adequate experiments design.

The framework of numerical codes for the purposes of the Deep Geological Disposal is being developed in the Nuclear Safety Institute. The long-term goal is ambitious: to provide integrated THMBC model of the disposal system that would take into account all relevant factors, multiple scales, subsystems interactions, all sources of uncertainties, etc.

In this work, we demonstrate the integration of two of these codes. Coupled simulation of thermal and mechanical processes is carried out in the FENIA code [Butov et al., 2017], and sensitivity analysis is provided by the MOUSE code [Saveleva, 2016]. Particularly, the model of the thermo-mechanical experiment is considered. The design of the experiment is the following (figure 1): two heaters are located in the parallel boreholes in the center of the tunnel at a separation of 4 m. The tunnel has an elliptical ceiling, 6m wide and 6-6.5 meter high. The goal of the experiment is to measure large-scale thermal and mechanical properties of the host rock, and to research the excavation-induced and thermal-induced stresses in a heterogeneous and fractured rock mass.

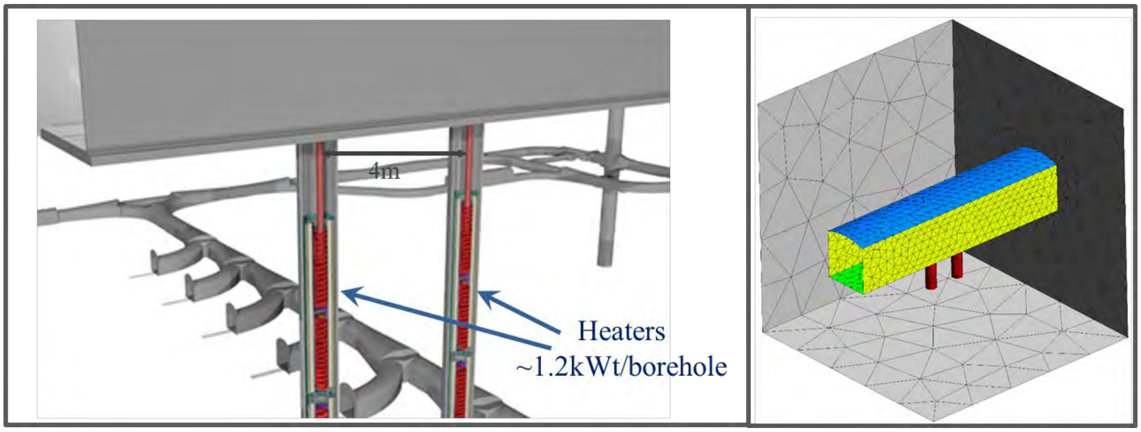

Figure 1: Schematic view of the experiment and computational domain

As a result of the simulation, the 3D fields of the temperature and the stress-strain state are obtained. For the sensitivity analysis, several points from the distinct areas of these fields were selected at different times. The varied input parameters were: heat generation, thermal conductivity, specific heat, heat transfer coefficient from the tunnel walls and floor, thermal expansion coefficient, Young's modulus.

For global sensitivity analysis, FAST (Fourier amplitude sensitivity testing) method [Saltelli et al., 1999] was applied. The results have shown the variability of the influence of the input parameters through different time scales and different locations. The stress-strain state is primarily influenced by the mechanical properties of the host rock (Young's modulus and thermal expansion coefficient). The impact of thermal conductivity is also considerable. The influence of heat removal at the tunnel floor, negligible initially, increases after the rock heats up. The heater power defines temperature maximum, and therefore its influence becomes important when the temperature field becomes quasi-steady.

The obtained sensitivity analysis results could be useful for more precise design of the experiment allowing better choice of instrumentation location and heating regime.

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3D Discrete Element Modelling of the Interference Tests in the Aspö HRL, Sweden

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Abstract

In 2011, SKB(Swedish Nuclear Fuel and Waste Management Company) submitted the applications of the license for constructing and operating a spent fuel repository at Forsmark. SKB suggested the deep geological repository as a strategy to dispose the spent nuclear fuel. To evaluate the performance of the geological repository, the mechanical and hydraulic stability of the natural barrier should be guaranteed during its lifetime. The transmissivity, especially, is a critical parameter representing the hydraulic stability of the repository, so the transmissivity of the host rock should be carefully monitored during the and operation. For the crystalline rock which is a bedrock at Forsmark, the fracture network tends to dominate the hydraulic behavior of the rock mass due to the low permeability of the host rock, so it is necessary to characterize the hydro-mechanical behavior of fractures. In the Aspö HRL(Hard Rock Laboratory), SKB already performed several in-situ tests to build the transmissivity model of the fracture rock. For instance, the interference tests were performed at the TAS04 tunnel to characterize the hydro-mechanical effects of the EDZ(Excavated Damaged Zone) on the host rock. In this research, the fractured rock is numerically modelled using the block based DEM(Discrete Element Method) tools to describe the hydro-mechanical behaviors monitored from the in-situ tests. The effects of EDZ are represented as the aperture changes induced by the deformation and shear dilation of fractures. The stress re-distributions from the opening of the TAS04 tunnel disturb the mechanical conditions of fractures and the transmissivity of the rock mass is also changed. The numerical simulation captures the quantitative changes of the transmissivity and the changes are compiled by the distance from the tunnel. Using the constructed tunnel model, the interference tests performed at the TAS04 tunnel are simulated, and the transient pressure responses from the observation wells are compared. The pressure responses from the interference tests are primarily dominated by the connectivity of the fracture networks, but the deformations of the fractures can contribute to the response significantly. Since the DEM model describes the hydro-mechanical behaviors of the fractured crystalline rock, this model can be applied on the further numerical simulations to evaluate the long-term stability of the repository.

DECOVALEX 2019 SYMPOSIUM
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Simulation of Hydro-Mechanically Coupled Processes in Rough Rock Fracture Intersections Using an Immersed Boundary Method and Variational Transfer Operators

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Abstract

Simulating hydro-mechanically coupled processes in the subsurface has to capture complex fracture surface topographies, highly non-linear processes and complicated fracture configurations in fracture networks. We present a methodology that resolves the small-scale roughness on fracture surfaces while capturing tightly coupled hydro-mechanical effects. This methodology is applied to fracture intersections, consisting of multiple solid bodies. Between all body surfaces (i.e. in the fractures), mechanical contact and the resulting fluid flow field are computed. The multibody contact problem and solid mechanics use linear elasticity. The fluid problem is formulated as incompressible Navier Stokes flow. The presented methodology employs variational transfer operators as a mortar surface projection to match the non-matching fracture surfaces, as a volumetric transfer operator to couple solid and fluid problem and to create solid domain specific unstructured fluid meshes. We present 2D and 3D benchmark simulations on fracture intersections and further demonstrate the capabilities of the approach on fracture intersections with complex geometries subjected to increasing load.

Numerical Study of Damage by Phase Field Method in Coupled THM Conditions and Application to Heating Test Simulation

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Abstract

In the context of short and long term safety analysis of facilities for geological disposal of radioactive waste, it is crucial to characterize and predict the nucleation and propagation of damaged and fractured zones around galleries and boreholes. The damaged and fractured zones are created under coupled thermo-hydromechanical (THM) conditions. In this study, we propose a new numerical method for capturing the damaged and fractured zones in coupled THM conditions. The proposed method is based on the phase-field approach. The damage density distribution is solved as an independent field which is governed by its own partially derivate equations. The damage field is coupled with the displacement field, temperature field and fluid pressure field. The advantage of this method is the possibility to easily describe the evolution process from diffuse damage to localized cracking (fractures seen as damage localization bands). We have proposed a new phase field model in order to better capture the specificity of mechanical behavior of clayey rocks under compressive stresses. Indeed, we have introduced two damage fields respectively corresponding to tensile cracking and shear cracking. The proposed model is first applied to modeling mechanical behavior of Cox claystone in different laboratory tests. With the help of proposed new phase field model, it is possible to capture the onset and propagation of localized cracks in samples and the post-localization responses. Then, the proposed model is applied to the simulation of THM responses during an in situ heating experiment (ALC1604) conducted by ANDR in the underground research laboratory at BURE. The evolutions of temperature, pore pressure, deformation as well as induced damaged zone are predicted and compared with in situ measurements. The efficiency of the proposed phase field method is clearly demonstrated.

Investigating the Thermal, Hydraulic and Mechanical Response of the Cox to Thermal Load at Experimental and Repository Scale

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Abstract

Disposal of heat generating radioactive waste at depth in low permeability clay host rock will result in changes to pore pressures and mechanical stresses within the host rock. These effects have been investigated in experiments at ANDRA's Underground Research Laboratory (URL) at the Meuse/Haute-Marne Centre. Two experiments have been examined here: the TED experiment in which three heaters at approximately 1/4 scale are emplaced parallel to each other; and the ALC experiment in which heaters at the full scale of a waste disposal canister are emplaced in series in a single tunnel. Modelling of these two experiments has been undertaken, starting with the TED experiment and then using the calibrated parameters from the TED experiment in blind predictive modelling of the ALC experiment. Comparison of the model predictions with data from the ALC allows some understanding of how well process models and parameterisation can be upscaled from 1/4 scale to the full scale of a waste disposal cell. The modelling work demonstrated that the predictive models were able to reproduce broad trends whilst further modelling in light of the data gave significantly improved results. Updates to the model included adding more of the sequence of construction of the experiment to the model, updating the shape of the excavation damage zone around the ALC tunnel and updating the parameter calibration. These model updates indicate that the properties of the COx are potentially scale and/or location dependent. Processes such as EDZ formation may be scale dependent, but for a true comparison between scales, observation points would need to be at consistent distances from the experiment.

Two different model formulations have been successfully used when modelling the TED and ALC experiments. The first is a fully coupled thermal-hydraulic-mechanical (THM) approach that solves momentum balance equations for the mechanical part of the problem and accounts for anisotropic mechanical properties, coupled with Darcy fluid flow via poro-elasticity and thermal diffusion. The second approach replaces the momentum balance of the mechanical equation with an equation for the elastic change in porosity as a function of temperature and pressure. This simplified approach does not calculate stresses and displacements but does consider the effect of volume changes on porosity and pore pressure. The approach produces good results and is less computationally expensive making it a potentially useful tool in upscaling to whole repository simulations if pore pressures are of more interest than stresses.

Finally, the processes and parameterisation used for the ALC experiment are used to model a series of waste disposal cells to investigate the effects of heat generation on the COx at the scale of the whole repository. A range of calculations are performed to determine the pore pressures and stresses that may occur in the COx given the uncertainty and spatial variability of the physical properties of the COx at the scale of the whole repository.

Acknowledgements: This work was funded by Radioactive Waste Management Limited (RWM; https://www.gov.uk/government/organisations/radioactive-waste-management) as part of participation in the international DECOVALEX project (https://decovalex.org/).

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Coupled Processes in Radioactive Waste Disposal and Other Subsurface Engineering Applications

Geomechanical Response of Carbonate-Rich Opalinus Clay to Carbonated Water

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Abstract

Geological carbon capture and storage is being adopted around the world as the means to reduce atmospheric CO_2 due to increased concerns on global warming accelerated by anthropogenic greenhouse gas. Whether or not the geological formation can successfully seal the injected gas depends on the type and state of materials that constitutes the subsurface. As the introduction of CO_2 to fresh soils or rocks may trigger chemical weathering, the material's resistance to acidic fluid should be investigated to guarantee long-term success. To study the behaviour of caprock material under CCS conditions, shales such as Opalinus Clay (OPA) are often adopted for modelling the response to CO_2 injection. OPA is regarded as one of the exemplar geomaterial that can serve as a caprock due to its low permeability, high air entry value, self-healing capacity and low reactivity to acid. OPA samples retrieved from Mont-Terri rock laboratory were mainly composed of clay minerals which were inert to CO_2. As it is often the case for sedimentary rocks to accommodate layers or sporadic lenses of carbonate minerals, the retrieved core samples also contained some highly concentrated lenses of carbonate. For this reason, the geomechanical response of carbonate rich OPA to acidic fluid were investigated with the objective of evaluating any changes in permeability and deformation induced by dissolution. For the experiment, high pressure oedometer cell developed at EPFL was used to conduct conventional consolidation and permeability tests. 3 LVDTs were installed to monitor vertical displacement during oedometer test any possible compaction induced by dissolution of minerals. For the start, installed specimen was saturated with deaerated water from two sides of the sample. The specimen was loaded to different degree of vertical stresses and followed by constant head permeability tests. After measuring hydraulic and mechanical properties of the sample, carbonated water was injected to the Opalinus Clay by pressurizing the upstream side with downstream side valve opened to the atmosphere. The entire experiment lasted for more than three months, where the CO_2 injection phase lasted more than six weeks. During the injection phase, LVDTs recorded continuous compaction with time. The trend of vertical displacement was clearly obvious, however, the recorded magnitude was not extreme for a given duration of injection. CO_2 treatment was followed by the constant head permeability tests to observe any change in fluid flow characteristics. With the compaction of the sample during CO_2 injection, changes in permeability before and after injection were recorded. Along with the experiments done using the high pressure oedometric cell, pore structural analysis are also discussed.

DECOVALEX 2019 Task E: Numerical Simulation of THM Processes in The Bure Heater Experiments Using A Failure Dependent Permeability Model

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Abstract

In this paper, we present the results of the DECOVALEX 2019 Task E by the BGR/UFZ team using the finite element code OpenGeoSys (Kolditz et al., 2012, Bilke et al. 2019). Task E is dealing with the analysis of the in-situ heater experiments in the Meuse/Haute-Marne Underground Research Laboratory (URL) at the Bure site in France, which is located in the Callovo-Oxfordian (COx) claystone (Armand et al., 2017). As a novelty in DECOVALEX, Task E is conducted at several relevant scales (i.e. a multi-scale study). Two in-situ experiments were analysed numerically to investigate the coupled thermo-hydro-mechanical (THM) behaviour of COx induced by excavation and under thermal load, which is assumed to be generated from the emplacement of radioactive waste: a borehole-scale experiment (TED) and the full-scale experiment (ALC). As a key parameter, the permeability of the rock and its spatial distribution are very important for the understanding of the THM behaviour. Therefore, a failure index-dependent permeability model based on the Mohr-Couloumb failure criterion is introduced into the THM model formulation in order to account for permeability changes in the excavation damaged zone (EDZ). The evaluated permeability distribution around the gallery fits well with the measured one. Integrating the permeability model into the simulations of the in-situ experiments enhanced the predictions of the full-scale experiment made by the THM model based on the parameterization of the borehole-scale experiment.

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Predictive HM-Modeling In The Heterogeneous Opalinus Clay Of The Mont Terri Rock Laboratory And Validation With Monitoring Data From A Mine-By Test

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Abstract

The Mont Terri rock laboratory was initiated in 1996 with 8 niches followed by a research tunnel in 1998. Since then the laboratory has been expanded every 10 years, mainly in the shaly facies of the Opalinus Clay. In March 2018, south of the existing laboratory, we extended the Mont Terri rock laboratory, mostly in the sandy facies of the Opalinus Clay (Ga18). In October 2019, this extension will be finished, resulting in more than 500 m of additional galleries and niches for new experiments. In the frame of this extension, we conducted for the first time a mine-by test investigating a sheet of sandy facies and carbonate-rich sandy facies sandwiched between shaly facies. This so-called MB-A experiment (hydro-mechanical characterization of the sandy facies before and during excavation) consists of two lateral niches for instrumentation and monitoring, and a test gallery of 30 m length oriented perpendicular to the lateral niches. Instrumentation based on 26 boreholes with lengths up to 40 m comprises pore-pressure transducers, extensometers, inclinometers and stress monitoring stations. It was finished several months before excavation of the test section was started to assure equilibration close to the initial conditions. We carried out excavation of the test gallery running parallel to bedding strike in May 2019 sequentially in daily advances of 2 m. The horseshoe-shaped gallery was lined with two layers of sprayed shotcrete of 20 cm total thickness. Concreting of the invert was done after finishing the entire gallery.

Here we present data from predictive modeling to estimate the hydro-mechanical behavior of the rock mass during excavation that was carried out for two heterogeneous, anisotropic cases: i) 3D-elastic and ii) 2D-APD (anisotropy, plasticity, damage). Initial predictive modeling was corrected to effective daily advances and sensor locations. We also present monitoring data and qualify the modeling results for the two different approaches. The elastic calculation predicts a rotation of early time, near-field pore-pressure reduction from perpendicular to parallel to bedding for later times. In contrast, the APD simulation predicts plastic volumetric dilation and a linked pore-pressure reduction along bedding. In general, monitored peak pore water pressures were higher than predicted, with a remarkable phase shift depending on distance and spatial position with respect to the drift. Compared to the elastic calculations, monitored deformations were clearly underestimated and are still low compared to the APD calculation. The overall behavior of the excavation in the sandy facies was, unexpectedly, not so different from earlier excavations in shaly facies. A large volume of the rock mass was influenced by the excavation works of Ga18, which became manifest in large-scale pore-water pressure changes and long-range deformations of existing galleries.

The acquired dataset of the mine-by test will be used in the future to calibrate our hydro-mechanical models. Adapted constitutive laws are needed to properly predict the hydromechanical response in stiffer claystone such as, for instance, the sandy and carbonate-rich sandy facies of the Opalinus Clay.

Mechanical and Hydraulic Characterization of the Excavation Disturbed Zone (EDZ) in the Opalinus Clay of the Mont Terri Rock Laboratory

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Abstract

The objective of the present study is to determine hydraulic and mechanical parameters in the excavated disturbed zone (EDZ) of the Opalinus Clay in the Mont Terri Rock Laboratory by applying three simple and inexpensive measuring field devices. For the estimation of the mechanical and also geophysical parameters the needle penetration test (NPT) is applied. In addition, the mechanical and hydraulic apertures of previously mapped joints (faults, splays, bedding joints and excavated disturbed fractures) are measured with a portable microscope camera and an air permeameter (TinyPerm 3, Fig. 1). The latter has been recently validated indicating its suitability to accurately measure hydraulic apertures down to 10 µm (Hale et al. 2019, Cheng et al. in preparation).

Figure 1: Measuring the hydraulic aperture using an air permeameter.

Our results show that the measured hydraulic apertures in the EDZ range between 20 and 100 µm with an average of 84 ± 23 µm. The latter is comparable with previously determined transmissivities from hydraulic cross-hole testing (Bossart et al. 2002). In contrast, the determined mechanical apertures range between 16 and 1400 µm. However, the study also demonstrates that two empirical equations by Kling et al. (2017) and Rasouli & Hosseinian (2011) can be successfully used to estimate hydraulic apertures from measured mechanical apertures and roughnesses (Fig. 2).

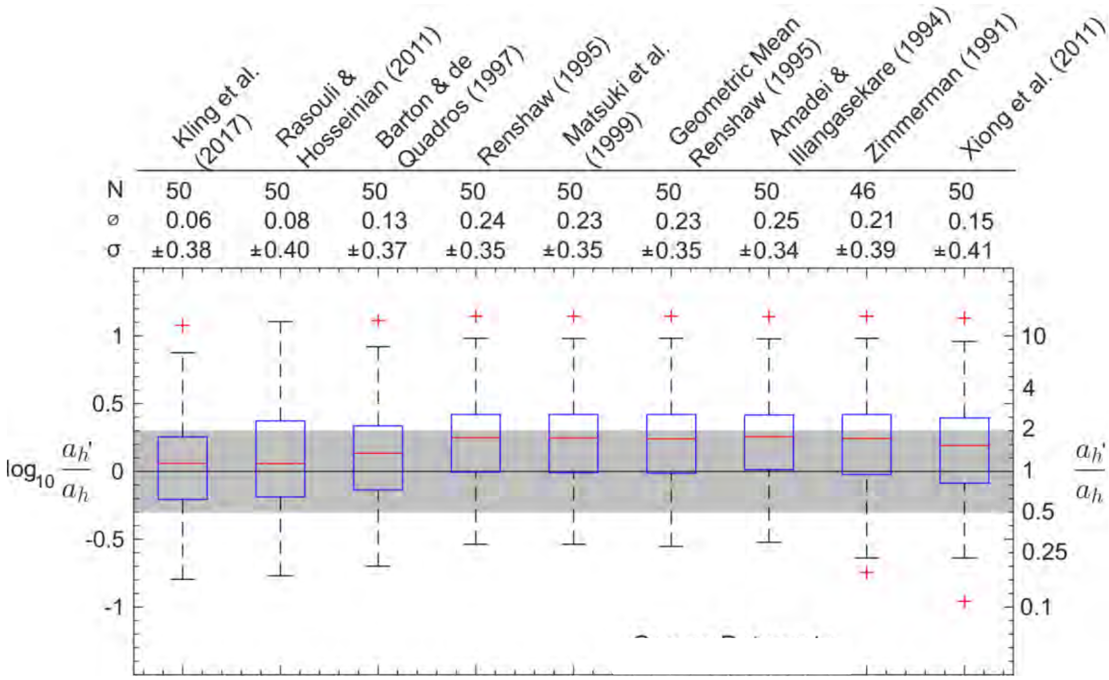

Figure 2: Relationship between directly measured hydraulic apertures (a_h) using an air permeameter and the empirically derived hydraulic apertures (a_h') using the mechanical apertures and roughnesses measured with the microscope camera.

Furthermore, the mechanical and geophysical parameters such as uniaxial compressive strength, elastic modulus, tensile strength, seismic velocities are comparable to previously determined values compiled by Jaeggi & Bossart (2014). To conclude, our results clearly demonstrate the suitability to determine mechanical, geophysical and hydraulic parameters of an excavated disturbed zone (EDZ) by using also simple, fast and inexpensive measuring field devices such as (1) needle penetration test (NPT), (2) microscope camera and (3) air permeameter. Further studies should however demonstrate the applicability also for other rock types and geological settings.

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Mineralogical, Structural and Geometric Properties of Old EDZ Fractures in the Opalinus Clay Shale

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Abstract

The Opalinus Clay shale (OPA) has been chosen as a potential host rock for Switzerland's high- and low-level nuclear waste repository. As such, a comprehensive characterization of the intact and damaged OPA rock mass is required to assess its short- and long-term behaviour with respect to repository safety and integrity. Rock sealing processes in the Excavation Damage Zone (EDZ) are considered important for safe, long-term storage and are the focus of the SE-P (SElf-sealing Processes) project within the frame of the Mont Terri Project. Specifically, sealing processes are investigated in ten and twenty year old EDZs (Williams et al., 2018, 2019). The project is supported by the Swiss Federal Safety Inspectorate (ENSI), the Swiss Federal Office of Topography (swisstopo), the German Federal Institute for Geosciences and Natural Resources (BGR), the German Federal Office for the Safety of Nuclear Waste Management (BfE), and Radioactive Waste Management Limited (RWM) from the UK.

In a first series of in-situ characterization experiments, we have conducted tunnel- and borehole-scale seismic and electrical resistivity tomographies to identify petrophysical and structural changes in rock volumes encompassing the EDZ in galleries 08 and 98. Based on refraction seismic tomography, we found that EDZ volumes in gallery 08 have either increased, not changed, or decreased in their seismic p-wave velocities over a period of ten years, i.e., they show a heterogeneous evolution. These results can be interpreted as an improved (i.e., sealing), stable, or even degraded EDZ. In order to investigate the underlying processes leading to sealing, we have taken drill core samples of induced and pre-existing rock fractures from ten boreholes to identify which sealing processes have occurred since gallery excavation. This study's focus is on the mineralogical and structural alterations and geometric properties of selected Opalinus Clay fracture samples.

We scanned about 70 fracture samples with an ATOS Core 300 3D scanner in order to conduct fracture roughness and morphology analyses prior to mineralogical and microstructural investigations (Figure 1). The latter include bulk and fracture XRD analyses, petrophysical and geochemical analyses, optical microscopy using a Keyence VHX-6100 digital microscope, and scanning electron microscopy (SEM) image analyses. Preliminary results show that EDZ fractures have a distinctly different roughness compared to tectonic faults and that secondary mineralization on fracture surfaces (one of many possible sealing mechanisms) is heterogeneous within the given time period. We will present a status update on the laboratory analyses focusing on microscale alterations of EDZ fractures in Opalinus Clay shale.

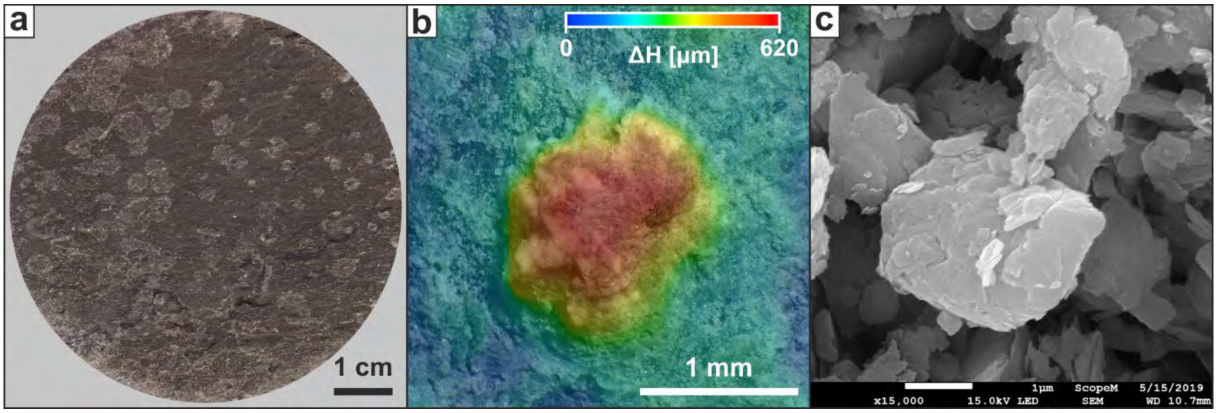

Figure 1: Examples of EDZ fracture surfaces and secondary mineralization at centimeter (a), millimeter (b), and micrometer (c) scales. Photos: D. Zangerl, M. Williams 2019.

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Modeling of Thermal Induced Pressurization in COx Claystone

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Abstract

The Callovo-Oxfordian claystone (COx) is utilized as a host rock in high-level or intermediate-level waste disposal underground. The heat emanated from the waste induced accumulation of pore pressure due to its low permeability and relative rigidity. As part of the international DECOVALEX-2019 project, TOUGH-FLAC is being applied for modeling of coupled Thermo-Hydro-Mechanical (THM) processes during in situ experiments in COx at an underground research laboratory in Bure, France. The in situ experimental program conducted by the French national radioactive waste management agency (Andra) consists of a step-by-step approach started by small scale heating to full-scale experiments. The main goal of these experiments is to study the THM behavior of the COx under thermal loads. Pore pressure build-up due to thermal expansion of the fluid and solid skeleton, stress evolution around a repository, and fluid flow in the rock matrix are researched in this task.

In this work, we simulate the THM processes during heating experiments. The fundamental theory developed in this simulator is based on thermoporoelasticity, which extends thermoelasticity to porous continua by considering an underlying thermoelastic skeleton. A sequential coupling scheme based on fixed stress-split is used in this method, in which flow problems are solved first under fixed stress in TOUGH, then pressure, temperature are passed to FLAC and prescribed during mechanical simulations. First, the model is benchmarked with a simple 3D consolidation test to verify the correctness of the code implementation on coupled THM processes against the analytical solution. Then, we present modeling results related to a small-scale in situ heating experiment (TED experiment) and a full scale heating experiment (ALC experiment) both at Bure. Some analysis of simulations results against the experiment observations are conducted. The simulation results illustrate the capability of our simulator to capture the THM behavior in host rocks, which is relevant for the design and safety calculation of a nuclear waste repository.

Keywords: THM modeling, heater experiments, Callovo-Oxfordian claystone, thermal pressurization.

Horizontal Borehole Experiments and Simulations to Understand Heat, Brine and Vapor Migration in Bedded Salt

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Abstract

Disposition of defense high level waste (DHLW) and civilian spent nuclear fuel (SNF) both create heat generating waste. Numerous concepts for the management of heat generating waste have been proposed and examined internationally, including geologic disposal in salt because of its low permeability and visco-plastic deformation that causes self-repair of damage. Evaluating the safety and technical challenges of storing thermally hot waste in a salt repository is an ongoing process involving experiments and supporting numerical simulations. An experiment is underway in the underground of the Waste Isolation Pilot Plant (WIPP in Carlsbad, New Mexico, USA), to address how phenomena such as brine migration, vapor transport, and mechanical changes to the salt might be effected by the presence of a heat generating source in bedded salt (Figure 1).

We report results from a shakedown test in a sub-horizontal borehole in the underground at WIPP that includes a 10.2 cm diameter borehole equipped with a heater surrounded with smaller diameter boreholes instrumented with thermocouples. The central borehole contains an inflatable packer, heater, and constantly flowing nitrogen gas circulation system. In the heated borehole, nitrogen gas circulation outflows to a desiccant container where water mass is measured daily during the experiment to quantify vapor removal. Thermocouples in the nearby boreholes allow us to determine the efficiency of several heater arrangements.

The shakedown test has allowed experimental issues to be addressed before a larger planned test that should be starting in the summer of 2019. Using data from the shakedown testing, we built simulations using the Los Alamos developed Finite Element Heat and Mass transfer code (FEHM) to evaluate the experimental results, and determine field-scale parameters. A 3-D numerical mesh has been built using LaGrit software (lagrit.lanl.gov; Miller et al., 2007) with increasing resolution around the central borehole (Figure 2). Simulations of the experiment allow us to confirm our conceptual model and provide checks on previously measure physical properties. Additionally, assumptions about brine and vapor flow and transport are being tested by comparing measured and simulated results. The combination of experimental data and model results provide additional data to help support the safety case for disposition in of heat

generating waste in bedded salt formations.

Figure 1: Installation of a heater into a horizontal borehole in the WIPP facility, Carlsbad, New Mexico, USA.

Initial results from this experiment show that water flow into the borehole agrees with previous experimental results and results from the TOUGH-FLAC simulator. Further, the shakedown test led to a design change to better transfer energy to the rock salt using an infrared heater. Simulations also show the impact of long-term pressure drainage during the 30 years that the drift was open before the heater testing.

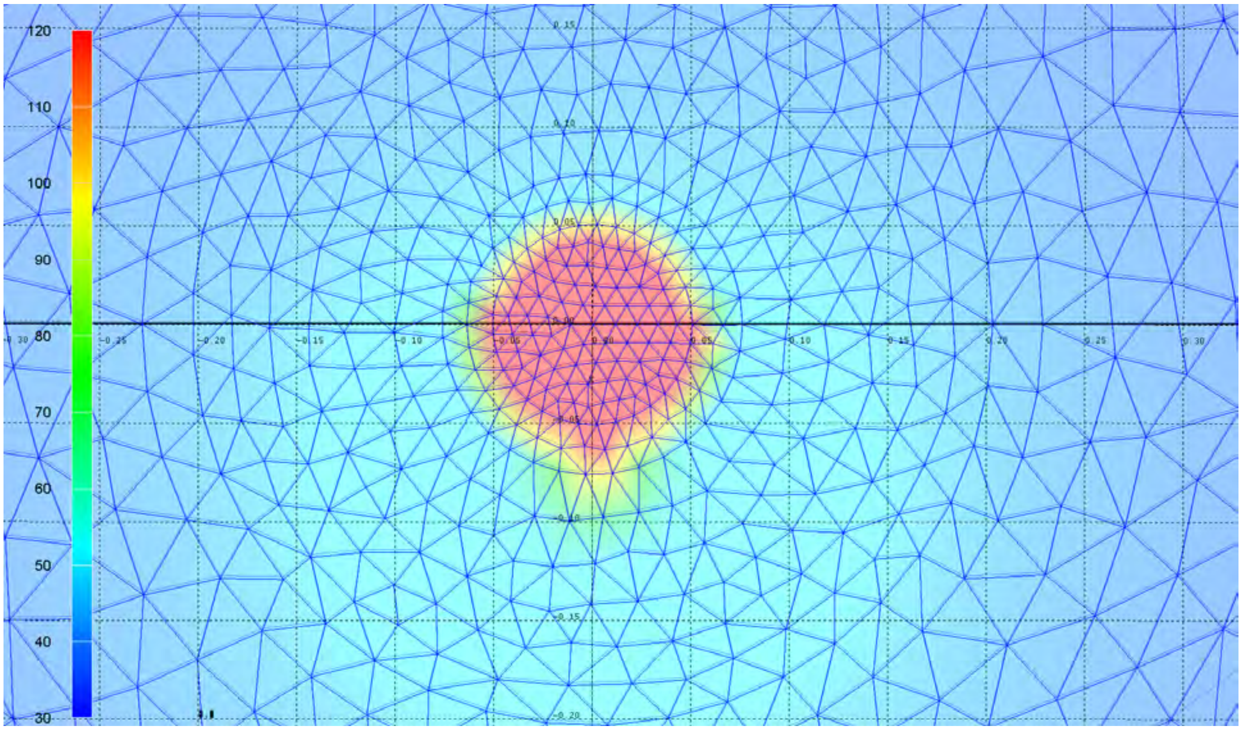

Figure 2: Slice through the heater in the 3-D computational mesh.

Coupled Thermo-Hydro-Mechanical Model of Ground Surface Deformation at Swiss Heat Storage Sites

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Abstract

High temperature (>40 °C) aquifer thermal energy storage (HT-ATES) is a promising technology that could decrease the carbon footprint and/or reduce the cost of the heating sector. Hot water is injected into aquifers in the summer when excess heat is in supply and extracted in the winter when excess heat is in demand. Due to coupled thermo-hydro-mechanical (THM) processes, there are several technical challenges associated with HT-ATES. For example, surface deformation could occur due to thermo-poroelastic expansion, which is poorly studied in the context of HT-ATES but could be problematic due to proximity of cities and infrastructure. The Swiss HeatStore consortium includes academic and industrial partners that are building pilot HT-ATES projects in Geneva and Bern, Switzerland, with the goal of accelerating the uptake of geothermal energy and HT-ATES. The well locations, injection/production strategy, and target formation(s) have not been finalized at these sites. Using the Multiphysics Object Oriented Simulation Environment (MOOSE), a parallelized finite element code, we run 3D thermo-poroelastic simulations in support of the Swiss HeatStore sites. Our model takes local geology and heat supply/demand into account to be site-specific. The model is run for several annual cycles and shows the importance of reservoir characteristics, placement of the well(s), and operational decisions (e.g. flow rate and temperature) on surface deformation. Results from this model can help to inform the design of the HT-ATES sites and could also offer insights into surface deformation driven by THM processes for other applications (e.g. geothermal energy, CO_2 sequestration, and nuclear waste disposal).

Coupled Hydro-Mechanical Modelling of Fault Slip Induced by Water Injection in Low Permeability Rock

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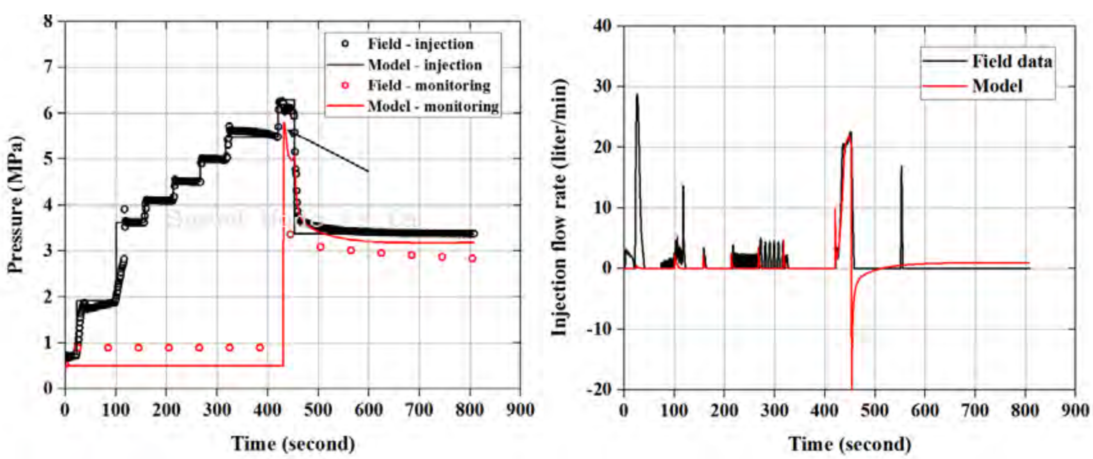
Abstract

This study presents the research results of the DECOVALEX-2019 project Task B. Task B is aiming at developing a numerical method to simulate the coupled hydro-mechanical behavior of fault induced by water injection. As the first step, benchmark simulations with simplified fault plane and geometry were carried out for participating groups to develop respective numerical codes by representing the coupling process between fault hydraulic transmissivity and the mechanically-induced displacement. We reproduced the coupled process regarding fault slip using TOUGH-FLAC simulator. The fluid flow along a fault was modelled with solid elements and governed by Darcy's law with the cubic law in TOUGH2, whereas the mechanical behavior of a fault was represented by creating interface elements between two separating blocks in FLAC3D. A methodology to link a solid element of TOUGH2 and an interface element of FLAC3D was suggested with hydro-mechanical coupling relations of two different hydraulic aperture models. In addition, we developed a new coupling module to consider the changes in geometric features of numerical mesh and hydrological properties of fault caused by water injection in TOUGH-FLAC. Transient responses of the fault, including elastic deformation, reactivation, progressive evolutions of pathway, pressure distribution and water injection rate, to stepwise pressurization were examined, and the effects of the transmissivity and storativity of the fault was assessed using uncoupled, one-way coupled and two-way

coupled models for various benchmark simulation cases. The results of the simulations suggest that the developed model can provide a reasonable prediction of the hydro-mechanical behavior regarding fault reactivation. The developed model was applied to the fault slip (FS) experiment at the ‘Main Fault’ intersecting the low permeability clay formation of the Mont Terri underground research laboratory in Switzerland. Several FS experiments were conducted in packed-off intervals at different sections of a borehole crossing the Main Fault core. A fault plane was stimulated by pressure-controlled water injection, and the hydro-mechanical behavior was observed from injection and monitoring boreholes in each test. The FS experiment for the numerical simulation corresponds to the test conducted during 800 seconds at 37.2 m depth below the Mont Terri gallery 2008 where the water was injected into a minor fault in the Main Fault hanging wall. We conducted a parametric study to understand the effects of in-situ stress condition and fault deformation and strength parameters and find the parameter set to reproduce the field observations. In the best matching simulation, the abrupt increases of flow rate and monitoring pressure at 420 seconds of injection showed good agreement with field data (Figure 1), which suggests the capability of the numerical model to reasonably capture the fracture opening and propagation process. In our model, the hydraulic aperture in non-elastic stage was increased mainly by shear failure rather than tensile opening, which resulted in overestimates of the fault displacement in shear direction and the range of reactivated zone. The numerical model will be enhanced by continuing interaction and collaboration with other research teams of DECOLVAEX-2019 Task B in a further study.



(a) (b)

Figure 1: Comparison of results obtained from field experiment and those simulated in numerical model: (a) injection and monitoring pressures and (b) injection flow rate

Modelling of Fluid-Injection-Induced Fault Reactivation in an Argillaceous Rock

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Abstract

Geological disposal is believed to be one of the best feasible options for long-term management of radioactive wastes, making use of multi-barrier safety functions in order to prevent the potential migration of contaminants towards the biosphere. However, faults in the host rock might exist in the vicinity of deep geological repositories for radioactive waste, which could enhance potential pathways for radionuclide migration. Therefore, there is an important issue related to contaminant transport through potential creation of permeable flow paths in low permeability argillaceous rocks. Such flow paths could be created by reactivating faults of various sizes by thermal, hydraulic and mechanical disturbance during operational or post-closure period. With the hydraulic fracturing process, critically stressed faults can be activated due to several processes and might trigger pore pressure increases in the faults and the decreased effective stress on the fault plane.

Based on DECOVALEX 2019 research project, the concerning technical item is referred to “Task B – the induced slip of a fault in an argillaceous formation”. The experiment setup of the corresponding in-situ test was done by Guglielmi, 2016. In this research, the paper is to perform a modelling of fault reactivation during an experiment of controlled water injection in a fault at the Mont-Terri Underground Research Laboratory in Switzerland. The effects of in-situ stress, fault shear strength parameters are all taken into. The computed results are compared with hydro-mechanical behaviour obtained from different code and indicate that the shear displacement path of host rock in the vicinity of water injection point is consistent with the initial shear stress direction on the fault surface, which is consistent with the results of in-situ test.

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Mathematical Modelling of Fault Reactivation from Water Injection at an Underground Research Facility

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Abstract

Faults that might exist near deep geological repositories for radioactive waste constitute potential enhanced pathways for radionuclide migration. Several processes might trigger pore pressure increases in the faults leading to fault reactivation and induced seismicity, and increase the faults' permeability. In this research, we developed a mathematical model to simulate fault activation during an experiment of controlled water injection at the Mont-Terri Underground Research Laboratory in Switzerland. Water was injected in a damaged zone around a Main Fault, with the injection pressure being increased in a stepwise manner. The injected water migrated towards the Main Fault, and at a critical injection pressure, triggered a sharp increase in pore pressure and fault movement across the Main Fault interface, and the generation of a microseismic event. We developed a mathematical model based on the theory of poromechanics to simulate the above experiment. The Main Fault structure is complex, and includes gouge at the Fault's interface, zones of scaly clays, and zones with discrete fractures. The mathematical model explicitly represents the damage zone, and the zones in the Main Fault as poro-elastoplastic materials, with different degree of anisotropy and hydro-mechanical properties. Such representation of the complex structure of the Main Fault and the damage zone is one of the key factors contributing to a successful simulation of the main processes that occurred during the experiment.

Modelling of Fluid Injection Induced Fault Reactivation by Hydro-Mechanical Coupled 2D & 3D Distinct Element Models

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Abstract

In this study, we present a series of numerical modelling results of simulation of fluid injection induced fault reactivation. The numerical modelling codes we used are Particle Flow Code 2D & 3D (PFC2D/3D), which are commercial softwares developed by Itasca Consulting Group on the basis of Distinct Element Model. For simulation of fluid injection, we further developed a fluid flow algorithm using the FISH programming. This is done by generating a 2D & 3D pore network models in a tightly compacted bonded particle assembly. The fluid flow from one pore to another pore is governed by Cubic law assuming that the flow is laminar and viscous between two parallel plates with a constant aperture for uncoupled modelling and with a stress dependent aperture for HM coupled modelling. The fluid pressure build-up in a pore space is governed by the fluid volume, pore space and the fluid compressibility. When the fluid pressure is big enough to break the bond strength at particle contacts, the strain energy is released in a form of a seismic wave that propagates and attenuates. Seismicity computation algorithm is implemented to capture the radiation pattern of the seismic energy released at the broken contacts to compute the seismic magnitudes. The faults in PFC models are simulated as a combination of finite thickness zone with core fracture running at the centre. The zone with a finite thickness has lower strength/stiffness to mimic a fault damage zone with relatively larger permeability compared to the fresh host rock. We simulated two models of fluid injection induced fault reactivation. Model 1 is the 2D case where the fault is reactivated by a long-term off-fault injection. The results demonstrate that the activation magnitude may differ depending on the hydraulic characteristics of the fault zone (fluid flow conduit vs. fluid flow barrier) which can also be discussed in term of fault maturity. The fault zone with fluid flow barrier character (immature fault) is reactivated with larger seismic magnitude due to build-up of a fluid overpressure zone next to the fault zone which added additional mechanical stress to the fault zone (poro-elastic stressing) and results in a larger stress drop at the time of reactivation. The Model 2 is the 3D case where we simulated the fluid injection experiment conducted in Mt. Terri (Guglielmi et al. 2015). The preliminary results of Model 2 demonstrate that the fluid injected into a conductive fault zone can trigger a sudden movement of a stressed fault intersecting the injection fault. In the Symposium, we will present more results on this Model 2 simulation.

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An Extension to the FE Method-Based Simulator OpenGeoSys to Represent Shear Rupture

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Abstract

Fault reactivation due to increased pressure in the vicinity of a deep geological disposal site may harm the repository and compromise its sealing. Here we present a numerical tool that is validated against experimental data collected during the execution of the Fault Slip (FS) experiment. The experiment was conducted in the Mont Terri underground rock laboratory (Switzerland).With the numerical tool we aim to correctly characterize the pressure evolution associated with the elastic and plastic deformation of the fault material. The application of the tool is not limited to a fault in a clay formation, but it has a more generic applicability.

The fault is represented with elasto-plastic elements, where the possible failure is due with an oriented Mohr-Coulomb failure criteria. Once the shear stress overcomes the shear strength of the element, plastic deformation takes place, with the strains prescribed to happen by the flow rule in the direction determined by fault orientation and shear stress, as well as the dilation or compaction of sheared material. At the same time, permeability of the material can be updated, depending on the stress state and on the plastic strain.

With the finite element approach, it is straightforward to include complex geometries and geological scenarios, such as multiple faults and/or the presence of damage zone. The successful validation and benchmarking of the numerical tool gives confidence on its capabilities of investigating such a large scale, complex scenario.

Measurement and Numerical Simulation of Thermally-induced Pore Water Pressures in Rock

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Abstract

For the past several decades, hydraulic packer systems have been used to measure the thermally-induced pore water pressures in many in-situ thermal-hydraulic-mechanical (THM) experiments in nuclear waste management programs. Measured pore water pressure is the average value of the pore water pressure in the interval of the measured bore hole between two packers. This is used to represent the value of the pore water pressure of the rock at the middle point of this measured interval between two packers. If the pore water pressure along the packer interval is not linear, the packer interval length and its direction have a significant influence on the pore water pressure measurement. This could result in significant errors when estimating the thermally-induced pore water pressure.

This paper examines the suitability of the hydraulic packer measurement system using a coupled THM model for fully saturated conditions developed with the finite element program COMSOL. Some suggestions regarding installation of a packer measurement system or numerical simulation of the thermally-induced pore water pressure are proposed to improve the validity of the pore water pressure measurements as follows:

- The variation in pore water pressure gradient along the packer interval should be small.
- If a substantial gradient variation is expected, the length of the packer interval should be made as small as possible. An interval of less than 0.5 m is suggested.
- If a packer system has been installed with a large interval length in a location where a large pore water gradient variation may exist, calibration of any associated numerical model should incorporate the packer measurement system.

This study is validated by comparing modelled results for the consolidation of an infinite homogenous saturated porous medium around a point heat source with the theoretical solution.

A Multiphysics Platform for Modelling Coupled Deformation, Damage, Flow and Transport in Fractured Rocks

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Abstract

We present a novel multiphysics computational platform for modelling coupled hydro-mechanical processes in fractured rocks including solid deformation, damage evolution, fluid flow and mass transport. We explicitly represent the geometrical complexities of natural fracture systems associated with various length distributions, anisotropic conditions and connectivity states based on the discrete fracture network approach. We resolve the stress and strain fields within the geological formations using a state-of-the-art finite element model with the damage of intact rocks captured by an elasto-brittle failure criterion and the displacement of natural discontinuities mimicked by a non-linear elasto-plastic constitutive law with strain-softening. We couple the solid deformation and damage processes with Darcy-type fluid flow within fully-saturated fractured porous media, such that important coupling mechanisms are simulated including stress-dependent transmissivity of natural fractures, poro-elastic deformation of intact rocks, and pore pressure-induced fracture slip and rock failure (Figures 1 and 2). We further link mass transport with the flow velocity field, permitting the capture of stress-induced anomalous transport behaviour like early arrival and late-time tailing of radionuclides. We deliver a few examples in the context of nuclear waste repository engineering to demonstrate the capabilities of our platform for hydro-mechanical modelling of fractured geological media.

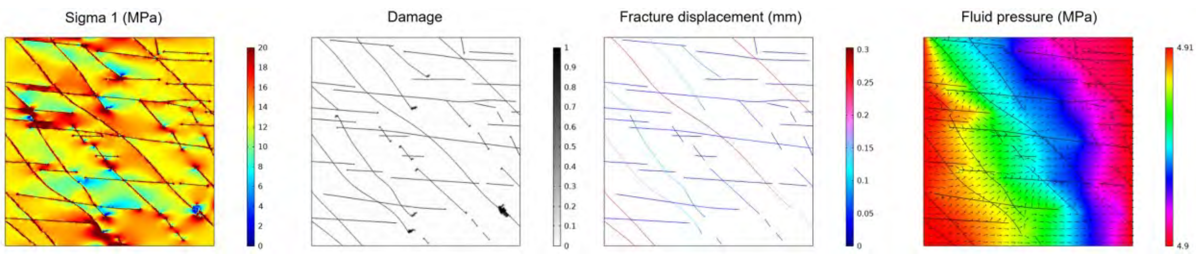

Figure 1: Simulation of stress distribution, damage evolution, fracture displacement and fluid flow in a fractured rock subjected to far-field stress loading and pore fluid pressure conditions.

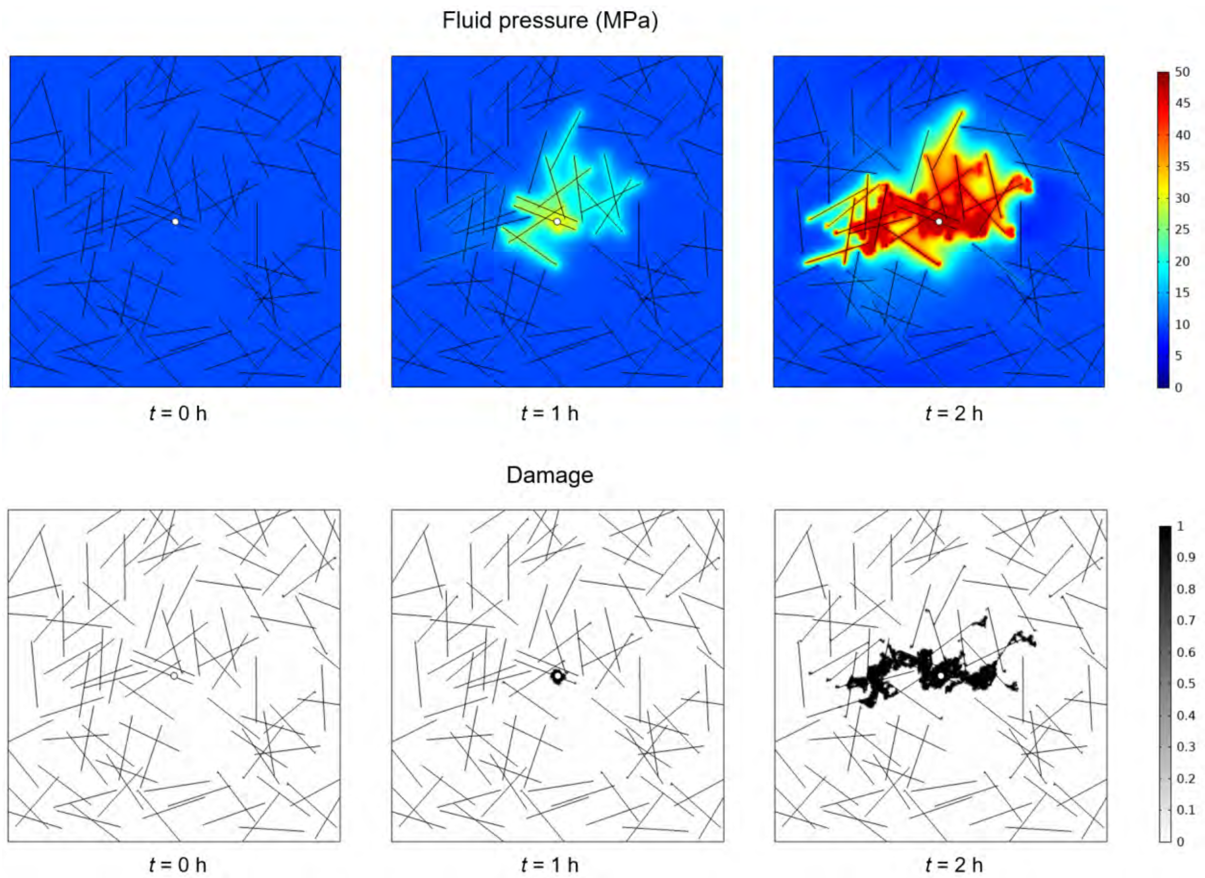

Figure 2: Simulation of fluid pressure distribution and damage evolution during the high-pressure fluid injection into a borehole through a fractured formation at a depth of 1000 m.

Accelerating Geochemical Equilibrium and Kinetics Calculations for Modeling Radioactive Waste Disposal

DECOVALEX, Brugg 2019, 4-5 November

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Keywords: geochemical modeling, reactive transport, machine learning, equilibrium and kinetics

Abstract

Reactive transport modeling is computationally expensive because it considers many coupled chemical and physical processes. We show, however, that the majority of computing time is spent, in most cases, on geochemical reaction calculations, performing chemical equilibrium and kinetics computations to model the chemical interactions among fluid species and between these and rock minerals (mineral dissolution and precipitation reactions). This is particularly severe when modeling radioactive waste disposal since chemical systems in such applications usually require many dozens to hundred of chemical species, a substantial number of pure minerals, and complex solid solutions. We present smart chemical equilibrium and kinetics algorithms that can speed up reactive transport simulations by orders of magnitude, using an on-demand learning technique in which previous geochemical problems are used for quick and accurate solution estimations of new ones. Simulations that would require weeks of computing time, could be made faster, in a couple of hours.

Decoding Nanoscale Chemical Mechanical Heterogeneity of Shale

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Abstract

Understanding chemical and mechanical properties of rock is essential for evaluating the long-term performance of subsurface rock engineering projects, such as radioactive waste storage and disposal, geological carbon storage, hydrocarbon production, underground gas storage and enhanced geothermal system. Fine-grained shales are usually caprocks, source rocks and host rocks for these projects. Shales are heterogeneous natural materials composed of inorganic minerals and organic matters including kerogen. Understanding the transport properties, stability, reactivity of shale for subsurface rock engineering projects requires a thorough understanding of material properties of shale such as pore morphology, mechanical properties and surface chemistry at the nanoscale. **This work reports a simultaneous chemical-mechanical mapping of a shale sample using a novel peak force infrared microscopy (PFIR) at a resolution of 10 nm.**

Shale core samples from the Lower Huron Shales (collected at a depth of 1721 meter) were obtained from a shale gas well at the Nora Gas Field of southwest Virginia (U.S.). Since the atomic force microscopy (AFM) measurements require a very flat surface, the fine shale powders were mechanically pressed into flat pellets under 40 MPa using a laboratory hydraulic mechanical press.

Peak Force Infrared Microscopy (PFIR) is a novel customized AFM-based infrared microscopy. It consists of an AFM with peak force tapping capability, an infrared laser source, a customized circuit for synchronization and triggering the laser, and a customized optical setup that delivers the focused infrared beam to the region of the tip and sample. The scheme of the PFIR microscopy apparatus is shown in Figure 1, where the blue arrow represents the synchronization and trigger of the laser pulse by the AFM peak force tapping cycle.

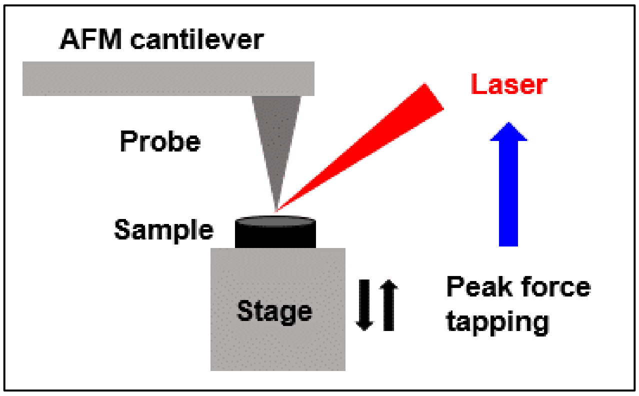

Figure 1 Scheme of the PFIR microscopy apparatus

During the measurement, the AFM is operated in peak force tapping mode. Infrared laser pulses illuminate the AFM tip and the sample when they are in contact and at every other peak force tapping cycles. Consequently, the subtraction of the cantilever deflection waveforms leads to the pure response from the laser-induced photo-thermal expansion. Subsequent analysis of the photo-thermal expansions extracts mechanical signals that correspond to the infrared absorption. Thus, both mechanical information from the peak force mode of AFM and the infrared absorption information induced by photo-thermal expansion can be simultaneously recorded and quantified.

PFIR reveals the distribution of infrared response from the composition of shales together with correlative surface tomography and mechanical properties of reduced Young's modulus and adhesion, as shown in Figure 2.

These measurements demonstrate that the PFIR has the capacity to reveal the nanoscale chemical-mechanical heterogeneity of shales. This high spatial resolution technique thus opens the door for researchers to probe the coupled chemical-mechanical processes pertinent to subsurface rock engineering projects at the nanoscale.

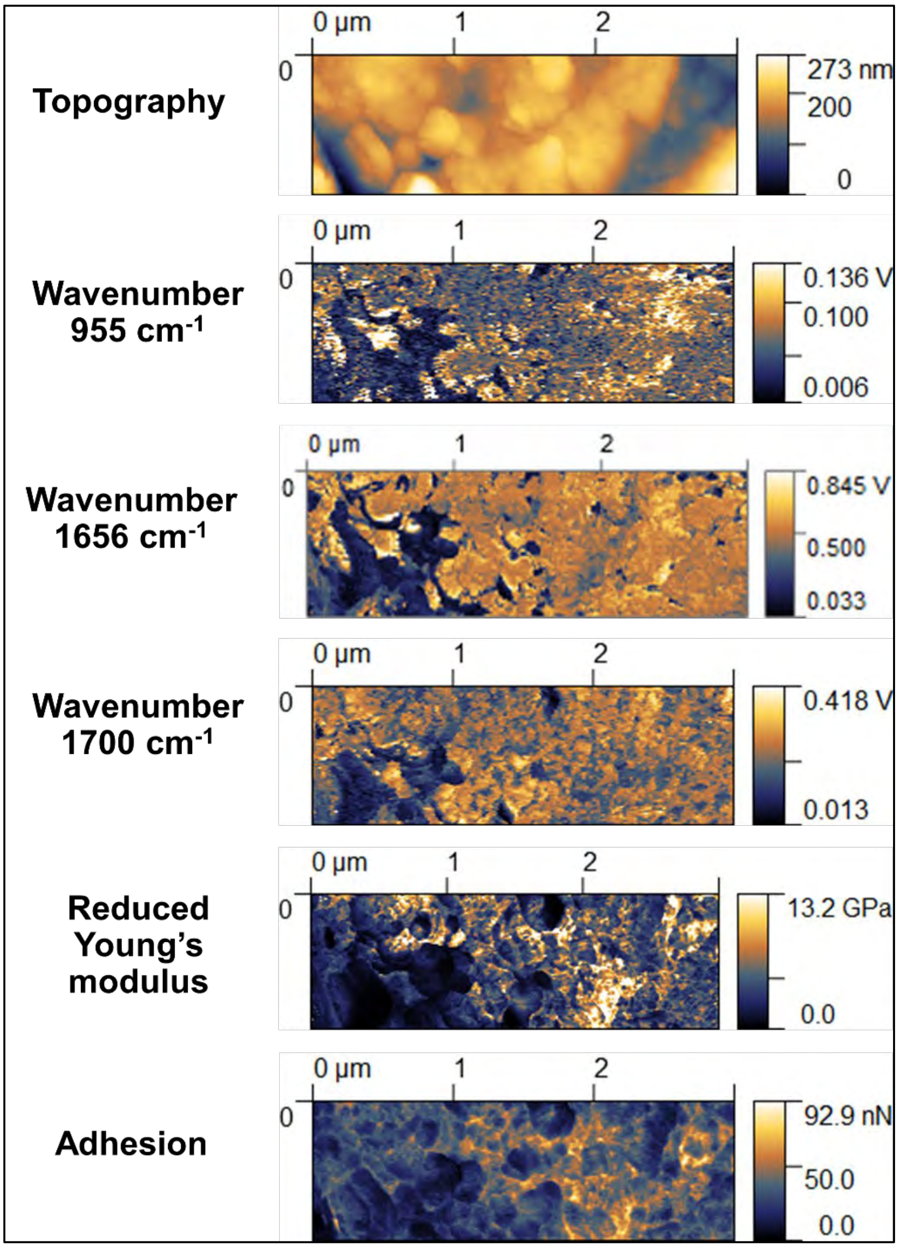

Figure 2 Nanoscale chemical and mechanical properties of the Lower Huron Shale

Hydro-mechanical processes in a single rough fracture: effect of fracture geometry

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Abstract:

The hydraulic behaviour of rock fractures is commonly approximated with the parallel plate model. However, it is well documented in the literature that this assumption leads to inaccuracies [1, 2] particularly pronounced when fractures have small apertures. Since fractures found in nature are under stress and generally have sub-mm apertures [3], it is important to improve the permeability models. Numerous efforts have been made in quantifying the impact of fracture geometry on its hydraulic behaviour [4, 5, 6]. The majority of the models were developed for static fracture geometries whereas in reality fractures are subjected to dynamic loading. Changes in loading alters the fracture geometry which affects both the mechanical and hydraulic behaviour of the fracture [3]. However, there has been little effort in characterizing the link between fracture geometry and its mechanical characteristics [7, 8].

In the current study, we investigate the effect of fracture geometry on the hydro-mechanical behaviour of a single rough fracture under dynamic loading using a light transmission technique. The novel experimental set up, designed in-house, enables us to visualize the flow field in a transparent replica of a rock fracture. The fracture replica is subjected to normal loading and the evolution of the fracture aperture and the permeability is recorded. The changes in the mean aperture of the fracture, evolution of the contact area and the average displacement of the fracture plane in every loading step are used to relate the mechanical behaviour of the fracture to its initial geometry. The hydraulic behaviour of the fracture in each loading step is characterized with the measured permeability.

The observations will also be compared against numerical simulations of the experiments and rock fractures of the same morphological properties. The employed numerical model enables us to extend and examine the experimental results for rough fractures with a wide range of geometrical properties. In future such data will be used in studying the tie between the hydro-mechanical behaviour of a rough fracture under stress with its geometrical attributes.

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BenVaSim—Introduction to a Benchmarking of TH^{2}M Simulators for Subsurface Applications with First Results

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The primary objective in many benchmarking projects in the context of radioactive waste disposal is to validate the participants' own internal approaches to the modelling of repository subsystems on the basis of measurement curves from in-situ experiments and laboratory investigations. Different ways of convert-ing the setting of a given task into a numerical model or applying self-developed mechanical constitutive models can be named as typical examples for such approaches. As a consequence, simulation results differ almost inevitably from each other and sometimes show significant mismatches. In many cases, the question, to which extent the underlying numerical methods and process-coupling relationships implemented in the simulators do have an influence on the obtained results, remains of secondary importance or simply unan-swered. Generally, it is assumed that the applied simulators work correctly, based on having verified them already to a certain extent.

The necessity of verification pertains especially for newly developed simulators as well as for the coupling of existing simulators which are each verified on their own, but not when interacting. Mainly this fact motivated the initiation of the simulator benchmarking project "BenVaSim" by TUC who has developed the simulator FTK coupling FLAC^{3D} to TOUGH2 for TH^{2}M processes in hard-rock structures in the past years. Teams from other organisations joined for verification of simulators they use for their own modelling or simply for confirmation of their simulators' correct functioning. The six different teams obtain unified model examples with geometric data and parameter sets which they subsequently simulate with their sim-ulator(s); TUC contrasts all results to each other and to analytical solutions, if available, in the end.

In order to be able to figure out reasons for possible irregularities in the results to be obtained, the range of model examples in the BenVaSim project starts with stylised one-dimensional models where causes and effects appear rather straightforward. Models covered in this stage of the project contain single- and two-phase-flow processes, poroelastic deformation behaviour, heterogeneous material properties, and the inter-action with heat and gas sources. Along with an introduction to the project, first selected results for 1D model examples are presented. Although these stylised model examples might appear trivial to simulate, issues already evolved around e.g. some simplifications and settings not being processable by some of the simulators, numerical divergence during system balancing, inconsistent consideration of HM coupling ef-fects, and inappropriate discretisations.

Integrating Near-Field THMC Processes into Field-Scale THC Simulations for Nuclear Waste Repository Performance Assessment

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Abstract

Performance assessment of subsurface nuclear waste repositories can require three-dimensional simulation of highly nonlinear, thermo-hydrological-mechanical-chemical (THMC), multiphase flow and transport processes on large length scales (many kilometers) and over long timespans (tens to hundreds of thousands of years). In the near-field, geomechanical changes immediately surrounding a repository can significantly impact radionuclide transport via alteration of permeability. While far-field transport is generally sensitive to permeability and thermal conductivity (as well as anisotropy in these properties), geomechanical changes over time are likely not as significant as in the near-field. The computational complexity involved in simulating all such fully-coupled processes at the near-field scale while also capturing far-field physics can pose a significant challenge to efficient PA simulation, especially when taking a probabilistic approach. This work presents an integrated approach to approximating near-field geomechanical behavior in PA-scale thermo-hydrological-chemical (THC) simulations using PFLOTRAN, a massively parallel reactive flow and transport simulator. This work demonstrates this approach by simulating a repository in a saturated shale host rock with a bentonite backfill. As the backfill re-saturates, it swells, which works to close fracture pathways in the disturbed rock zone (DRZ) between the repository and intact host rock. A fractured DRZ presents possible high-permeability radionuclide transport pathways that can link the repository to the far-field; therefore, simulating the evolution of DRZ permeability may be important for prediction of PA-scale radionuclide transport. This work employs TOUGH-FLAC using the Barcelona Basic Model (Rutqvist et al., 2011) to simulate fully coupled THMC processes in near-field 3D simulations to derive a functional relationship describing swelling stress of the bentonite backfill as a function of water saturation. This function is then implemented in PFLOTRAN 3D THC simulations at far-field scale through a permeability-effective stress relationship in the DRZ to model DRZ permeability evolution as a function of bentonite swelling stress via water saturation in the bentonite. This work shows that this implementation is able to adequately approximate the effects of geomechanical processes on permeability in the near-field while also providing a computationally efficient means of approximating effects of nearfield geomechanical behavior on far-field radionuclide transport.

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Thermal-Hydrologic Design Constraints for the Disposal of High-Heat Waste Packages in a Deep Geologic Repository

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Abstract

In the absence of licensed geologic repository for spent nuclear fuel (SNF), the U.S. nuclear reactor fleet is accumulating more than 2000 metric tons of SNF per year in on-site dry storage systems. Most of the fuel-rod assemblies are containerized in dual purpose canisters (DPCs) that can be used for both on-site storage and transportation to an interim storage facility or final repository site. Several commercial DPC designs are currently in use, with a trend toward more SNF assemblies per DPC, but generally in the range of 21 to 39 PWR assemblies per DPC. In the interest of worker safety, it would be desirable to directly dispose each DPC in the final geologic repository without having to repackage the assemblies into smaller disposal canisters. However, DPCs have a much greater energy output at the time of disposal than previously considered waste packages. Consequently, DPCs represent unique challenges in tightly-coupled multi-phase thermal/hydrological modelling during the first few hundreds of years after disposal, while the packages generate large amounts of heat that must be dissipated through the engineered and natural barriers. In this work, simulation models at various scales are used to explore engineering design parameters for DPC disposal.

The DPCs considered in this work represent existing 24 PWR arrays of 40 GWd/MTU fuel, 100 years out of reactor. The hypothetical host rock is a partially-saturated alluvium formation 250 m below the surface with small infiltration and a water table 550 m deep. Models are built to study the near and far-field impacts of various engineering criteria using PFLOTRAN, a massively parallel reactive flow and transport simulator.

The smallest-scale model represents a single DPC in the center of a large waste-package array and is used to study the thermal conductivity and permeability of engineered backfill necessary to avoid temperature over 350°C and pressure build-up at the waste package and within the emplacement drifts. The intermediate model represents an array of 16 DPCs in four drifts and is used to explore the drift spacing required to moderate temperature and avoid dry-out of the formation between the drifts. The largest simulation model is a performance-assessment (PA) scale array representing disposal of 1350 DPCs with parameters informed from the two near-field studies.

The range of temperatures and pressures encountered in the DPC scenarios present a challenge to simulate, as both fluid saturation and pressure change very quickly in the near-field. For several combinations of parameters temperature in the waste packages exceeds 350-400°C. Simulations are halted when 350°C is reached anywhere in the domain, as such extreme temperature could change rock and backfill properties and would not be acceptable at a disposal site.

The parameter study indicates that high thermal-conductivity engineered backfill will be needed for disposal of 24 DPCs in an unsaturated alluvium formation. Unexpectedly, disposal in the higher permeability rock in the formation is favorable because the lower initial water saturation results in a smaller pressure increase caused by steam generation. Finally, large drift spacing will be needed to. prevent complete dry-out of the formation.

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Diffusion Simulation of Radionuclide Transport and Sorption Processes in the Opalinus Clay

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Abstract

One of the major challenges for future generations is the storage of nuclear waste for more than 1 million years. According to current knowledge, deep geological repositories are the safest way to store especially high-level radioactive waste over long time periods.

This work focuses on the migration of radionuclides from a hypothetic repository through its host rock. Besides crystalline and salt rocks, claystones are favourable host rocks for geological storage of nuclear waste due to low permeability and retardation of transport by sorption. In the present study, the Opalinus Clay is considered as an example host rock due to the availability of a comprehensive database elaborated during more than 25 years of scientific activities in the Mont Terri underground research laboratory (Switzerland). We apply numerical reactive transport simulations to assess the long-term safety of a repository.

Diffusion models are employed to quantify the migration of radionuclides in claystones by means of the diffuse double layer theory, anion exclusion and interlayer diffusion between the clay layers, taking into account sorption processes on the different clay minerals. In this context, porewater is divided into three different types at the micro-scale: free porewater, porewater bound in the diffuse double layer and that bound in between the clay layers.

Simulations are conducted by coupling a Python-based 1D finite difference diffusion model with PHREEQC to model the transport of radionuclides through the Opalinus Clay, quantifying sorption processes via inner- and outer-sphere complexes and ion exchange. Diffusion models are applied to assess the upward radionuclide migration into shallow groundwater aquifers, depending on the different facies and resulting variations in porewater composition.

Our simulation results show, that the different facies of the Opalinus Clay and with it their variations in geochemical composition affects the sorption capacity. An individualized approach is required for any host rock.

Use of High Performance Computing Cluster for Reactive Transport Modelling

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Abstract

There are several software tools for the simulation of reactive transport problems which can be usually used for description of small 2D transport problems with full geochemistry or of real-world 3D transport problems using simplified chemical reactions. High performance computing seems to be the only possible way to solve real-world 3D problems with full chemistry, but not many applications have been presented due to high computing time requirements.

In the frame of project supported by the Technology Agency of the Czech Republic (project number TH02030840) such an HPC tool is being developed and tested for use for long term deep radioactive waste repository simulations for the Czech Radioactive Waste Repository Authority and also for any other purpose for other customers.

The solution is based on FEFLOW (Finite Element subsurface FLOW system) software for simulation of groundwater flow, mass transfer and heat transfer in porous media and fractured media offered by DHI A/S (www.dhigroup.com). It uses finite element analysis to solve the groundwater flow equation of both saturated and unsaturated conditions as well as mass and heat transport, including fluid density effects. It is very efficient for 3D transport problem modelling. Coupling FEFLOW with widely used PHREEQC software for equilibrium and kinetic reaction calculations, specifically PhreeqcRM code available on USGS web site and use of supercomputer power allow combine full 3D transport simulation with full reaction including minerals, exchangers, surface complexers, gas phases, solid solutions, and user-defined kinetic reactants.

The coupling component is based on the operator-splitting approach. Flow and transport simulation in FEFLOW are performed sequentially over time steps of size according to the robustness conditions of the numerical solution. The reaction module is being called for all spatial elements within one time step which allows massive parallelization. The coupling component uses several tricks to parallel this call in order to reduce the total computing time.

Testing of the coupled software shows that for successful real-world problem solution the chemical model should be also constituted “a tricky way”. The computational performance of the PHREEQC software strongly depends on the length of the used thermodynamic database and the accuracy of PHREEQC computations strongly depends on the completeness of the database.

The way of a clever cutting of the database will be presented together with principles of the efficient coupling.

Another problem being solved is a parallelization of sensitivity analysis. It is based on FePEST calibration software (DHI A/S), which implements PEST - "Model Independent Parameter Estimation and Uncertainty Analyses" (Doherty, 2015). When PEST calculates derivatives of model outcomes with

respect to adjustable parameters using finite parameter differences, successive model runs are completely independent (the parameters used for one particular model run do not depend on the results of a previous model run). It allows a parallelisation of the whole process distributing independent model runs to different HPC cluster nodes.
The presented coupled software tools on the HPC cluster at IT4I in Ostrava are intended be accessible for users out of the project during the year 2020.

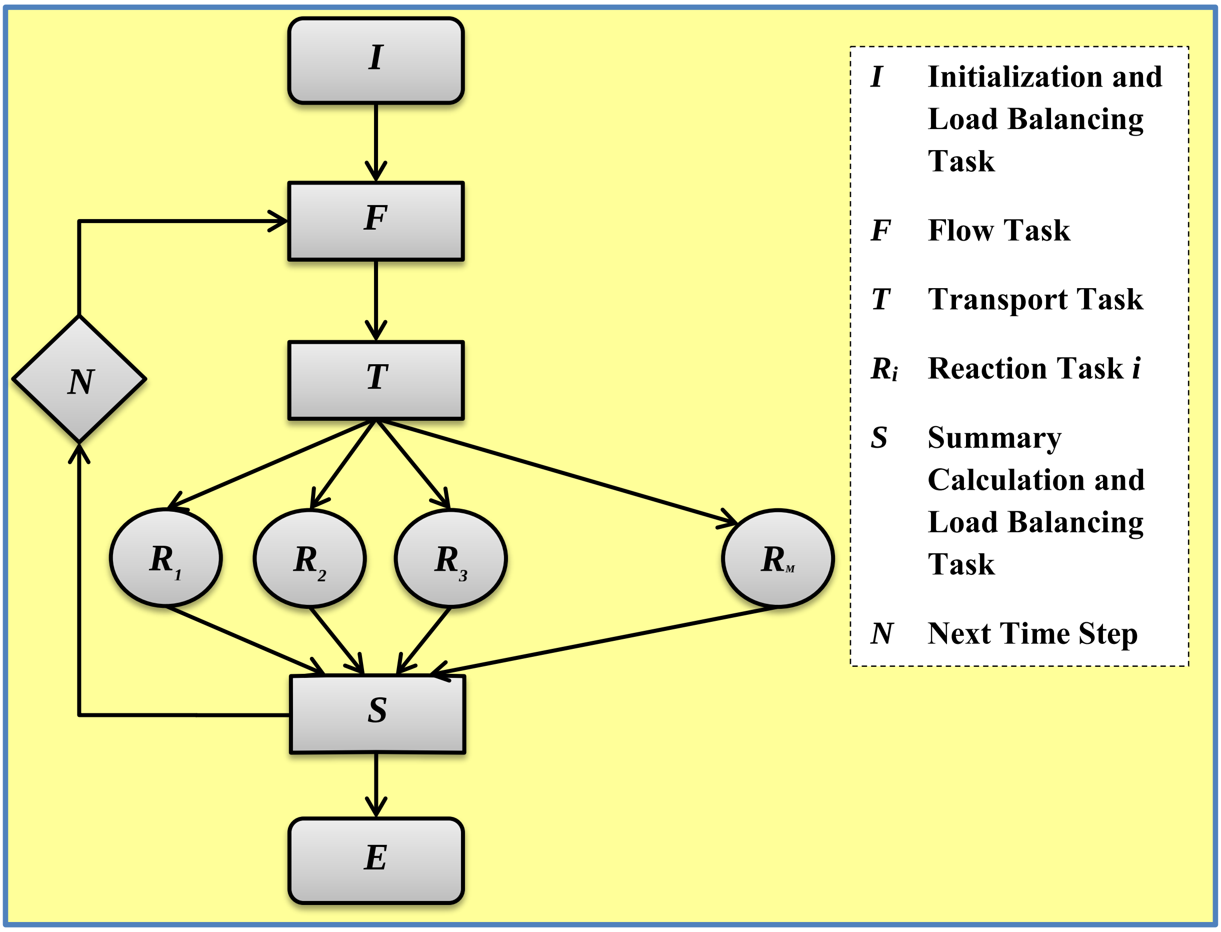

Figure 1: Scheme of the parallel reactive transport computation

On Conceptual Models of Chaotic Advection and Diffusion in Fractured-Porous Media

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Abstract

Nonlinear dynamical hydro-thermo-chemical processes in fluid-saturated porous media have been considered in the past few decades for wide ranges of scientific and practical applications, such as petroleum reservoirs, geothermal science, hydrology, and environment pollution. Experimental and theoretical studies indicate that nonlinear dynamical processes, such as chaotic advection and chaotic diffusion, are inherent to flow and transport through fractured-porous media, including sediments (granular media) and fractured rock. These processes are generated due to the intrinsic topological complexity of the pore-scale and fracture network architecture. The flow path network causes multiple saddle points even under steady flow boundary conditions. This network causes fluid stretching and forms a 3-D fluid mechanical analogue of the baker's map, which is a typical diagnostic feature of chaos, and which generates chaotic advection. The persistent and ubiquitous nature of this phenomenon has profound fundamental implications for the study and upscaling of a wide range of fluid-borne processes including thermal convection, transport, mixing, chemical reactions, and biological activity.

Fluid dripping and film flow are typical for in fracture flow, causing chaotic advection in fractured-porous media. Chaotic advection provides a mechanism for anomalous transport and accelerated dispersion in fractured-porous media, and leads to enhanced chemical reaction kinetics. Anomalous diffusion, which exhibits nonlinear growth of mean square displacements, can be caused by a chaotic mechanism of fluid diffusion.

For the case of thermal convection in high-porosity media with heat source, Lorenz and Ginzburg-Landau models can be used, which both demonstrate phenomena of nonlinear instability of thermal convection. The transition from steady convection to chaos can also be demonstrated based on application of the effect of Darcy-Brinkman couple stress parameter model.

Quantification of nonlinear dynamics involved in chaotic advection, chaotic diffusion, and thermal convection in various types of fractured-porous media would be an essential component of research on hydro-thermo-chemical processes related to the long-term performance of nuclear waste disposal sites.