DEVELOPMENT AND VERIFICATION OF MODELLING METHODS FOR THMC PROCESSES WITHIN THE INTERNATIONAL PROJECT DECOVALEX 2019
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Annex 2: DECOVALEX 2019, Task D – Modelling the EB experiment: model formulation, implementation, results from 3D model, p. 34 (Blaheta et al., 2018)

List of electronic attachments:
Task C – “TASK_C_GREET(Zadani).ppt” (Iwatsuki, 2016)
Task D – “INBEB Task description - Stage 1 v1.pdf”, “INBEB Task description – Stage 2 v0.pdf” (Gens, 2016b, 2016c)

Data provided for Task D – files in a directory structure located on the Sievert server of SÚRAO
Data provided for Task C – files in a directory structure located on the Sievert server of SÚRAO, source http://www.jaea.go.jp/04/tono/miu/dataset/greet/greet.html

Data provided for Task G – ZIP archives located on the Sievert server of SÚRAO
Data files with results of the models (files in a directory structure located on the Sievert server)
List of abbreviations:

CTD Closure Test Drift
DECOVALEX Development of Coupled Codes and Their Validation against Experiments
DGR Deep Geological Repository (of radioactive waste)
EB Engineered Barrier Emplacement Experiment
EBS Engineered Barrier System
EDZ Excavation Damaged Zone
ENRESA Empresa Nacional de Residuos Radioactivos (Spanish radioactive waste authority)
FEBEX Full-scale Engineered Barriers Experiment
FEM Finite Element Method
GREET Groundwater REcovery Experiment in Tunnel
GWB Geochemist’s Workbench
HM Hydro-Mechanical
INBEB HM and THM Interactions in Bentonite Engineered Barriers
JAEA Japan Atomic Energy Agency
KAERI Korea Atomic Energy Research Institute
LSFD Lower Sparsely Fractured Domain
RAW Radioactive Waste
RN Radionuclide
SKB Svensk Kärnbränslehantering (Swedish spent nuclear fuel authority)
SNF Spent Nuclear Fuel
SNL Sandia National Laboratories
SNU Seoul National University
SSM Strålsäkerhetsmyndighetens (Swedish radiation safety authority)
SW Software
THM, THMC Thermo-Hydro-Mechanical (-Chemical)
TUL Technical University of Liberec
IGN Institute of Geonics AS CR
UOS Waste Packages of Spent Nuclear Fuel
UPC Polytechnic University of Catalonia
URL Underground Research Laboratory
Abstract
The report describes model calculations made within the participation in the DECOVALEX-2019 international project. Its content is solving tasks of numerical simulations of thermo-hydro-mechanical processes according to experimental data. The tasks are selected by deep repository implementors in participating countries, hiring the research teams for their solutions. The tasks represent processes important for the repository safety assessment. The Czech institutes TUL and IGN participated in three Tasks. In Task C, the effects of the excavation of the experimental tunnel in the granite in the Mizunami Underground Laboratory in Japan were predicted in terms of pressures and water movements detected by the concentration of the tracers, and the groundwater geochemical composition throughout the laboratory was then evaluated to support the transport modelling. In Task D, the EB experiment in Mont Terri, Switzerland, in clay rock was modelled – the prediction of the effect of artificial hydration of bentonite blocks and pellets is calculated, obtaining e.g. the homogenization of the dry density. Task G firstly solved synthetic problems demonstrating EDZ phenomena around the tunnel, with expression of a differently defined fracture network on the distribution of water pressures and rock stress, then continued with evaluation of hydraulic tests in boreholes from the TAS04 experimental tunnel in the Äspö Underground Laboratory. In all cases, the results have already been compared with other investigators in international teams and the eventual difference have been explained.

Keywords
Thermo-hydro-mechano-chemical phenomena, modeling, simulation, model validation, DECOVALEX, GREET, EDZ, EB experiment, Mizunami, Mont Terri, Äspö
Abstrakt


Klíčová slova

Termo-hydro-mechano-chemické jevy, modelování, simulace, validace modelu, DECOVALEX, GREET, EDZ, EB experiment, Mizunami, Mont Terri, Åspö
1 Introduction

This report was prepared as a part of the SÚRAO project “Research support for the safety assessment of a deep geological repository” which forms an important part of the preparation phase for the construction of deep geological repositories for radioactive waste (hereinafter DGR). The aim of the project is to obtain the selected data, models, arguments and other information required so as to be able to evaluate potential sites for the location of such a repository in terms of long-term safety. Following the conducting of a public procurement procedure, a four-year contract was signed in July 2014 with ÚJV Řež, a. s. and its subcontractors: The Czech Geological Survey; The Czech Technical University in Prague; The Technical University of Liberec; The Institute of Geonics of the CAS, v. v. i.; ARCADIS CZ a. s.; Progeo, s. r. o.; Chemcomex Praha, a. s.; and Research Centre Řež s. r. o. concerning the provision of research support for long-term safety assessment purposes in the following areas:

- The behaviour of spent fuel and radioactive waste (which cannot be accepted for near-surface storage) in an underground repository environment;
- The behaviour of storage casks for spent fuel and radioactive waste in an underground repository environment;
- The behaviour of damping, filling and other construction materials in an underground repository environment;
- The final design of the storage wells and their influence on the properties of the surrounding geological environment;
- The behaviour of the rock mass;
- The transport of radionuclides from the repository;
- Other characteristics of the sites which might potentially affect the safety of the repository.

It is a complex project, containing individual subprojects – one of them is the project DECOVALEX-2019 (the acronym is used both in the sense of the subproject as mentioned above and in its primary sense as the particular stage of the international project described below). Its aim is a comparison of model solutions for the evaluation of a range of selected phenomena in the rock environment related to the transport of radionuclides, in the framework of an international team. For SÚRAO, the purpose is to understand the phenomena in the rock environment and the engineered barrier based on data from foreign experiments (recovery of groundwater conditions after closure of a repository, interaction of rock with the engineering barrier and the relevance of tests in boreholes for the real rock properties), which will also be significant in the Czech DGR program, and verification of the professional level of the project members by comparing them with foreign modelling teams.

The international project DECOVALEX (Development of Coupled Models and their Validation against Experiments) is a project of international collaboration in the field of the development of tools and methods for mathematical modelling of coupled thermal, hydraulic, mechanical and chemical (THMC) processes in a geological environment. In order to evaluate the safety features of engineering barriers over thousands of years under the influence of THMC processes, it is necessary to obtain appropriate methodological procedures to predict the development of the engineering barriers and the rock environment of the repository. The involvement of SÚRAO and Czech organizations in this project will facilitate the development and validation of modelling codes for these processes for conditions in the Czech Republic.
DECOVALEX is a platform for the long-term collaboration of organizations responsible for SNF disposal in different countries, with a history since 1992. These institutions act as so-called Funding Organizations, appoint their representatives to a Steering Committee, which defines the task descriptions and their Task Leaders. Research teams working on the solution are tied to one of the funding organizations. The project is organized in four-year stages, in which a fixed set of Tasks is solved; the current stage is known as DECOVALEX-2019 and lasts for the period 2016-2019.

In order to gain a deeper understanding of THMC modelling, SÚRAO is involved in the following tasks through the project team:

- Task C (GREET) Hydro-mechanical-chemical-biological processes during groundwater recovery,
- Task D (INBEB) – Hydro-mechanical interactions in bentonite engineered barriers,
- Task G (EDZ) Evolution – Reliability, feasibility and significance of measurements of conductivity and transmissivity of the rock mass for the understanding of the evolution of a repository of spent nuclear fuel).

These selected Tasks have the closest factual connection to the knowledge acquiring needs for building DGR in the Czech Republic and also best correspond to the professional focus, experience and software background of the project team.

Experimental data for Task C - GREET was provided by the Japanese Atomic Energy Agency (JAEA) from the Mizunami underground laboratory. This laboratory was built in 2004-2011 and serves to gain experience on the behaviour and development of the geological environment, including a study of the THMC processes. The Task C project team modelled processes during the flooding of one branch of the gallery located at a depth of 500 m as an analogue closure of the repository for the purposes of assessing the recovery of the hydraulic and chemical conditions of the groundwater to conditions prior to the excavation. The development of pressures and the chemical composition of water during the excavation and flooding was monitored. Teams from JAEA and Sandia National Laboratories (USA) participated on this Task.

The aims of the participation and solution for the requirements of SÚRAO were to evaluate data of the flooding process, mediate in the conclusions of other teams and use the data on the flow and solute transport on a medium scale to demonstrate and validate the Flow123d software and in general the possibility of the concept of multidimensional interconnection. The connection of flow and transport modelling with geochemical analysis represents a unique feature of the participation, and the site also contains a specific distribution of concentrations with depth dependence, which provides an opportunity to use the data for the model as a natural tracer. Because of the complexity of the environment, however, this theme remains as an open issue for future solutions.

Task D - INBEB (Interactions in Bentonite Engineered Barriers) deals with HM and THM interactions in bentonite barriers. The first part of the DECOVALEX 2019 project, described in more detail in this report, is dedicated to the modelling of HM processes in the bentonite barrier EB experiment conducted by a team led by the Spanish ENRESA institution in the Mont Terri underground laboratory in Switzerland. A total of five research teams were involved in the modelling during Task D.
In the EB experiment, a horizontal concept of storing and sealing the space around a dummy storage canister is used. The combination of bentonite blocks with buffering of the remaining space with bentonite pellets and a duration of 8.5 years are some of the unique features of the experiment. In addition to data from the monitoring of hydro-mechanical processes during gradual saturation, data from the disassembly of the experiment and verification of the homogenization of the fill are now available. These data were used to verify the model. In terms of the interests of SÚRAO, which are related to the design of DGR in the Czech Republic, the model is created and verified as a tool for assessing various different concepts of bentonite barriers.

Experimental data for Task G - EDZ was provided by the Swedish SSM institute (in collaboration with SKB) in the Åspö underground laboratory. The aim of the project team was to verify the feasibility, reliability and relevance of in-situ hydraulic conductivity measurements of the rock matrix and the transmissivity of fractures at the time of closure of the repository by means of mathematical modelling of HM processes. The mathematical models are based on data obtained from the TAS-04 experiment. In addition to the domestic project team, this Task was also performed by researchers from Germany (Geomecon) and South Korea (SNU under the authorization of KAERI).

The report is organized into chapters based on the individual Tasks. The internal breakdown of each Task contains a part with the task description and a part with an evaluation and discussion; the remaining subchapters are structured according to the material content of the solution (stages, model types, etc.). The extent of the chapters is based on the different needs of the presentation of the partial steps of the solution process. In the case of Task D, the final results are included in a separate report for the DECOVALEX project (Annex 2 in English), while for Task C, an interim report for DECOVALEX (Interim Report, Annex 1 in English) was prepared reflecting the situation up to approximately September 2017, and the subsequent process of the solution is consequently included in its entirety without further reference.

For the sake of clarity, Task C is divided into two main chapters. The first corresponds to the above-mentioned structure and follows the main line of the task description. The second processes the provided geochemical data with respect to their wider significance, additional to the task description itself. The task description also covers the geochemical development, but in the case of granite processes, it first requires an understanding of the situation prior to the experiment, i.e. the natural conditions subsequently affected by the mining work. The analysis of geochemical data is more extensive, it is a different subject and has a different set of methodologies compared to the simulation of flow and transport, which are at the core of the task description; therefore, the authors consider the used breakdown as being expedient.

With regard to the ongoing solution of the Task in the framework of the international DECOVALEX-2019 project, this report describes the final status of the solution in relation to SÚRAO’s project contract, but only the partial status in relation to the international team and Task Leaders.
2 Task C – GREET

Task C of the DECOVALEX project is based on the issue of “groundwater recovery”, i.e. the processes leading to the return of the conditions of the groundwater in the surroundings of the repository after its closure to the state before the excavation, which include the hydraulic conditions (pressures, movement), chemistry, and parameters controlling these phenomena (opening of fractures). This supports the question of how to verify whether conventional means of monitoring phenomena in underground laboratories or during investigation and construction works are able to provide data on rock conditions that will subsequently be relevant also for determining the conditions for the stability of engineering barriers and radionuclide migration in a later period. This is a hydraulic and geochemical task, with geomechanics also playing a significant role (the coupled hydro-mechano-chemical problem).

The designer and Task Leader of Task C is Dr. Teruki Iwatsuki of the Japan Atomic Energy Agency (JAEA). The research teams involved are from JAEA, Sandia National Laboratories USA and TUL.

The task description is based on the use of data from the GREET project performed in the Japanese Mizunami underground laboratory under conditions relevant to crystalline rocks (Iwatsuki, 2016). During the time used for the project, the experiment consists of one drainage stage and one stage of flooding of the end section of the gallery of approximately 50 m (updated as opposed to the multiple cycles mentioned in the first version of the task description from 2016). Pressure conditions of water and rocks are monitored in the nearby boreholes (both from the gallery and parallel to it). Inhomogeneity, i.e. fissures, fractures, is also included in the process. According to the proposed time schedule, the project is divided into experimental stages (drainage, flooding, steady state), as well as the initial prediction stage (blind, without monitoring data) and the subsequent calibration stage (evaluation against monitored data and modification of the model). This structure was also slightly modified compared to the original proposal in the framework of DECOVALEX (which also included a breakdown in the contract for SÚRAO’s sub-project).

The modelling partially includes a long-term time scale prior to the experiment, i.e., the course of changes in the conditions during the excavation process, in order to obtain the relevant initial state at the beginning of the experiment.

The Task also includes modelling and data processing of chemical processes in the groundwater and the flooded CTD gallery. Due to its extent and the looser factual links to the specified time stages of the project, there is a separate chapter devoted to this issue (ch.3).

2.1 Summary of the task description and evaluation of the data provided

The data is provided to the project investigators directly from JAEA, a Japanese institute with a wide competence in the field of nuclear energy, including the issue of spent fuel storage and the operation of the Mizunami underground laboratory (http://www.jaea.go.jp/04/tono/miu_e/, Fig. 1). A special website is set up for DECOVALEX-2019 for the transfer of data http://www.jaea.go.jp/04/tono/miu/dataset/greet/greet.html (JAEA, 2018)
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where links are available for downloading individual data packages divided based on form and individual fields of science (also an electronic annex to this report). The data are divided into three sets (Set1-Set3) corresponding to the individual stages of the performance of the GREET experiment so that it is possible to combine prediction modelling (without knowledge of the monitoring from the time period, which is the subject of the simulation) and subsequent calibration and validation of the model using an extended data set from the monitoring. The links include a list of literature published in scientific journals and conferences, as well as in reports of radioactive waste management organizations.

2.1.1 Location and experiment

The Mizunami underground laboratory is located in central Japan, approximately 50 km northeast of Nagoya, in a crystalline rock environment. The elevation of the terrain is 150-200 m, the laboratory reaches a depth of 500 m below the surface (Fig. 1), i.e. 300 m below sea level (the distance from the coast is approximately 50 km). The underground spaces were mined between 2004 and 2011 (reaching a depth of 500 m), and individual wells and horizontal galleries for specific research tasks were added in the subsequent years. The boreholes are numbered with a code, where the first two digits indicate the year of drilling and the end is a global sequence number (an example for the surroundings of the experiment is included in Fig. 3).
The GREET experiment is located at a height of -500 m in the northern gallery. It consists of a sloping access gallery and a closure test drift (CTD), approximately 50 m long (Fig. 2). At the beginning, the approximately 100 m long pilot borehole 12MI33 was drilled for performing hydraulic tests and sampling and subsequently for monitoring the pressures and chemical composition of water during the excavation, drainage of the experiment and flooding. After the corridors were excavated, several other shorter boreholes were made directly from the section for flooding, for the placement of additional monitoring points during the flooding phase (Fig. 3).

![Diagram of the GREET experiment](based on Iwatsuki, 2016)

**Fig. 2** Diagram of the GREET experiment (based on Iwatsuki, 2016)

![Overview of data used for the calibration model](Step 3a – complete system (based on Iwatsuki, 2016).

**Fig. 3** Overview of data used for the calibration model in the flooding phase (Step 3a) – complete system (based on Iwatsuki, 2016).
2.1.2 Hydraulic data

The provided data are mainly in the form of rock permeability data and monitoring of changes in pressure in a large number of locations, both in deep boreholes and in horizontal and vertical boreholes in the underground laboratory. The packer sections for measuring vary from 0.7 m to 100 m. The monitoring period for the first and the second of the provided data sets (Set 1) is defined by the date 31 March 2013 (preceding the excavation of the CTD, which should be simulated as a predictive model), in the next step of the project (Set 2) by the date 31 March 2014 (which contains the first data from new boreholes in the surroundings of the CTD after excavation) and 31 December 2016 (after a period of less than a year of flooding).

An MS Excel table was provided with data on individual pressure/pump tests for the evaluation of the permeability and the time development of the pressure in the monitored sections, as well as the more globally processed hydrogeological concept of the whole site (Fig. 4) and statistically processed data for selected rocks/aquifers or fractures - horizontal and vertical hydraulic conductivity (longitudinal and transverse), porosity and specific storability.

Other auxiliary data from geological mapping and from well logging in boreholes are provided in the form of graphical diagrams - lithostratigraphic descriptions, numbers and orientation of fractures, classifications of rock quality, weathering/alteration, geophysical quantities. The results of the initial hydrogeological studies are also presented in scientific publications (Saegusa et al, 2003 and Watanabe et al., 2004).

![Fig. 4 Hydrogeological model of the site elaborated by the Task Leader (Iwatsuki, 2016).](image-url)
The data show several of the phenomena and properties that are the basis for the presented modelling:

- The interface between the overlying rock (sediment) and the granite massif, which is the subject of the investigation, is located at an elevation of -50 to +100 m, i.e. approximately 100-200 m below ground level. This is evident from the well-logging diagrams, the layout of the hydrogeological model and the pressure monitoring (below).
- The groundwater level in the upper aquifers is at an elevation of approximately 200 m (max. first tens of meters below the surface) and is minimally affected by the excavation of the underground space, whereas in the granite the piezometric head decreased during the excavation from approximately 150 m to 50-100 m. In addition, in most cases, the piezometric head is virtually without any vertical gradient within the rock blocks or layers, and has a distinct discontinuity on the upper boundary of the granite block.
- The determined water inflows and permeability in borehole 12MI33 along the prepared experiment are irregular and confirm the inhomogeneity of the granite permeability along the irregularly located fractures and faults - the measurements made on six sections of 100 m are relatively inaccurate for distinguishing the individual permeable structures.
- Although they should be a subject of the prediction, the graphical outputs of the reaction of pressure in borehole 12MI33 on the excavation of the CTD and the communication test between the two boreholes across the CTD were shown in the presentation of the Task. It provided examples of both the significant communication and minimal impact on distances of a few meters. This shows that the model needs to focus on inhomogeneities; on the other hand, it could be expected that it would be very difficult or impossible to predict communication in the CTD only on the basis of a pilot borehole (12MI33) and partial knowledge of faults from mapping of the inclined access gallery and its effect on the monitored pressures. On the contrary, this proved to be a challenging task for the calibration in Step2a.

From the monitoring data provided after the model was processed, the following main findings were made relating to the previous blind prediction:

- There were varying degrees of pressure drop, from slight to severe, due to the effect of drainage during the excavation. In addition, various irregularities were seen, partly explained by the mechanical consequences of seismic phenomena (their location on the timeline is included in the provided xls files). However, these were not taken into consideration in the models.
- The pressure drop was only very roughly captured in the data due to an interruption of the data recording during the excavation.
- For a more effective calibration, there was a lack of detailed spatial distribution of discharges (only the total amounts from the inclined drift and the CTD), only one time was originally provided, but minimal changes were seen in the subsequently provided data.
- Partial changes during the tests before final closure of the plug were complicated and were ignored in the modelling.
After closing the plug and buffer the CTD, the pressure increased to varying levels as predicted, the pressure directly in the CTD reached a maximum after several days and then gradually decreased in the subsequent months.

2.1.3 Data on chemical composition

Data are provided from the regular chemical analyses at varying intervals (typically quarterly, in selected periods weekly) in almost all of the defined packer intervals of the boreholes and in the shaft discharges. The monitored intervals are the same as for the pressures. They are evaluated in detail in Chapter 3. The chemical composition is in some cases supplemented with concentrations of isotopes used for dating, i.e. stable isotopes $^2$H and $^{18}$O, tritium, carbon $^{13}$C and $^{14}$C.

The provision of data, similar to the pressure patterns, is divided according to the planned stages of prediction and calibration: the first section up to the beginning of the CTD excavation (March 2013), the period during the excavation and shortly thereafter and the third period during the flooding of the CTD gallery.

For the task description of Task C, the main components were chloride ions, which are the dominant components and were considered unreactive in the formulation of the task, with the role of a tracer - the concentration in an unaffected condition is significantly dependent on the depth with relatively small variations compared to the regression function (see Chapter 3 for more details). An increase in concentrations over time can then be interpreted as the effect of “upconing” and a decrease in concentrations as the effect of downward flow. However, the actual conditions at the site are more complex: the range of concentrations for the model in the surroundings of the CTD determined in the task description based on the dependence of concentration at depth does not cover the monitored course in the next period, and there were several irregularities in spatial distribution and time trends observed in the data.
2.2 Description of the model

The tasks in this section are designed for modelling the flow (hydraulics) and transport of chloride ions as a non-reactive tracer in the individual stages of the GREET experiment, i.e. the situation in the existing underground laboratory prior to excavation of the experimental gallery (CTD), the subsequent effect of the excavation of the CTD, drainage at the time of opening the gallery, and subsequently the situation when the CTD is flooded after installing the plug.

Although the geometry and boundary conditions were defined by the Task Leader for this phase (the model is hereinafter referred to as the “CTD model”), a large-scale model was considered for the purpose of the task as part of the entire URL laboratory (the large-scale model is hereinafter referred to as the “URL model”). A large-scale model was also mentioned by other project teams in the framework of the project, and was given a specific form by the Task Leader in the conclusion of the project in order to explain the monitored course of chloride concentrations. The purpose of this model in the first phase was to estimate the pressure field in areas with the boundary conditions of the CTD model. In the case of the CTD model, several alternatives with various different boundary conditions and distributions of permeability inhomogeneity and other gradual modifications were considered in relation to the experience gained during the performance of the project and the gradually released data for use in the calibration.

The descriptions of alternatives in this final report are organised according to the individual blocks of data defining the model (geometry, parameters, boundary conditions, discretization), and not according to how they were gradually used. Only the alternatives relevant for the final evaluation of the results are described (e.g. without the configurations identified later as being inappropriate). The results included in the following chapters are then described in the order of their relationship to the steps of the task description, i.e. within the time series of the project work.

2.2.1 Definition of the large-scale model (URL model)

The large-scale model (URL model) was designed with a square base of 5,000 m edge and a height of 1,300 m. The URL laboratory was modelled as a single vertical cylinder represented by two tubes (5 m in diameter) and one horizontal cylinder representing the access shaft to the CTD experiment. For simplicity, even the experimental part was designed as a horizontal tube.

The geometry and boundary conditions are shown in Fig. 5. The model was designed as being flat on the surface without the influence of elevation above sea level. The side walls are considered impermeable (in the sense of symmetry between the outside and the inside, i.e. assuming a position out of the reach of the URL laboratory’s drainage). Excavation of the URL laboratory is simulated in the model by switching the individual sections from zero flow to zero pressure on the walls of the shaft tube (the same principle is described in detail for the CTD in Chapter 2.2.7). On the upper and lower walls of the model, the pressure values are determined with respect to the on-site measurements in two alternatives:
- Higher pressure: groundwater level is at the surface, i.e. $p=0$ (piezometric head 200 m) on upper wall of the model and $p=11$ MPa (piezometric head is 0 m) on the lower wall of the model.
- Lower pressure and higher gradient: groundwater level is 40 m below ground level, i.e. $p=-0.4$ MPa (piezometric head is 160 m) on the upper wall of the model and $p=9.6$ MPa (piezometric head is -140 m) on the lower wall of the model (the piezometric head at the laboratory level of -300 m is 45 m).

The parameters were set based on the data provided for the hydrogeological unit (UHFD, LSFD) and the data of the individual packer tests. Hydraulic conductivity was entered slightly higher than the geometric mean obtained from the packer tests $K=10^{-7}$ m/s (considered scale effect) and the storativity $S=10^{-5}$ m$^-1$.

![Diagram of the large-scale model](image)

**Fig. 5 Geometry and boundary conditions for the large-scale model (vertical cross section)**

### 2.2.2 Definition of the CTD model

From the point of view of the basic features of geometry, the conceptual model shown here is common for all of the alternatives. The external dimensions are based on the design of the Task proponent JAEA and are the same for all of the following alternatives. The model was considered as a rock block measuring 150 m in the direction of the gallery and 100 m perpendicular to the gallery in the horizontal and vertical direction (Fig. 6). A single invariable geometry is used where the CTD tunnel is represented by an empty space at its maximum range and the gradual excavation is represented only by the time variable boundary condition described in the special chapter 2.2.7. The geometry of the model retains the basic features of the real shape of the tunnel, i.e. the vertical position of the inclined drift and the CTD, and the shape of the profiles of both sections are consistent with the documentation. Therefore, the tunnel is not directly in the centre of the model in the vertical direction (Fig. 7). The geometry of the tunnel is composed of a horizontal floor, vertical walls and a semi-circular ceiling. The size is different for the inclined part and the CTD. This geometry was later changed for the fracture model, and the tunnel is approximated by the cylinder in order to facilitate the creation of the discretization mesh due to the intersections of the tunnel with the fractures. The boundary conditions on the outer sides are based on the assumption of a negligible impact of the excavation (the inclined part plus the CTD). However, various alternatives of approximation of the situation around the CTD are considered.
All of the model alternatives address the issue of the non-steady flow and non-reactive transport of chloride ions. For this task, we need to define the following additional input data:

- Hydraulic conductivity,
- Specific storativity,
- Porosity,
- Coefficient of molecular diffusion and longitudinal and transversal dispersivity.

The data were designed by the Task Leader and JAEA and are summarized in Tab. 1 for Toki granite (restructured part of the table from the Interim Report). The alternatives with spatial inhomogeneity differ gradually from these data. Hydraulic data were very well supported by other specific measurements (pressure tests in many boreholes throughout the URL, including 12MI33), the transport data were not available in a more specific form with spatial distribution.

The above-mentioned table was used to set the default and homogeneous model parameters (referred to below as REF - Chapter 2.2.8). Porosity of 0.01 is used based on the table of the defined hydrogeological units (another xls file also included in the dataset), which differs from the value of 0.001 in the table but is consistent with the values for granite in the literature. Dispersivity values, 4.3 m longitudinal and 0.43 m transversal, are lower than the usual 1/10 of the model scale, but correspond to the fact that the study is actually on a smaller scale only in the surroundings of the tunnel. The selected pore diffusion coefficient \( D_p \) is \( 5\times10^{-10} \text{ m}^2/\text{s} \), in the same order as the data in the table (the effective diffusion coefficient will be different due to the factor based on the porosity value), but its effect is small due to the dominant advection.

The gradually specified non-homogeneous model alternatives are especially important in the further solution. Only the hydraulic conductivity is considered to be variable, while the other parameters are constants due to a lack of available data. The spatial structure for the inhomogeneity was designed from two different conditions:

- The prediction phase, based only on the data of the pressure tests in the borehole 12MI33, resulted in the following “heterogeneous model” (TUL1 and TUL2 in Chapter 2.2.8) with zones of permeability perpendicular to the tunnel (differentiation of permeability in the direction of the tunnel) and the model with fractures extrapolate up to the boundary of the model (which is not part of the evaluation – see the Interim Report (Maryška et al., 2017)).
- The calibration phase, based on observation of the pressure pattern at different locations, which was explained by different modes of communication perpendicular to the tunnel and subsequently solved by a conceptual model differentiating the permeability at different distances perpendicular to the tunnel, as explained below. This resulted in a model with fractures in the block in the surroundings of the tunnel in the part of the model area – the final structure is described in detail below (hereinafter referred to as the “fracture model”).
The latter concept was based on the need to realistically capture the measured pressures in the borehole. In several borehole monitoring sections, the pressure was either higher, closer to the unaffected pressure on the boundary condition, or lower, approaching atmospheric pressure on the tunnel wall (Fig. 8 on the left), which is assumed to be controlled based on whether the monitored zone communicates in a direction towards the tunnel or away from it. To achieve this qualitative distinction, the model has to be divided into two parts – the outer average permeable zone and the inner zone with less permeable blocks and deterministic
fractures providing hydraulic communication between the tunnel pressure and pressure in the monitored sections of the borehole. The geometry of the model is composed of two embedded parts: the inner block of 30×30×100 m (alternatives are included in Chapter 2.2.5), with a combination of fractures and a matrix (equivalent of a small-scale continuum), and the outer block with a homogeneous equivalent continuum (larger scale). Selection of the interface is based on the assumed spatial scale of observation on the wall of the tunnel and in the borehole, i.e. in the order of single units of meters to the first tens of meters. Subsequently, communication at the level of the unaffected pressure through the outer block may be considered as a boundary condition with the borehole being isolated from the tunnel (the upper line of Fig. 8 on the left) or the effect of drainage, i.e. the dominant communication between the boundary condition in the tunnel with the fracture and the monitored section in the borehole (the lower line of Fig. 8 on the left).

The hydraulic conductivity of the continuum in the inner block had to be considerably lower than the hydraulic conductivity of the outer block (massif) in order to achieve higher pressure at the site of the monitoring borehole. Conversely, the permeability in the fracture is always higher than in both zones of the continuum and leads to a decrease in pressure, even in a homogeneous model (Fig. 8 on the right).

![Model boundary](image)

**Fig. 8** Concept explaining the differing responses of the borehole pressures in the surroundings of the tunnel, depending on the range of inner/outer permeability and a quantitative illustration with data from the Fracture Model alternative.

### 2.2.3 Model with non-homogeneous permeability (heterogeneous model)

A heterogeneous model was considered with several important simplifications, which were designed based on the use of local information prior to the excavation of the experimental gallery, i.e. still in the role of a blind prediction. The model consists of blocks arranged in series in the direction of the gallery/borehole covering the whole space perpendicular from the gallery to the boundary condition (Fig. 9). It was assumed that the spatial scale of the hydraulic tests is sufficient to cover the distance between borehole 12MI33 and the CTD and to predict the permeability near the tunnel wall with a possible shift in position in the range of meters. The domain was extended up to the boundary of the model as one of many options, but was left out in the following alternatives in the calibrated model (see the comment in the previous section).
Fig. 9 Concept of the heterogeneous model - the blocks with differing permeability are arranged based on the sections of the packer tests and the positions and numbering of the monitored sections of the borehole are stated at the bottom (in reverse order).

Tab. 2 Parameters of the heterogeneous model – the positions of the blocks and hydraulic conductivity. In the unmeasured sections, the data source of the estimated hydraulic conductivities is labelled as “own”. The last line shows the monitoring section in borehole 12MI33.

<table>
<thead>
<tr>
<th>Label</th>
<th>No.0</th>
<th>No.1</th>
<th>No.2</th>
<th>No.2’</th>
<th>No.3</th>
<th>No.4</th>
<th>No.5</th>
<th>No.5’</th>
<th>No.5''</th>
<th>No.6</th>
<th>No.6’</th>
</tr>
</thead>
<tbody>
<tr>
<td>Data source:</td>
<td>Own</td>
<td></td>
<td>Packer test</td>
<td></td>
<td>Own</td>
<td></td>
<td>Packer test</td>
<td></td>
<td>Own</td>
<td></td>
<td></td>
</tr>
<tr>
<td>K [m/s]</td>
<td>1E-9</td>
<td>2.6E-8</td>
<td>1.1E-7</td>
<td>6.1E-9</td>
<td>8.4E-9</td>
<td>4.8E-10</td>
<td>9.5E-10</td>
<td>1E-8</td>
<td>1E-9</td>
<td>2.73E-7</td>
<td>1E-9</td>
</tr>
<tr>
<td>Start [m]</td>
<td>0</td>
<td>12.1</td>
<td>37.1</td>
<td>20.1</td>
<td>44.2</td>
<td>53.2</td>
<td>65.2</td>
<td>90.0</td>
<td>95.0</td>
<td>105.2</td>
<td>107</td>
</tr>
<tr>
<td>End [m]</td>
<td>12.1</td>
<td>18.9</td>
<td>42.6</td>
<td>36.1</td>
<td>54.5</td>
<td>63.5</td>
<td>90.0</td>
<td>95.0</td>
<td>105.0</td>
<td>107.0</td>
<td>End</td>
</tr>
<tr>
<td>Monitoring</td>
<td>Section 6</td>
<td>Sec.5</td>
<td>Sec.4</td>
<td>Sec.3</td>
<td>Sec.2</td>
<td>Sec.1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Heterogeneous hydraulic conductivity is based on a packer test performed in borehole 12MI33. Data from the packer tests do not cover the entire model. There is a gap in the measurement at the point where one packer test ends and the second begins. This location was chosen for the interface between two blocks of continua with differing hydraulic conductivity. The remaining volume was considered to be a background with a hydraulic conductivity value of $K=10^{-9}$ m/s, which is a general estimate for the lower range of the packer tests. It can be assumed that higher hydraulic conductivity will correspond to the higher inflow into the borehole. The inflow is continuously monitored and has an almost continuous character.
Tab. 2, the blocks of the model are marked based on the packer test, and further blocks are defined either sequentially by numbers or by a symbol, similar to how the two sections in the packer test are numbered. The interval from 86 to 105 m is not covered by the packer test. Monitoring of the inflow indicates a location with a higher conductivity at a distance of about 90 m. Two different sections, No.5’ and No.5”, are considered for this location. The hydraulic conductivity value is estimated in the order of magnitude of the measurement values at the other intervals, not on the basis of a calculation.

### 2.2.4 Selection and parameters of fractures

Selection of the conductive fractures for the model geometry was based on two sets of source data: (1) mapping of the tunnel wall in the access (inclined) drift and in the CTD section, including classification of the water inflow, (2) monitoring in borehole 12MI33 and pressure packer tests. These sources are partly complementary, but they also confirm their consistency. The idea was to determine a limited set of hydraulically dominant fractures and use the concept and capability of Flow123d, i.e. a combination of a discrete fracture network and an equivalent continuum for rock blocks between these fractures.

The data was processed as follows:

- Only fractures with a type of flow - either F (flowing) or D (dripping), i.e. with the assumption of their interconnection and effect on the pressure field, were taken into consideration. This means 78 from a total of 2,023 fractures. Fractures labelled as W (wet) were neglected, because there were too many for the model concept and subsequent processing of geometry.
- The selected fractures were approximated as vertical (for simplicity, because most of them are almost vertical), from the ground plan in the height of the tunnel they were projected in a vertical direction.
- A drawing was made showing the penetration of the fractures with borehole 12MI33 and its packer intervals (Fig. 10).
- The “main” fractures were selected so that at least one of them would fit each interval of the packer tests with a higher hydraulic conductivity, with F fractures being preferred. Fractures with a similar position and direction could be represented by a single fracture (as a fracture zone). A total of 14 of these fractures were selected and subsequently digitized from the manual drawing.
- The transmissivity of the individual fractures was determined based on the packer tests and their intervals. The hydraulic conductivity was also determined for the rock blocks between the fractures.

Fig. 11 shows the fractures and intervals of borehole 12MI33 with an evaluation of the measurements and other supporting information – flowing (F) and dripping (D) fractures and openings are labelled. The overall idea is to set the model parameters so that they can reproduce the packer data, simply by adding the contributions of the rock blocks and the individual fractures in each packer interval. This captures the overall real hydraulic effect of multiple fractures in the interval (also a single fracture in the model may represent several “real” fractures). The conductivity of the “rock matrix” (including the fractures not explicitly represented) is estimated so that the contribution to less conductive sections (4 and 5) is equal to the contribution of the given fracture. The issue is underdetermined, but most of the relationships are unique with one fracture for one interval in the borehole.
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Fig. 10 Manually processed data - sketch on a printout of the fracture system from data entered in a horizontal cross-section at the level of the tunnel, together with borehole 12MI33 and its intervals. The 14 model fractures selected from the mapping in areas of larger clusters of fractures are marked in pink. The orientation is given by the coordinate system, the entrance to the tunnel is at the bottom of the image, and the CTD is inclined to the left.

Fig. 11 Determination of the transmissivity of the fractures from the packer tests in borehole 12MI33 and other data references (our own estimates are in red). The “x” symbolizes an existing intersection and its contribution to the transmissivity measurement. The blue numbers are set manually so that the sum of the transmissivity intervals at the bottom of the table corresponds to its measured equivalent or to its selected value.
2.2.5 Fracture model with an inner block

Whereas the result of the fracture model described above is merely a description of the individual fractures, i.e. the position of the fracture, direction, and transmissivity, the input geometry of the simulation code requires a full hierarchy of points, lines and volumes, including all geometries and boundary conditions. This part was performed using the SALOME software (an open source CAD program). The specific issues of the discretization are included below.

The fracture model was considered in two geometry and computational mesh alternatives. The position of the interface between the inner (fractures + continuum) and the outer (continuum) blocks is based on the approximate scale of the spatial measurement range, but this leaves a large space for our own choices. The interface between the external and the internal rock mass was first set at twice the distance of the borehole from the tunnel and then the distance was reduced by one third (i.e. interfaces 7.5 m or 2.5 m from the borehole towards the boundary of the model). Based on this, the following two model geometry alternatives (Fig. 12) were determined:

- Interface distance of 15 m from the tunnel axis – a block with the base edge of 30 m with the tunnel in the centre and with a 5 m overlap of the fractures to the outer conductive zone
- Interface distance of 10 m from the tunnel axis – a block with the base edge of 20 m with the tunnel in the centre and with a 3 m overlap of the fractures to the outer conductive zone

The second alternative was discretized into two further alternatives with different steps, i.e. a course and fine mesh. The number of elements for the optimized mesh is shown in Tab. 3 (a homogeneous model is also included for comparison). Calculations are limited by memory and computational time in order to calculate the transient hydraulics and the transient transport of the tracer. The discretization was optimized with the aim of reducing the number of degrees of freedom (Tab. 3).

Tab. 3 Number of nodes and elements of the computational mesh

<table>
<thead>
<tr>
<th>Distance of interface from the tunnel axis</th>
<th>Overlap of fractures to the outer conductive layer</th>
<th>No. of nodes</th>
<th>No. of elements</th>
<th>Type of mesh</th>
</tr>
</thead>
<tbody>
<tr>
<td>15 m</td>
<td>5 m</td>
<td>6,987</td>
<td>46,426</td>
<td>Rough</td>
</tr>
<tr>
<td>10 m</td>
<td>3 m</td>
<td>5,060</td>
<td>32,252</td>
<td>Rough</td>
</tr>
<tr>
<td>10 m</td>
<td>3 m</td>
<td>6,269</td>
<td>39,852</td>
<td>Fine</td>
</tr>
<tr>
<td>Homogeneous model</td>
<td></td>
<td>4,269</td>
<td>22,036</td>
<td>X</td>
</tr>
</tbody>
</table>
The discretization of the working versions of this model concept uncovered the general numerical property of the mixed-hybrid finite element method in Flow123d, where the discrete unknown pressure and flow in the fractured domain cannot be directly associated with the discrete unknowns in the 3D domain across the edge of the fracture. Therefore, the hydraulic communication between the “internal” domain of the fractures and the “external” domain of the continuum was possible only through the individual elements of the matrix within the internal domain. This is shown in Fig. 13 on the left (the 2D-3D communication is perpendicular to the 2D area). This creates additional (artificial) hydraulic resistance between the inner and outer domains, which depreciates the value of the results (which are not further presented).

The above-mentioned model was then created in such a way that the fractures were extended to the outer block (i.e. the 3D domain of the continuum) and the triangular elements of the fracture became the walls of several tetrahedrons from the 3D domain, ensuring correct numerical communication (Fig. 13 on the right). The partial increase in hydraulic communication is no longer relevant in this situation.
2.2.6 Outer boundary conditions

The boundary conditions for hydraulics and transport are shown in Fig. 14. The outer boundary conditions include the piezometric heads and the concentrations corresponding to an intact state, which is based on simple regression of the measured data. The hydraulic conditions of the tunnel are described below. The transport conditions in the tunnel wall were set to “free outflow”, which is defined as the total mass flow equal to the advective flow corresponding to the hydraulic model. Two other alternatives were considered:

- Selection of the hydraulic state on the boundary (field not affected by the CTD)
  o Hydrostatic alternative with a single piezometric head (proposed by JAEA)
  o Non-uniform pressure fields as a result of a larger scale model, i.e. involving the drainage effect of the entire URL structure, particularly vertical shafts (other horizontal objects outside the CTD are not included). Values from a larger scale model are interpolated to the boundary elements of the CTD model (i.e. other positions).

- Selection of conditions on the “front” vertical wall (the wall intersecting the tunnel)
  o In the default settings, the boundary condition is set to the same value as on the other walls (default input of JAEA), resulting in pressure/piezometric head discontinuities at the edge of the tunnel/boundary condition
  o Zero flow corresponding to the assumption of symmetry, i.e. the assumption of a long open tunnel on both sides of the boundary condition, which is justified in the later stages of the excavation (except for deviations in the tunnel from the straight line), as if a similar boundary condition distribution would be the result of a pressure field model.

Fig. 14 Boundary conditions for hydraulics and transport (based on Iwatsuki, 2016).

2.2.7 Modelling the excavation of the gallery – specification of the boundary conditions

In principle, the excavation of a tunnel means a change in geometry. This is impractical for the implementation of the model, and can be replaced with an almost equivalent solution by switching the boundary conditions: if zero flow is applied on the tunnel wall, then it is the
equivalent state to the tunnel filled with an impervious environment and the hydraulic effect is manifested by a deviation of the flow out of the tunnel volume (which would be negligible assuming that the gradient across the tunnel is negligible). Technically, zero pressure is applied to the excavated part and zero flow to the remaining part. The interface between zero pressure and zero flow varies with increasing time. Neglecting the flow in the unexcavated part of the tunnel is negligible over time. Although the excavation process is documented in detail, and the upper and lower surfaces are distinguished, a constant rate of excavation is considered as a sufficient approximation for the model. The difference between a detailed excavation and the model simplification is shown in Fig. 15. Alternatives correspond to Tab. 4, which focuses on the properties of the model as well as the non-homogeneity and sources of external boundary conditions. The REF model alternative applies a piezometric head on the front wall of the model, while the other three alternatives apply a zero flow (symmetry, intersecting the tunnel are considered).

In all cases, we can see a decrease in pressure due to the excavation of the tunnel. The time series of the decrease corresponds exactly to the point-of-point tracking process. All non-homogeneous models are characterized by more gradual decreases, which correspond to the intersections of the different conductivity interfaces.

Movement of the boundary interface is suitably reached in Flow123d by the Robin (third-type) standard condition and by using formulas expressing the dependence of the coefficient on the spatial coordinate and time. The boundary condition for the total flow includes both types of boundary conditions, the Dirichlet (first-type) and Neumann (second-type) condition depending on the coefficient (see equation 2.1):

\[-q_a \cdot n = \delta_a \left( q^N_a + \sigma_a (h^P_a - h_d) \right)\]

where \(q^N\) is the applied flow (in this case zero), \(h^P\) is the applied pressure head (in this case the value is dependent on \(z\), corresponding to zero pressure) and \(\sigma\) is the coefficient - if the

![Fig. 15 Course of the excavation – detailed documentation and linear regression used in the model.](image)
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dominant flow is applied then it is near zero, whereas if the dominant pressure is applied then it is infinite. In this case, the values of $10^{-12}$ and $10^{+12}$ were selected (it is not necessary to consider the units). The use of the formulas in the input file (the so-called “parser”) is a specific property in Flow123d, the relationship between the coordinates $x$, $y$ and time $t$ is used to determine the position of the entire excavation and the command “if” (with similar syntax as in MS Excel) is employed with the corresponding extreme values of the coefficient (specifically indicated in the Interim Report - Annex 1).

2.2.8 Summary of the alternatives for evaluation

The above-described alternatives of the structure of the inhomogeneity and boundary conditions create several combinations, only a few of which have been calculated; and those selected in the summary report are important for the evaluation (for example, selections with unrealistic velocity and discontinuities on the edges at the entrance to the tunnel are not presented).

Tab. 4 Alternatives of the considered models with different heterogeneities and boundary conditions. Only the filled variants in the table were calculated (BC - boundary conditions, IC initial conditions)

<table>
<thead>
<tr>
<th>Label:</th>
<th>Boundary conditions set by the Task assignment</th>
<th>Boundary conditions set by the URL model</th>
</tr>
</thead>
<tbody>
<tr>
<td>CTD model</td>
<td>REF</td>
<td>X</td>
</tr>
<tr>
<td>Homogeneous model</td>
<td>BC+IC: Piezometric head = 110 m + front wall zero flow</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$K = 1 \times 10^{-8}$ m/s</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Sp. storativity = $1 \times 10^{-8}$ 1/m</td>
<td></td>
</tr>
<tr>
<td>Heterogeneous model</td>
<td><strong>TUL1</strong></td>
<td></td>
</tr>
<tr>
<td></td>
<td>BC+IC: Piezometric head = 110 m + front wall zero flow</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$K$ directly from borehole 12MI33 of the packer test</td>
<td></td>
</tr>
<tr>
<td></td>
<td><strong>TUL2</strong></td>
<td></td>
</tr>
<tr>
<td></td>
<td>IC from a steady state</td>
<td></td>
</tr>
<tr>
<td></td>
<td>BC from the URL model + front wall zero flow</td>
<td></td>
</tr>
<tr>
<td>Fracture model</td>
<td><strong>Fracture model</strong></td>
<td></td>
</tr>
<tr>
<td></td>
<td>BC+IC: Piezometric head = 110 m + front wall zero flow</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$K$ inversely from borehole 12MI33</td>
<td></td>
</tr>
</tbody>
</table>
To solve the task, alternative models with an equivalent continuum based on the task description were first considered. Various inhomogeneities were then gradually added. For each alternative, a model was created with different boundary conditions. The basic model alternatives are included in Tab. 4, to which references are further made in the text. The fracture model is considered to be final at this stage and is used for all of the prediction and calibration steps in the following chapters and is compared to the homogeneous reference model (REF) to see the differences caused by the inhomogeneities. Various alternative fracture models (labelled TUL3 Fractures, Rock1 and Rock2) were dealt with in the interim reports. These models either had fractures in the solid mass without subdivision into two embedded equivalent continua (TUL3 fractures) or had no embedded fractures in the outer volume (Rock1 and Rock2 models). The embedding of fractures is described above. These models can be understood as a precursor to a fully functional Fracture Model. This was referred to in the interim reports as “Rock3”, but it is no longer used in this text.

A separate alternative was then created to predict the flooding, only in the case of the fracture model. However, the change is not based on the properties used to distinguish alternatives above. Surface 2D elements on the CTD wall defining boundary condition were adapted to 2D continuum elements representing the physical properties of the volume of water in the flooded area.
2.3 Step 1 – Results of the prediction during the excavation

This chapter is divided into the results of the prediction of hydraulics and transport, and at the end of the chapter is a section comparing the results of the Fracture Model with the monitoring. In terms of time development, the period under review corresponds to the excavation period from April 2013 to October 2013.

2.3.1 Course and distribution of pressure

The hydraulic conditions are evaluated by the project teams in the form of pressure (MPa). This value is more illustrative than piezometric head (m), especially when focusing on the groundwater level related to the boundary condition applied on the tunnel wall.

The results for the three model alternatives or their combination(s) are compared in Fig. 16. The alternatives and their labelling correspond to Tab. 4, which explains in particular the combination of heterogeneity and the source of the external boundary conditions. The REF model uses the applied piezometric head throughout the boundary condition. The other three models use zero flow on the front wall (which intersects the tunnel).

In all cases, we can clearly see a decrease in pressure caused by the excavation and pumping. The time progress corresponds to the excavation process and the position of the observation points. All of the model heterogeneities are characterized by multiple decreases in pressure in sequential steps, which correspond to intersections with the blocks with differing conductivity and fractures.

The asymptotic pressure values of the alternatives differ after the excavation. Sections 3-5 achieve lower final values between 1.5 and 2 MPa, Section 2 remains at the centre of the range and Section 1 shows a very strong decrease in the homogeneous model REF but it is negligible for the model with the block (TUL1 and TUL2). As expected, using the boundary condition of a large model does not have a major effect on the time trend, but it determines the overall pressure level with a difference of approximately 0.1-0.2 MPa (10-20 m of pressure). The difference in asymptotic values for Section 6 in the REF model is due to the boundary condition on the front wall with the applied pressure. Hence, the boundary condition on the front wall for the models TUL1 and TUL2 is set to zero, and the pressure for Section 6 is more realistic. This corresponds to the settings for Sections 3-5.

Given the future comparison of model prediction and measured data, it should be noted that the observation point at the centre of the monitoring interval for a given model output is not necessarily realistic. In principle, the measured pressure from the packer test is determined by the dominant conductive structure intersecting the borehole. On the other hand, it would be inappropriate to evaluate the pressure by a type of weighing along the borehole line within a given interval, due to the current level of gross prediction. To illustrate the possible influence, the development of pressures in the fracture/borehole points for the fracture model (Fig. 23) was plotted. The colours are the same for the same packer sections, and the effect of the time response is visible.
Fig. 16 Results of the modelled pressure development in the observation points corresponding to the monitored sections - top left: Heterogeneous model (original boundary condition - TUL1); top right: Heterogeneous model (URL boundary condition - TUL2); bottom left: Homogeneous model (with piezometric head on the front wall of the model – REF. Date in MM.DD.YYYY format on the horizontal axis.

The following figures show the spatial distribution of pressures and the differences between the two boundary conditions - hydrostatic pressure and pressure from the URL model (Fig. 17). A horizontal gradient directly towards the gallery can be seen at the top of the model (Fig. 17 on the right). Fig. 18 shows the spatial extent of the decrease in pressure due to the excavation. The front wall is considered to have zero flow. A normal gradient is also seen up to the edge of the model (upper, lower, lateral), indicating that the boundary condition may affect the model or, on the contrary, was not constant over time.
2.3.2 Inflow to excavated areas

Inflow to the access tunnel and CTD tunnel was evaluated from a steady-state hydraulic model. The time changes were not evaluated. The final values of the model were compared with the measurement values (one value for the total leakage rate in the inclined drift and one value for leakage to the CTD).

Fig. 19 shows the two model alternatives where the effect of the heterogeneity can be observed. The effect of the boundary condition did not manifest itself in the results. It is clear that the inflow to the tunnels in the Homogeneous model is quite uniform with the same
contribution from the inclined part as from the CTD part. In the heterogeneous model, the inflow to both parts varies due to several factors. The inflow is more a direct result of the lower conductivity in the rock in the surroundings of the CTD than in the whole massif. The time trend is uniform for the homogeneous model, while the heterogeneous model shows a staggered increase. Moderate peaks following increased flow are the result of sudden fracture intersections, followed by a reduction in flow and a reduction in the pressure gradient.

![Graph](image)

*Fig. 19 Time development of the outflow into the inclined part and the CTD – left: results of the homogeneous model (REF); right: results of the heterogeneous model (TUL2).*

### 2.3.3 Results of the transport model

Advection-diffusion transport was evaluated for the homogeneous and heterogeneous models. The results are tailored to the expected structure of monitoring data, i.e. chemical samples from sections of borehole 12MI33. In addition, the concentrations in the outlet water from the tunnel were also evaluated, which can also be used to validate the representativeness of both conductivity spatial distributions.

The values in the borehole sections are calculated inside the simulation code as a direct result. Their values are interpolated from the nearest mesh point values to the desired observed point. The time development is shown in Fig. 20 for the two representative model alternatives. Small differences between the models and time changes appear to be the effects of numerical errors for which there are physical arguments related to the configuration of the model as explained below:

Firstly, the borehole is not horizontal (Fig. 7) so it crosses the concentration field at different heights above sea level in the non-constant profile. Therefore, the initial values (visually the same for all models) are ranked from the lowest to the highest concentrations in Section 6, with the exception of the unexpected relation between Section 2 and Section 3.

Secondly, the time change trend should be controlled by the relative positions of the borehole and the tunnel. Assuming symmetrical drainage of the tunnel, the water from the lower space is transported to a point below the tunnel axis and vice versa. This, on the other hand, is complicated by the non-circular shape of the tunnel profile. This consideration is only relevant from a theoretical point of view for understanding the model because the measured data have a much lower accuracy (chemical analyses are typically reported with up to tens of percent of uncertainty) than the model alternatives discussed (with differences of less than 1 percent).
Fig. 20 Chloride concentrations during excavation of the tunnel in borehole 12MI33 for the two model alternatives - homogeneous (REF) with a hydrostatic boundary condition and heterogeneous (TUL2) with a pressure field from the large-scale URL model.

The effect of the lower concentrations at inflow from upwards and higher concentration at inflow from downwards can in principle lead to a sharpening of the boundary between the lower and higher concentrations at the level of the tunnel axis (mean height). This is visible in the concentration field plotted in the vertical section perpendicular to the tunnel and especially through the block with high conductivity (Fig. 21).

Concentrations in water discharging to the tunnel are evaluated directly from the available software outputs – fluxes through the boundary condition: volume flux from the hydraulic model (volume per time) and mass flux from the transport model (mass per time). The ratio of these quantities is equal to the concentration in the mixture of outflowing water in the “mass per volume” units. Evaluating the weighted average of the concentrations along the boundary condition of the elements or points is therefore simple. These results are shown in Fig. 22. The values are in line with the values in borehole 12MI33 with the differences corresponding to the vertical position. The significant fluctuations in the results are probably caused by numerical errors in the calculation process. Firstly, the volume and mass fluxes of the model are calculated from discrete unknowns within the software, and secondly, the concentrations are calculated as ratios of mass flux and volume flux (see above) beyond the simulation software.

Fig. 21 Concentrations of chloride with the areas of concentration changes during the excavation labelled.
Fig. 22 Concentrations of chloride in water flowing from the tunnel wall at the time of the tunnel excavation in the two model alternatives - right REF and left TUL2, defined in Tab. 4.

2.3.4 Results of the Fracture model

This chapter can be understood as a pre-stage for the fully automatic calibration in step 2a in the next chapter. The parameters for the calculation are taken from the table in Fig. 11. The results of the model are compared with the monitoring. The model with the set of parameters obtained in this way coincides with at least some but not all of the quantitative and qualitative features of the monitoring. Therefore, manual correction of the specified parameters was performed for this stage in order to achieve better agreement in several of the sections (Tab. 5). Modifications were made in the hydraulic conductivity parameter in the outer domain: $K = 5 \times 10^{-9}$ m/s except in fracture 108, where $K = 3 \times 10^{-9}$ m/s.

Tab. 5 Input parameters used in the Fracture model – modified data

<table>
<thead>
<tr>
<th>Fracture model</th>
<th>Hydraulic conductivity m/s</th>
<th>Specific storativity 1/m</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inner block (matrix)</td>
<td>1e-10</td>
<td>1e-10</td>
</tr>
<tr>
<td>Outer block (massif)</td>
<td>5e-9</td>
<td>1e-6</td>
</tr>
<tr>
<td>Fracture108</td>
<td>3e-9</td>
<td>5e-8</td>
</tr>
<tr>
<td>Other features</td>
<td>Original values</td>
<td>5e-8</td>
</tr>
</tbody>
</table>

The results of pressure development are shown in Fig. 23. The model is usually in reasonable agreement with the measured data. The pressure in Section 6 captures measurement trend but is significantly shifted. Section 2 captures the decrease in time, but does not capture the exact value. Sections 1 and 3 capture the measurement trend and the final value is not far from the measurement. Curves 5 and 4 are off their measured counterparts.
The spatial distribution of the pressure shown on the left of Fig. 24 confirms the realistic hydraulic communication between the fractures and the inner and outer rock blocks. It is evident that the fractures penetrating the outer domain have greatly helped the development of the gradient at the connection between the outer and inner domains (details of the previous results are included in the interim reports). The pressure gradients on the fractures are shown in Fig. 25. The difference between the permeable fractures and the less permeable fractures is obvious from this cross-section. In addition, the exposed fractures are visible penetrating the outer conductive block.

The results of the chlorine concentrations in the fracture model are shown on the right of Fig. 24. The less permeable rock block between the fractures is clearly separated from the more permeable outer block. The spatial contrast of the concentrations in and around the fractures is clearly visible.

![Graph showing pressure development](image)

**Fig. 23** Pressure development in the fracture model, comparison of measurements (upper legend) and calculations (lower legend, with a definition of the observation points).

![Spatial distribution of piezometric heads and chloride concentrations](image)

**Fig. 24** Spatial distribution of the piezometric heads [m] (left) and chloride concentrations [g/l] (right) for the fracture model.
Fig. 25 Spatial distribution of the piezometric heads [m] for the fracture model (the outer domain is removed, the fractures are visible with the overlapping part, and the inner block is also partially cut off).
2.4 Step 2a – Calibration of the model

The basic idea of model calibration during tunnel excavation is based on the use of all available data until the end of the drainage period. These are monitoring of the pressure and concentrations in six sections of borehole 12MI33 (labelled 1 to 6), data on the structural mapping of the surface of the tunnel wall, and the inflow into the CTD tunnel from the rock. Unfortunately, a significant part of the model data was not available due to the planned interruption of the monitoring during the excavation.

New data were made available at the end of this step. These are further pressure tests and monitoring in the CTD boreholes (13MI39-41) as well as monitoring and packer testing in a second borehole that is parallel to the CTD (13MI38). The new data are used to “validate” the previous agreement of the model and the measurements during the excavation.

A fracture model was created for this step and was used for all calibration alternatives and subsequent prediction of the flooding in the next chapter.

2.4.1 Agreement with the observed measurements

The main feature of the model calibration was the choice of hydraulic properties of non-homogeneous structures (fractures) and the two embedded rock blocks. The following properties were selected from the entire period of the time development and the relationship between the sections, on which the calibration was focussed:

1. The order of pressure reduction corresponds to the excavation process: In the sections with a pressure reduction (Sections 2, 3, 4, and 6), the positions of the pressure decrease correspond to their position. Several connections are not entirely unambiguous, due to a relatively long interval with missing data.

2. The final pressure value after the excavation - it is different for each section - some final values decrease to a similar predicted value, while others are almost constant. They are controlled by the effects of the boundary conditions and the internal geometry. In order to influence the behaviour of the model with a simple boundary condition, it is necessary to include inhomogeneity along transport routes between the tunnel and the boundary condition – the low pressure is the effect of high conductivity between the tunnel and the monitored sections and the high pressure is the effect of high conductivity between the boundary condition and the monitored section (and low conductivity between the tunnel and the sections).

3. The pressure slope during the decrease: it is influenced by the inhomogeneity of the model, in which there is a sharp decrease (including the Fracture Model) compared to the gradual decrease in the Homogeneous Model. On the other hand, the measured data have gaps in measurements, which means the quick and gradual reduction for sections 2 and 3 cannot be distinguished, but the remaining data show a faster reduction.

For the calibration, chlorine concentration measurements were also available, which are also a good feature of inhomogeneity in the flow field. In this stage, the chlorine transport data were not used for the calibration, and the chlorine concentrations were evaluated for illustration only. The issue of chlorine concentrations for calibration of the model is discussed later (chapter 2.6).
2.4.2 Methodology for the automatic calibration of hydraulics

The UCODE automatic calibration tool (Poeter and Hill 1998), i.e. inverse problem solver, was used to calibrate the hydraulics. The manual calibration values given in Tab. 5 were used for the initial calibration values. The calibration took place in two steps. Firstly, all of the available monitoring data were used and the hydraulic conductivity obtained from the pressure tests was later added to the calibration. The hydraulic conductivity from the pressure tests was considered as being important data characterizing the hydraulic processes in the massif. A drawing of the calibration procedure is included in Fig. 26. The automatic calibration uses the following observation data:

- Pressure monitoring in borehole 12MI33
- Pressure tests and the resulting hydraulic conductivities are used as part of calibration and not as input values
- Inflow to the tunnel

For a correct calibration, it was necessary to set the weights for each set of source data. The weights were set to compensate for the different number of measurements for each set of data and thus the disproportionate effect of the residuals from one set at the expense of the other to their sum.

The automatic calibration was performed in several successive steps with respect to the size of the task and the number of parameters and hence the computing cost of the calibration. The hydraulic conductivity of the outer massif was included in the calibration because of the need to transfer pressure through the fractures to borehole 12MI33. The procedure was as follows:

1. Firstly, the hydraulic conductivity of the fractures was calibrated for sections where the model values most closely matched the measurements. The hydraulic conductivity of the fractures opening into the sections where the model roughly corresponded to the monitoring was omitted and the effect of the calibration of the other parameters on this section was monitored.
2. Subsequently, the results were evaluated with respect to the measurements and a different combination of parameters was selected, where again the greatest potential was to improve agreement.
3. In the next step, each parameter that was still outside the measured data was calibrated, or sections that fit but were not yet included in the calibration were tested in terms of whether they can affect the results in other sections.
4. In the last step, the pressures from the monitoring of borehole 13MI38-40 were added as additional observations.

The best parameters were evaluated by minimizing sum of squared weighted residuals, with the algorithm implemented in the UCODE software. Furthermore, the agreement of the model with the measurements was examined in the form of a graph - a comparison of the measured values of pressure monitoring in borehole 12MI33 and the model. New monitoring of borehole 13MI38-41 that was put into operation after the excavation of the tunnel was used to confirm the accuracy of the previous calibration. This can be considered a “validation”. The final values of the hydraulic parameters were selected from the best agreement of the model and the measurements.
2.4.3 Results of the automatic calibration

The results of the pressure development are shown in Fig. 27 and the resulting hydraulic conductivity values are summarized in Tab. 6. In general, the pressure is not as low as in previous models and shows better agreement with the monitoring (Fig. 22). No.1 captures the unchanging trend relatively well and the final value is slightly lower. For No.2, the curve drop time is captured very well, but the exact final value is no longer affected. No.3 also shows a relative improvement over the previous results, both in terms of the measurement trend and the final value, which is slightly higher. Section 4 is more below the measurement, and Section 5, which does not cross any of the fractures, shows a more modest decrease than the previous results, yet it is significantly below the measurement. No.6 is almost consistent with the measurement, although the model responds slightly faster. Compared to the previous results (Fig. 22), this is a significant improvement.

From the table of calibrated hydraulic parameters Tab. 6, we see that most fractures have a change in transmissivity value within a single order of magnitude, and some fractures are almost closed. These include fractures 109, 111 and 114, which converge on a value of $1 \times 10^{-12}$ m$^2$/s, which is the lower limit value entered into the calibration software. The fractures transfer pressure through intersections from the surrounding fractures and their closure will help achieve the desired pressure values in the surrounding sections.
Tab. 6 Comparison of the calibration results of the Fracture Model with the previous estimate of conductivity obtained from the Rock2 pressure tests (in more detail in the interim reports).

<table>
<thead>
<tr>
<th></th>
<th>Manual calibration (results from the interim report)</th>
<th>Fracture model</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Rock2 model</td>
<td></td>
</tr>
<tr>
<td>Hyd. conductivity of the outer zone [m/s]</td>
<td>5 × 10⁻⁹</td>
<td>1.83 × 10⁻⁸</td>
</tr>
<tr>
<td>Hyd. conductivity of the inner zone [m/s]</td>
<td>1 × 10⁻¹⁰</td>
<td>6.91 × 10⁻¹⁰</td>
</tr>
<tr>
<td>Thickness = 1 m</td>
<td>Transmissivity [m²/s]</td>
<td>Transmissivity [m²/s]</td>
</tr>
<tr>
<td>Fracture 101</td>
<td>1 × 10⁻⁸</td>
<td>1 × 10⁻⁹</td>
</tr>
<tr>
<td>Fracture 102</td>
<td>1 × 10⁻⁷</td>
<td>1 × 10⁻⁸</td>
</tr>
<tr>
<td>Fracture 103</td>
<td>5 × 10⁻⁹</td>
<td>1.15 × 10⁻⁷</td>
</tr>
<tr>
<td>Fracture 104</td>
<td>9.5 × 10⁻⁸</td>
<td>1.18 × 10⁻⁷</td>
</tr>
<tr>
<td>Fracture 105</td>
<td>6 × 10⁻⁸</td>
<td>3.7 × 10⁻⁹</td>
</tr>
<tr>
<td>Fracture 106</td>
<td>6 × 10⁻⁷</td>
<td>5.41 × 10⁻⁷</td>
</tr>
<tr>
<td>Fracture 107</td>
<td>8 × 10⁻⁸</td>
<td>7.03 × 10⁻⁸</td>
</tr>
<tr>
<td>Fracture 108</td>
<td>3 × 10⁻⁹</td>
<td>1.47 × 10⁻¹⁰</td>
</tr>
<tr>
<td>Fracture 109</td>
<td>1.5 × 10⁻⁸</td>
<td>1.93 × 10⁻¹²</td>
</tr>
<tr>
<td>Fracture 110</td>
<td>5 × 10⁻⁹</td>
<td>5.87 × 10⁻¹⁰</td>
</tr>
<tr>
<td>Fracture 111</td>
<td>4.5 × 10⁻⁸</td>
<td>1 × 10⁻¹²</td>
</tr>
<tr>
<td>Fracture 112</td>
<td>5 × 10⁻⁹</td>
<td>4.74 × 10⁻⁸</td>
</tr>
<tr>
<td>Fracture 113</td>
<td>1.2 × 10⁻⁸</td>
<td>5.39 × 10⁻⁸</td>
</tr>
<tr>
<td>Fracture 114</td>
<td>4.5 × 10⁻⁷</td>
<td>1 × 10⁻¹²</td>
</tr>
</tbody>
</table>

Fig. 27 Pressure development after the tunnel excavation and results of the model calibration using the UCODE auto calibration tool (Section 1 – Section 6 correspond to No.1 - No.6, the indexes “fr” and the numbers designating the fractures in the model)
2.4.4 Results of the pressure development in boreholes 13MI38-41

After excavating the CTD, boreholes 13MI38-41 were drilled and equipped with pressure monitoring equipment. Data from these new boreholes were provided after calibrating the model (time interval during the excavation). A comparison of the model results with the pressure monitoring is shown in Fig. 28. Overall, the model captures the range of pressures well. The ranges in boreholes drilled from the CTD are captured the best, in particular borehole 13MI39, even with the final pressure values. Section 4 of borehole 13MI40 (closest to the tunnel) has a final value below the measurement. Borehole 13MI41 has nearly identical pressure values for Sections 2 to 4. Borehole 13MI38, drilled along the tunnel on the opposite side from borehole 12MI33, captured the range very well, but the order of the sections is reversed.

The new boreholes used during the automatic calibration were also successful and had a minimal effect on the resulting permeability. However, it will be necessary to make possible improvements to the structure of the model during future work in order to achieve a better agreement between the model, the measurements and these new boreholes.

2.4.5 Comparison of the effect of geometry

The effect of the mesh spacing on the results was checked due to the complexity of the model, i.e. the intersection of the fractures and the tunnel plus the interfaces of the outer and the internal conductive blocks. The calibration was performed on the coarsest model (a 15 m interface on each side of the tunnel axis and a 5 m fracture overlap) – the mesh and the results of the pressure field on the vertical section along the fracture are shown in Fig. 29a. When comparing the pressure field in the model with a smaller range of the internal conductive block (a 10 m intersection on each side of the tunnel axis and a 3 m fracture overlap), there is a difference in the pressures in the surroundings of the tunnel, which do not reach such a distance (Fig. 29b). The final result of the pressure calculation is on a fine mesh with an internal block range of 10 m from the tunnel axis. The figure shows a faster pressure change in the pressure field of the inner conductive block and a slightly longer range in the outer conductive block.

Fig. 30 shows the development of the pressure monitoring and the results of the models with two alternatives meshes a) a range of 15 m on each side of the tunnel axis; and b) a coarse mesh of 10 m on each side of the tunnel axis. The changes are relatively small compared to the final mesh used (Fig. 27). A description of the results for the final set of parameters is included in the previous chapter 2.4.3.
Fig. 28 Pressure development in the newly added boreholes 13M138-41 with the results of the model calibration using the UCODE automatic calibration tool. Horizontal axis with date in DD.MM.YYYY format.
Fig. 29 Pressure field with a cross-section along the tunnel axis and various meshes a) mesh with a 15 m extent on each side of the tunnel axis and a 5 m fracture overlap b) 10 m on each side of the tunnel axis and a 3 m fracture overlap – course alternatives c) 10 m on each side from the tunnel axis and 3 m fracture overlap – fine alternative.

Fig. 30 Pressure monitoring and results of the model with the final parameters a) mesh with a 15 m extent on each side of the tunnel axis and a 5 m fracture overlap b) 10 m on each side of the tunnel axis and a 3 m fracture overlap – course alternatives. The fine alternative is included in Fig. 27.
2.4.6 Chloride transport—effect of drainage

A fracture model with calibrated hydraulic parameters was used for a transport model simulating the chloride ions (as a non-reactive tracer). The results of the transport are compared with the monitoring (Fig. 31). The modelled concentrations exhibit an almost steady state, which is due to the position of the borehole at the same vertical level with respect to the tunnel, and hence a “symmetrical” mixing for a flow controlled by the drainage.

We also attempted to calibrate the transport to the measurements, but without a great deal of success. This is due to the use of the boundary conditions (in the range of 332 to 428 mg/L), set by the task description, which do not let the results have a concentration corresponding to the monitoring beyond this range. Therefore, the task was performed with a change in the range of the boundary condition of the concentrations. The limits were set to 214 mg/L of chlorides on the upper wall of the model and 566 mg/L on lower wall of the model. Even after this modification, the results of the model did not significantly approach the monitoring. Therefore, the results are not presented in this report (they were presented at the DECOVALEX-2019 meeting in Nancy, April 2018). The effect of the boundary conditions and possible changes in the concept of the model are discussed below.

![Fig. 31 Development of the concentrations in the individual sections in borehole 12MI33 (left); Development and values of concentrations from the monitoring (right).](image-url)
2.5 Step 2b – Prediction of the flooding

The next step in modelling was to predict the changes in the monitored boreholes after closing the CTD gallery with a watertight plug. As in the previous versions, the fracture model was used with little modification. The model was implemented in two approximation alternatives:

- By changing the boundary conditions – specifying the zero flow on the tunnel wall at the location of the CTD. In this case, the volume of water in the filled tunnel is not considered as part of the model.
- By changing the function of the surface elements - 2D elements on the tunnel wall (where the boundary condition was originally applied) were used to represent the volume of water in the closed part of the tunnel. The volume is represented by the thickness of the 2D elements and corresponds to the volume of the CTD tunnel. This approximation also made it possible to capture the effect of the seepage into the tunnels. No boundary conditions were used on the wall of the tunnel except for a small portion at the start of the CTD where a zero flow was applied. This part simulated the area with the impervious plug and also separated the 2D elements simulating the water in the CTD from 2D elements representing the boundary condition of free seepage applied for the rest of the tunnel. The parameters for the 2D domain were set to values corresponding to free water (K=1 × 10^2 m/s as the extreme value beyond the most permeable rock, storativity 10^-9 1/m (compressibility) and the initial chlorine concentration of 475 mg/L (prescribed, known by the measurement).

Due to the difficulty in changing the boundary conditions in the area of the CTD in the first alternative and the inability to change the function of the elements in the mesh during the calculation of the second alternative, the flooding was approximated by a discontinuity in time, i.e. the state of draining the wall of the tunnel is immediately followed by the state of the filled CTD. This corresponds to the calculation in the time period of the flooded state from 10 January 2016 to 10 May 2016 (the date was chosen due to the model already being set). The model in the period of flooding is called the “flooding model” and the model in the period of drainage is called the “drainage model”. Shortening the period of the calculation to the flooding model only leads to its faster development. The flooding model uses the initial conditions of the previous drainage model after its stabilization.

The model does not consider the effect of the gradual flooding of the CTD and the effect of the mixing of the inflowing water on the whole volume of the CTD. For a comparison with the work of the other teams, the pressure in the CTD was determined roughly in the centre of the CTD on the upper and lower walls at the point of a discretization node, and the resulting value was calculated as the mean of the two values.

2.5.1 Results of the development of pressure in borehole 12MI33

The pressure values in borehole 12MI33 stabilized very rapidly after flooding the CTD and remained at a steady value throughout the calculation of the drainage model (Fig. 32). Compared to the steady state of the drainage, the pressures are higher but do not return to the original values observed before the excavation (the difference is in the effect of the inclined access gallery that remains open). The smallest change was observed in the pressure in
Section 6, located immediately next to the unflooded inclined gallery. The pressure values were again ordered from the most distant section from the CTD entrance to the nearest (No.1 – No.6). After the excavation, there was an exception in the order due to the permeable fractures near No.3, which showed the highest increase in pressure values from all of the flooding model alternatives. By comparing all of model alternatives, it is clear that the greatest increase in pressure is in the homogeneous model (Fig. 32c). In the fracture model, the pressure increase is likely to be prevented by the communication of the fractures. The difference between the two alternatives of the fracture model is minimal, both in the trend and in the steady pressure values, which are almost identical. This is not surprising, the effect is only due to the compressibility of the water in the transition phase and the hydraulic communication through the 2D elements, which may not reach the monitoring borehole.

2.5.2 Results of the chloride transport

Fig. 33 and Fig. 34 show the development of the concentrations for boreholes 12MI33 and 13MI38, respectively, with a specified range of initial concentrations on the walls of the tunnel of 214–565 mg/L for the flooding model. The graphs show the entire calculation period of two consecutive concentration models – the drainage model and the flooding model. The flooding model had the initial conditions of the drainage model. In the first steps, technical issues with the implementation of this condition were observed (they will be subject to further analyses by the Flow123d development team), so the initial values in the flooding model do not follow the previous drainage model in some cases. After flooding, the concentrations stabilize very rapidly to the final values for the model with zero flow in the CTD. For the model with 2D surface elements, there is a slight increase and then a decrease in the concentrations in Sections 2 and 3. The rapid stabilization corresponds to the fact that the concentrations are determined...
by the boundary condition and the change of the velocity field only changes the location on the boundary with the initial trajectory. Fluctuations in the case of the surface elements correspond to the effect of mixing with water in the flooded gallery.

![Concentration plots](image1)

**Fig. 33** Concentrations in borehole 12MI33 for the zero flow model (left) and the 2D elements model (right) with an initial concentration of 214–565 mg/L. The drainage period followed by the flooding period.

![Concentration plots](image2)

**Fig. 34** Concentrations in borehole 13MI38 for the zero flow model (left) and the 2D elements model (right) with an initial concentration of 214–565 mg/L. The drainage period followed by the flooding period.

### 2.6 Supplementary analysis of the transport of chlorides

Although the use of chloride concentration data should have provided a convenient means of monitoring the flow in the surroundings of the CTD and checking the accuracy of the model and its calibration, the comparison between the model and the measurement proved to be much more complicated for all of the investigators. Therefore, the analysis in this chapter is in addition to the input steps (1, 2a, 2b). The main limitation of the model is the above-mentioned concentration range in the initial and boundary conditions proposed by the Task Leader for the model in the surroundings of the CTD, with a range of 100 m vertically (50 m above and 50 m below). In addition, a specific flow configuration has to be established in order for the water to flow to the borehole location from either the top or the bottom. The TUL models are symmetrical in terms of the permeability distribution and the deviation is only the slightly inclined orientation of the tunnels or boreholes and the shape of the tunnel profile. Although the DFN-based models may create unsymmetrical conditions, but with no deterministic input, the distribution
of the communicating fractures is statistically equal, which is confirmed by the results of the models with a small range of calculated concentrations.

In order to explain the measured development and range of concentrations corresponding to the combination of flows from different directions in the individual parts of the experiment, synthetic permeability configurations were analysed, with an emphasis on asymmetry above and below the level of the CTD and with a larger vertical geometric range. These models led to changes in concentrations in the monitoring borehole of up to 50 mg/L, i.e. still less than the measured changes.

The general configuration of the task is shown in Fig. 35 on the left and the resulting concentration field is included in Fig. 35 on the right. The model is based on the CTD model, the tunnel is circular with a diameter of 5 m, the size is doubled, i.e. the edge of the square is 200 m, with a corresponding double concentration range on the boundary (278 to 482 mg/L). The difference in permeability (e.g. factor 10) is significantly reflected on the velocity, but changes in the shape of the trajectories are relatively small, just slightly above the vertical level of the tunnel, so the concentrations in the borehole located horizontally from the tunnel are still a mixture of water from the top and bottom. The effect is more significant above and below the tunnel in the speed of movement from the edge of the model to the tunnel (a fully saturated “cone” of min/max boundary concentrations). The difference in the borehole area is only partially increased by shifting the interface, which distorts the trajectory more. The effect of the interface position can be seen in Fig. 36, which shows the time development of the concentrations in the monitored borehole (a point in the model at a horizontal distance of 7.5 m from the tunnel axis).

Based on the agreement of the individual investigators at the Nancy meeting, April 2018, further options were proposed: (a) to look for the effect of permeable “channels” from a number of communicating fractures; and (b) to consider the effect of the hydraulic field due to other exposed areas of the underground laboratory. Recommendations to configure the model at

![Fig. 35 Left: Configuration of the model task demonstrating the effect of vertical inhomogeneity on the transport of chlorides. Right: The resulting concentration distribution over 100 days for an upper and lower zone permeability ratio of 10:1 and an interface position at 10 m below the tunnel axis, the linear colour scale range is 278 to 482 mg/L.](image-url)
the scale of the entire URL were subsequently made by JAEA during the preparation of the report.

![Graph showing development of concentrations for various alternatives of the synthetic 2D chloride transport problems due to tunnel drainage with a homogeneous permeability distribution. The legend defines the ratio of the permeability of the upper and lower parts (10:1) and the position of the interface to the tunnel axis (-15 m to +10 m ... lower/higher divide). The comparison is with a homogeneous model with symmetrical mixing of water from above and below.]

**Fig. 36** Development of concentrations for various alternatives of the synthetic 2D chloride transport problems due to tunnel drainage with a homogeneous permeability distribution. The legend defines the ratio of the permeability of the upper and lower parts (10:1) and the position of the interface to the tunnel axis (-15 m to +10 m ... lower/higher divide). The comparison is with a homogeneous model with symmetrical mixing of water from above and below.

### 2.7 Summary and discussion of the results

The output of the Task C participation is a model explanation of the hydraulic and transport processes during the experimental simulation of the excavation process and the closure of the repository. From a comparison of the model calculation and the measured data, it is possible to compare to what extent and at what rate the rock environment and groundwater can recover to the conditions prior to the excavation (so-called groundwater recovery). Modelling of the phenomena in the granite (generally crystalline rock) is hampered by inhomogeneities and discontinuities in the form of fractures. Therefore, any possible disagreement between the measurements and the blind prediction model, i.e. without knowledge of data from the modelled time period, does not necessarily mean a wrong or inappropriate solution, but it expresses uncertainty in the processes using data of the same type of rock from another position of the same site. Subsequently, the calibration of the model on the measured data was a verification of how the different investigators can qualitatively estimate the character of the inhomogeneity distribution, and determine the parameters expressing the optimal agreement between the model and the measurements using algorithmic means.

The Task Leader proposed a specific formulation of the model problem and geometric configuration in the first step of the solution. In this model, with an approximation of the homogeneous rock, the individual teams achieved good agreement between each other. In the subsequent solution, investigators from JAEA and Sandia (SNL) used Discrete Fracture Network (DFN) models, which stochastically generate a large number of fractures and applied
them variably. Since the statistical distribution of the fractures in the space is homogeneous, this approach alone is not sufficient to reproduce the observation of a different pressure pattern in the individually monitored sections, which can be achieved by adapting the generated fracture network at specific points, i.e. by adding deterministic information (called fracture network conditioning in the solution). This procedure has been quite successful in reproducing the pressure pattern. The level of agreement was comparable for each model, although particular differences were spatially localized. The success of the TUL solution was that the results were achieved using the original model, i.e. a multidimensional configuration of selected deterministic fractures and continua with which there is hitherto little experience in modelling at this spatial scale of meters to tens of meters, but it has potential advantages in terms of portability and scalability, i.e. combining solutions at different spatial scales. Additional findings were as follows:

- The use of an inverse resolver (UCODE software) had a limited effect on getting the model closer to the experiment, but technically the algorithm worked.
- Projection of the model conditions at a larger-scale onto the model of the experiment did not have a significant effect on the pressure pattern, but proved to be important for the transport.
- The calculations are largely limited by the pre-processor options, i.e. by efficiently entering the underground geometry and the fractures and discretization without unnecessary refinement outside the area of interest.

The individual teams focused differently on solving the transport tasks and geochemical reactions. The common basis was the modelling of non-reactive transport of chloride ions, which have a significant role at the site as an indicator of the depth of the groundwater origin. This model in the original form of the task description did not provide interesting results because the data used led to very small changes in the monitored concentrations, inadequate for the measurements. The partial analyses demonstrated by TUL with concepts potentially leading to a larger range of chlorine concentrations at the monitoring points, motivated the Task Leader to formulate a specific model problem at the scale of the entire URL, including flow and transport at a greater vertical distance.

When modelling the development of chemical composition, the investigators from TUL focused in detail on identifying the processes leading to the observed chemical composition of groundwater on a wider scale as a necessary basis for simulating the specific steps of the GREET experiment. Sandia investigators, on the other hand, focused directly on the behaviour of the granite-cement system on the wall of the gallery after the excavation and during the flooding, using the typical chemical composition of the rock and the water. The geochemical analysis performed by J. Zeman from TUL brought a new perspective on the spatial and temporal distribution of the groundwater composition in the surroundings of the laboratory, as a mixture of water from selected analyses in various proportions (see Chapter 3). This highlighted the dominant role of transport (advection and dispersion) over the reactions between the components and between the water and the rock, and defined the initial conditions for more relevant modelling of transport in 3D connected to the inhomogeneous flow field from the hydraulic model. This may be the subject of the next stage of Task C until the end of 2019.

The importance of TUL’s results and their collaboration in general can be summarized as follows:
• The use of a multidimensional model of flow and transport was demonstrated in a new type of configuration involving fractures and matrix in the near field and an equivalent continuum in the far field.
  o The model was able to capture the main features of the effect of inhomogeneity on the spreading of the hydraulic effect of the excavation.
  o Most of the information obtained from the investigations at the site can be included in the model.
  o In terms of calculating and incorporating flow and transport phenomena, Flow123d is able to capture complicated conditions during the excavation and changes in configuration over time, and we expect it to be more usable in the future due to the ongoing development of pre-processor tools.
• Suggestions for possible reasons for the data observed by TUL have led the Task Leader modifying the model and data specifications, as well as to major new specifications in the task description. This confirms the active role in the collaboration.
• Participation in the solution provided a detailed insight into the results of the experiment and an assessment of the groundwater behaviour in the granite and the processes leading to a return to the conditions before the excavation – for example:
  o Hydraulically, the environment of the CTD returns to a state close to the original, irreversible rock changes can be expected due to the effect of mechanics (deformation and opening/closing of fractures), whose modelling was not part of the solution.
  o Movement of dissolved substances with flowing water due to drainage causes changes in chemical distribution over long distances and the equilibration of pressures will not lead to a direct return of concentrations to the original state, i.e. there will be a new or other imbalance between the water and the rock.
  o Phenomena and changes occur that are not predicted by standard models or THMC process equations.
  o For the purpose of assessing the behaviour of the rock in relation to safety of the DGR, it is beneficial to perform a similar type of experiment and model evaluation, as it proves the extrapolability of the data obtained during the investigation (excavation) and after closure of the repository (even if the flooding only partially creates the relevant conditions).
3 Geochemical development of groundwater at the MIU

3.1 Introduction

In the framework of the assessment of the geochemical development at the Mizunami Underground Research Laboratory (MIU), in relation to Task C (Chapter 2), the spatial and temporal development of chloride concentrations on the individual sample profiles of all of the boreholes was evaluated. The geochemistry of the groundwater in the surroundings of the closure test drift (CTD) at depths of -500 m was evaluated in detail.

The data provided on the official website of the Japanese Atomic Energy Agency (JAEA, 2018) for the project DECOVALEX-2019 Task C: GREET Hydro-mechanical-chemical-biological processes during groundwater recovery were used as source data. The horizontal position and the vertical profile of the individual boreholes with the labelling of the source data files are included in Fig. 37–Fig. 39. The positions of the individual zones in borehole 12MI33 are shown in Fig. 39.

The data were processed in The Geochemist's Workbench (Bethke and Yeakel 2018).

Fig. 37 Horizontal position of shafts and monitoring wells at the MIU underground laboratory. Boreholes with geochemical data are marked in red, source data is listed in the file Step1a_GW_chemistry_Facility_scale.xlsx. Source: JAEA (2018), modified.

Fig. 38 Position of shafts and monitoring wells at the MIU underground laboratory. The yellow background indicates wells with geochemical data, the coloured labels show files with geochemical source data, the legend is in the top left of the image. Source: JAEA (2018), modified.
3.2 Trends in the depth development of chloride concentrations

A detailed image of depth and time development is provided by the groundwater monitoring on the main shaft A-WR and the ventilation shaft B-WR. In the upper part, to a depth of approximately 80 m, the chloride concentrations have long been in the range of several mg/L. Chloride concentrations in the groundwater below this level are approximately 100 mg/L and then systematically increase to approximately 300 mg/L at a depth of 500 m. This trend is primarily confirmed by the shallow boreholes MSB2 and MSB4, which reach a depth of 176.1 and 99.0 m, respectively.
At the start of the sampling there was a significant fluctuation in the concentrations, which lasted approximately two years until they stabilized into a clear trend. In shallow zones up to 80 m, the chloride concentrations rapidly increased and then decrease to a long-term stable level of several mg/L (Fig. 40a). From the start of the sampling at depths of approximately 100 m to 200 m, the concentrations in both shafts were typically approximately 150 mg/L, and decreased slightly over time (Fig. 40b). At depths below 200 m, the development of the concentrations in both shafts differed markedly. Apparent seasonal trends are visible in shaft A-WR (Fig. 40c), while at the beginning of the sampling in the shaft B-WR there was a significant increase in concentrations, which decreased over two years and continued to show seasonal changes, while concentrations were comparable to the same depth of the level of shaft A-WR (Fig. 40d). Another distinct change in trends occurred at depths below 400 m. In shaft A-WR, there was a slight increase in chloride concentrations without significant fluctuations at the beginning of the sampling (Fig. 40e), while shaft B-WR showed a significant decrease in concentrations from 2012 (Fig. 40f).

In addition, in shaft A-WR at depths of 136.2 and 151.8 m, the concentration transition between two levels of chloride concentrations was unusual (Fig. 41). At both depth levels, the chloride concentrations jumped between the higher and the lower levels, and from 2010 (in the displayed time scale +7), the concentrations at a shallower depth remained high and at a greater depth remained low. In 2011, there was again a sharp transition at both sampling depths, with higher concentrations of chlorides at greater depth.

As can be seen, it is not easy to select the typical concentrations for the evaluation and graphical depiction of the depth trend of the chlorine concentration development. Average concentrations are unsuitable because very different time developments occur on the individual sampling profiles, and the values from the beginning and during the sampling vary widely for several of the profiles. Therefore, the last values that correspond to the stationary values or were part of a moderate long-term trend were selected. Fig. 42 shows the trends of chlorides concentrations with depth in intervals up to 500 m and 1170 m. The concentrations distributed with 2nd degree polynomials were not physically or geochemically interpreted.
Fig. 40 Examples of typical time developments in chloride concentrations in groundwater in the shafts and vertical wells of the MIU. Details are provided in the text.
Fig. 41 Development in chloride concentrations in the main shaft A-WR at a depth of 136.2 and 151.8. The start of the time axis is set to 1 Jan 2003. Details are provided in the text.

Fig. 42 Trends in chloride concentrations in groundwater in the shafts and vertical boreholes at the MIU. (a) and (c) with the shafts and boreholes highlighted, (b) and (d) without the objects highlighted and with the trends plotted, (a) and (b) to a depth of 500 m; with borehole MIZ-1.
The monitoring of the spatial and temporal development of chloride concentrations in the vertical and horizontal boreholes performed at the MIU can be summarized in the following conclusions:

1. In the vertical boreholes, the chloride concentrations in the groundwater samples ranged from 1.4 to 492 mg/L.
2. In the deep borehole MIZ-1, the chloride concentrations were between 1800 and 1900 mg/L.
3. The chloride concentrations in the vertical boreholes increased systematically with depth.
4. Chloride concentrations in the horizontal boreholes vary widely, and in individual cases reach up to 800 mg/L.
5. In most cases, the chlorides concentrations fluctuated in the interval of 6 months to one year from the start of the sampling, in the next period they range around a stable stationary value.
6. Typical chloride concentrations in the horizontal boreholes are in good agreement with the concentrations found in the vertical boreholes.
7. Most of the horizontal boreholes are characterized by a stable trend in the development of chloride concentrations between the individual zones from the beginning to the end of the borehole. However, in several zones, the concentrations fluctuate greatly step, and for these zones there is a characteristic increase in chloride concentrations over time.

3.3 Geochemical development of groundwater in the surroundings of the exploration gallery – 500 m

In the surroundings of the exploration gallery at a depth of -500 m, extensive research is carried out on the parameters of the rock environment. Consequently, a detailed assessment of groundwater geochemistry was carried out for the hydrochemical wells around the gallery. The configuration of the boreholes in the surroundings of the gallery is shown in Fig. 38 and Fig. 39.

3.3.1 Borehole 12MI33

The total concentration of dissolved solids is relatively stable over the reporting period and stabilized by mid-2013 (27 June 2013) after initially fluctuating. In most zones, there was no clear development. The exception is the groundwater sampled on 7 July 2014, which is characterized by large deviations with a significant decrease (zone 1, 3 and 5) or increase (zones 2 and 6). A comparison of the Stiff diagrams for groundwater with a clear deviation with groundwater in a “steady” regime is shown. A decrease in the total concentration of dissolved solids is associated with a decrease in the relative concentration of calcium ions (zones 1 and 5) and a positive deviation of the total concentration of dissolved solids is also associated with a higher relative concentration of calcium ions (zone 2).

The total concentrations of dissolved solids systematically decreased from zone 1 to zone 4, in zone 5 they increased rapidly, and in zone 6 they were comparable to zone 1. Similar trends
in total dissolved solids concentrations applied to zones and other sampling times except for zone 5, where the concentrations increased systematically over time. The decrease in total concentrations of dissolved solids was accompanied by a decrease in the relative concentration of calcium ions in the groundwater. This was not due to simple dilution of the groundwater. It is evident on the Piper and Durov diagrams (Fig. 43), where the groundwater composition from the last two sample rounds of 13 October and 15 December 2015 was plotted to maintain consistency. It is clearly visible that the change in the nature of the groundwater in the various zones of borehole 12MI33 involves a change in the relative proportion of cations, whereas the relative proportion of anions is almost unchanged. With the increasing proportion of calcium ions, there is a marked increase in mineralization (total concentration of dissolved solids).

Fig. 43 Piper and Durov diagrams for the composition of groundwater from borehole 12MI33.

3.3.2 Borehole 13MI38

In contrast to borehole 12MI33, there was no significant deviation in the total concentration of dissolved solids in borehole 13MI38 and a steady state is maintained for a long period of time. Exceptions are small positive deviations in zones 2, 3 and 4 during the sampling performed on 18 April 2014 and in particular the development in zone 5, characterized by a significant systematic increase in the total concentrations of dissolved solids.

The development of the concentrations of the individual groundwater components shows that sodium, calcium and chloride ions are practically exclusively involved in the changes in concentrations, and that the concentrations of other components remain virtually unchanged. The increase in the total concentration of dissolved solids, similar to borehole 12MI33, is accompanied by an increase in the relative ratio of calcium ions to sodium ions. This development is clearly evident from the Piper and Durov diagrams (Fig. 44), where the values of the major cations and anions for the last three samples are plotted.
3.3.3 Borehole 13MI39

The development in the total concentration of dissolved solids in borehole 13MI39 shows a similar trend over time to borehole 13MI38. After the first or second sampling rounds in the first half of 2017, when there were significant changes, the development stabilized. Then there was no change at all, or the total concentration slightly increased.

The main change in the groundwater composition in borehole 13MI39 was the change in the relative ratio of calcium ions to sodium ions. The total concentration of dissolved solids from zone 1 to zone 4 markedly and almost monotonically increased. In the cationic part, the increase was mainly due to the calcium ions, with the increase in sodium and potassium ions being only minor. The overall differences between the relative cation proportions and the increase in total mineralization between the zones are clearly shown on the Piper and Durov diagrams (Fig. 45), only chlorides are almost exclusively present in the anionic part.
3.3.4 Borehole 13MI40

Significant changes in total concentrations of dissolved solids occur in borehole 13MI40 only during the first two sampling rounds in 2014 (zone 1 and zone 4) or there are none at all. In the next sampling round on 7 July 2014, only small variations are visible, and only a moderate increase is comparable to the size variations.

The total mineralization is comparable (almost the same) in the individual zones, which is also evident from the Piper and Durov diagrams (Fig. 46).

![Piper and Durov diagrams for the composition of groundwater from borehole 13MI40.](image)

3.3.5 Borehole 13MI41

Similar to the previous drillings, there were marked changes in borehole 13MI41 during the first two sampling rounds in 2014. In zone 1, the total concentrations of dissolved solids were stable. In the other zones, the development was different from the previous boreholes and also from zone 1 of borehole 13MI41. The total concentrations of dissolved solids in the other zones decreased until 24 October 2014 when they reached a minimum. At the same time, the total concentrations of dissolved solids from zone 2 to zone 4 continued to decrease and in zone 4 to as much as a third of the value at the beginning of 2014.

By comparing the chemical compositions of the water in the individual zones of borehole 13MI41, it can be stated that the total concentrations of dissolved solids in zones 1 and 2 are comparable, they increased by half in the direction of zone 4. All three major cations were involved in this increase, but the increase in the calcium ion concentration was so steep that the groundwater character changed to water with a predominance of calcium ions. The overall development is also evident from the Piper and Durov diagrams (Fig. 47).
3.3.6 Boreholes 13MI45–13MI48 around the plug

These are short boreholes with a length of 2 m. The mutual ratios of the concentrations of the major cations and anions in the boreholes do not show any noticeable development over the monitored period of one year (Fig. 48). The water is virtually identical in terms of the representation of the main constituents. Total concentrations of dissolved solids ranged from 800 to 850 mg/L. The predominant cations were 60% Na+, the concentrations of K+ were negligible, and Ca2+ made up 40%. Only the chloride ions Cl− were present in the anions. Values of pH were only measured on 18 November 2014, and ranged around 7, with borehole 13MI45 having a value of 8.25.
3.3.7 Overall development

From the assessment of the chemical composition of groundwater in borehole 12MI33 and the other boreholes in the area of the exploration gallery, it is clear that the total concentration of dissolved solids in most of the groundwater ranges approximately from 400 mg/L to 1200 mg/L. The main constituents of the groundwater that participate in the increase in total mineralization are chloride ions in the anionic part, and sodium and calcium ions in the cationic part. In this context, the relative proportion of calcium ions increased in relation to the increase in the total concentration of dissolved solids, at the expense of the sodium ions. The chemical composition is characteristic of the whole groundwater group from the area under investigation around borehole 12MI33 well, regardless of the borehole in question.

The behaviour of the groundwater at the MIU site, sampled in borehole 12MI33 and the boreholes monitoring its surroundings, leads to the assumption that the water results from the mixing of two or more types of groundwater. This assumption can be verified by geochemical modelling of the mixing of the assumed initial types of water.

3.3.8 Summary

The results of the evaluation of the geochemical development of the groundwater from borehole 12MI33 and the related boreholes at a depth of -500 m below the surface of the MIU can be summarized as follows:

1. The total concentrations of dissolved solids range widely from 273.1 to 1265 mg/L.
2. For low mineralized water, there is a significant predominance of sodium ions above calcium ions, in the case of highly mineralized water the concentrations of calcium ions are slightly higher than sodium ions concentrations.
3. The low mineralized water can be attributed to shallow and highly mineralized groundwater to deeper layers of the rock environment.
4. The chemical composition of more than 90% of the groundwater of the area can be derived by simple mixing two types of groundwater irrespective of their position in the borehole and sampling date.

The differing trends in the time development of the chemical composition of the groundwater in the individual zones of borehole 12MI33 in its surroundings, as well as different trends in changes in chemical composition between the zones of the individual boreholes, can be attributed to the change in hydrodynamic conditions during the drilling of the boreholes and other changes over time after completion of the drilling. These then lead to a gradual change in the ratio of the mutual mixing of two main types of groundwater in the rock environment.

3.4 Model of the geochemical development of groundwater in the surroundings of the exploration gallery −500 m

The assumption that the groundwater parameters in the surroundings of the exploration gallery at a depth of −500 m is determined by mixing two types of water was verified on a model mixing selected typical groundwater with high and low mineralization.
3.4.1 Geochemical model of mixing groundwater

To model the geochemical development of groundwater in borehole 12MI33 and its surroundings, waters from borehole 13MI38 with high mineralization (sample 13MI38-37.6-151014) and groundwater from borehole 13MI41 with low mineralization (sample 13MI41-10.1-151019) were selected to estimate the initial groundwater end members composition. The results of the mixing of both end member water types are shown in Fig. 49.

![Fig. 49 Geochemical groundwater development in the surroundings of borehole 12MI33 (circles) with the results of the modelling of mixing water with high and low mineralization represented by groundwater from borehole 13MI38 (13MI38-37.6-151014) and 13MI41 (13MI41-10.1-151019), respectively. The model values are represented by lines (a) Piper diagram, (b) Durov diagram, (c) Changes in the concentrations of the main groundwater components in relation to the total concentration of dissolved solids, and (d) Dependence of the total concentration of dissolved solids on the mixing ratios of both types of water.](image)

3.4.2 Composition of the modelled water

The previous chapter describes a geochemical model, which shows that it is possible to derive all of the groundwater in the surroundings of the exploration gallery by mixing two basic types of groundwater. The first is a low mineralized type of 499.5 mg/L from borehole 13MI41
(sample 13MI41-10.1-151019) and the other is a high mineralized type from borehole 13MI38 (sample 13MI38-37.6-151014).

The difference in the chemical composition of the groundwater and the relative ratios of the major cations are best illustrated using Stiff diagrams (Fig. 50).

Water with low mineralization has a distinct predominance of sodium ions above calcium ions in the cationic part, whereas highly mineralized water has calcium ions very slightly above sodium. These groundwaters belong to common groundwater of deep circulation and were selected for the construction of a geochemical groundwater model because they are located at the opposite ends of the chemical composition of the waters of the exploration gallery area. Their complete physical and chemical parameters and composition are shown in Tab. 7.

A comparison with the assessment of the vertical development of the groundwater composition in the area of the MIU shows that the low mineralized type 13MI41 belongs to shallow groundwater and type 13MI38 to the mineralized waters from deeper layers.

Fig. 50 Stiff diagrams for the composition of groundwater used to prepare a geochemical model of groundwater mixing from the area of borehole 12MI33.
Tab. 7 Physical and chemical parameters and chemical composition of the water used for the geochemical groundwater mixing model of area of borehole 12MI33.

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3.5 Spatial development of groundwater

For the purpose of transport-reaction modelling, the profiles of the main components at the intersection of boreholes 13MI39, 13MI40 and 13MI41 perpendicular to the exploration gallery at a depth of -500 m beneath the surface, were prepared and supplemented with data from the respective zones of boreholes 12MI33 and 13MI38, which run horizontally and parallel to the tunnel.

3.5.1 Profiles of the horizontal boreholes 13MI40 and 13MI41

For the basic evaluation of the concentration trends around the exploration gallery, horizontal boreholes 13MI40 and 13MI41, which are perpendicular to the gallery, were selected. The sampling zones of the boreholes are arranged consecutively from the front of the gallery and their positions are marked with a number (labelled “Position” on the graphs). A detailed configuration of the zones is shown in Fig. 51.

![Fig. 51 Frontal view of the tunnel, indicating the positions of boreholes and profiles for plotting the concentration dependencies from the zones of boreholes 13MI40 and 13MI41. The white numbers in the circles indicate the sampling zones of the individual boreholes, their colours show the colour coding of the individual zones in the graphs, and the black numbers of the positions as each zone is plotted consecutively (labelled “Position” on the graphs). The boreholes and zones are plotted schematically and are not to the relevant scale.](image)

The overall trend in the development of dissolved solids (mineralization) shows a continuous decrease from the end of borehole 13MI40, through the tunnel to the end of zone 1 of borehole 13MI41 borehole (Fig. 52c). In the area of zone 4 of both boreholes perpendicular to the tunnel, there is a marked increase in concentrations. In terms of time development, after an initial decrease in concentrations there was a systematic increase in all of the zones from the start of sampling on 4 March 2014 to the last sampling date of 1 February 2016 (Fig. 52d). Trends
in the increase in concentrations of dissolved solids are comparable in the individual zones of borehole 13MI40 but differ from the norm in the zones of borehole 13MI41.

The development of chloride concentrations shows the profile time trends in the individual zones. However, the significant difference is that there are no elevated chloride concentrations in zones 4 of either borehole perpendicular to the tunnel and the concentrations show a linear trend from zone 1 of borehole 13MI40 to zone 1 of borehole 13MI41.

The development of the concentrations of the components from the first to the last sampling, i.e. an interval of almost two years, is shown in Fig. 53 and Fig. 54 as a comparison of the distribution of concentrations in the first and last sampling times (4 March 2014 and 1 February 2016). At the time of the first sampling, the trend of the main groundwater components, with the exception of carbonate concentrations, is the same. Concentrations from zone 1 of borehole 13MI40 to zone 1 of borehole 13MI41 decreased, in zones 4 of both boreholes perpendicular to the tunnel, the concentrations are clearly higher than the trend line. For carbonates, the situation was the opposite. The overall trend of carbonate concentrations shows an increase from zone 1 of borehole 13MI40 to zone 1 of borehole 13MI41, whereas there is a marked decrease in zones 4 of both boreholes.

The situation clearly changed at the end of the sampling period on 1 February 2016. Concentrations of dissolved solids in the individual zones of borehole 13MI40 were comparable, whereas in borehole 13MI41 they showed a marked decrease in the direction away from the tunnel. Sodium ion concentrations had virtually the same trend as total mineralization. For chlorides, there was a decrease in zone 4 in both boreholes compared to baseline values and the concentrations remained on a continuous line. The trend in calcium ion concentrations remained unchanged, i.e. higher concentrations remained in zone 4 in both boreholes. Concentrations of carbonates increased compared to the baseline, but it is difficult to determine any specific trend.
Fig. 52 Piper, Durov and concentration diagrams of the individual zones of boreholes 13MI40 and 13MI41, the tunnel is located between profiles 4 and 5: (a) Piper diagram, (b) Durov diagram, (c) concentrations of dissolved solids in the individual zones for all of the sampling dates, d) the same as (c) with the sampling dates included, the first is always the sample taken on 4 March 2014, the last sample of the given zone was taken on 1 February 2016, (e, f) chloride concentrations.
Fig. 53 Concentration of dissolved solids, chlorides, sodium and calcium ions in individual zones of boreholes 13MI40 and 13MI41. In the left column, the values are from the beginning of the sampling on 4 March 2014, in the right column from the last sampling on 1 February 2016.
Fig. 54 Total concentrations of carbonates in individual zones of boreholes 13MI40 and 13MI41. In the left column, the values are from the beginning of the sampling on 4 March 2014, in the right column from the last sampling on 1 February 2016.

Fig. 55 Frontal view of the tunnel, indicating the positions of boreholes and profiles for plotting the concentration dependencies from the zones of borehole 13MI39 and comparing with zones 4 of boreholes 13MI40 and 13MI41. The white numbers in the rings indicate the sampling zones of the individual boreholes, their colours show the colour coding of the individual zones in the graphs, and the black numbers of the positions as each zone is plotted consecutively (labelled “Position” on the graphs). The boreholes and zones are plotted schematically and are not to the relevant scale.

3.5.2 Profile of the vertical borehole 13MI39

The last trends to be evaluated were in the vertical borehole perpendicular to the profiles of boreholes 13MI40 and 13MI41. For comparison, these trends were complemented by zones 4 of boreholes 13MI40 and 13MI41, perpendicular to the tunnel and located higher than borehole 13MI39. The configuration of the zones on the evaluated profiles is shown in Fig. 55.

There is an overall decreasing trend in the total concentrations of dissolved solids and concentrations of chlorides with depth (Fig. 56c and Fig. 56e). The time development from the first to the last sampling is clearly more complex than in the zones of the horizontal boreholes 13MI40 and 13MI41 (Fig. 56d and Fig. 56f). After an initial decrease in concentrations, they
increase and then decrease again. At the same time, the trends in zones 2-4 of borehole 13MI39 are comparable.

Compared to the highest zone 4 of borehole 13MI39 perpendicular to the tunnel, the concentrations in zones 4 of boreholes 13MI40 and 13MI41, which adjoin the tunnel from the sides, are clearly lower.

### 3.5.3 Summary

The comparison of the concentrations of the main components in the profiles of boreholes 13MI39, 13MI40 and 13MI41 perpendicular to the tunnel and boreholes 12MI33 and 13MI38 leads to the following conclusions:

1. **Horizontal development:**
   a. In the horizontal profile from zone 1 of borehole 13MI40 to zone 1 of borehole 13MI41 there was a clear decreasing trend in the concentrations of all of the components, with the exception of carbonates, which showed the opposite trend.
   b. Concentrations in all of the zones of the two boreholes increased with time.
   c. All of the components with the exception of carbonates were significantly higher in zone 4 of borehole 13MI39, which adjoins the tunnel from the bottom.
   d. The concentrations of the individual components in zone 2 of borehole 12MI33, which perpendicularly intersects borehole 13MI41, were in good agreement with the trends found in borehole 13MI41.
   e. The concentrations of the individual components in zone 2 of borehole 13MI38, which perpendicularly intersects borehole 13MI40, clearly differ from the trends found in borehole 13MI40 and with the exception of carbonates were significantly lower.

2. **Vertical development:**
   a. Vertical development of the concentrations of the components in borehole 13MI39 from the exploration gallery to depth markedly decreased with time.
   b. In zone 4 of borehole 13MI39, which adjoins the tunnel from the bottom, the concentrations were significantly higher than in zones 4 of boreholes 13MI40 and 13MI41, which adjoin the tunnel from the sides.
Fig. 56 Piper, Durov and concentration diagrams for the individual zones of the vertical borehole 13MI39 and the addition of zones 4 of the horizontal boreholes 13MI40 and 13MI41: (a) Piper diagram, (b) Durov diagram, (c) concentrations of dissolved solids in individual zones for all sampling dates, d) same as (c) with the sampling dates included, the first is always from the sample taken on 4 March 2014, the last sample of the given zone was taken on 1 February 2016, (e) concentrations of chlorides in the individual zones for all of the sampling dates, (f) the same as (e), with the sampling dates included, the first is always from the sample taken on 4 March 2014, the last sample of the given zone was taken on 1 February 2016.
4 Task D – INBEB

Task D entitled “HM and THM interactions in bentonite engineered barriers” (INBEB) is focused on the modelling of hydro-mechanical and thermo-hydro-mechanical processes related to the function of bentonite engineering barriers, which are a key element of most spent nuclear fuel (SNF) and highly radioactive waste repository projects.

The Task Leader is Prof. Antonio Gens from the Polytechnic University of Catalonia (UPC). Five research teams are involved in the task: Institut de Radioprotection et de Sûreté Nucléaire (France), Japan Atomic Energy Agency, Korea Atomic Energy Research Institute, National Central University (Taiwan) and IGN.

The data from two long-term in-situ experiments conducted in Switzerland - the EB experiment conducted in the Mont Terri laboratory (duration 10.5 years) and the FEBEX experiment in the GRIMSEL laboratory (duration 18 years) are used to validate the models in Task D. Both experiments are performed using the same bentonite and are currently dismantled, providing unique data for model validation and study of the causes of heterogeneity of the final state of the bentonite barrier.

The present report deals with the performance of the project in the period 2016-6/2018 and is therefore devoted to the creation of a hydro-mechanical model for the modelling of a sealing element consisting of a combination of bentonite blocks and pellets. This model was validated on the data from the EB experiment. This chapter describes the layout of the experiment, the data used, and the model developed and implemented by the IGN team. It also describes the final results of the simulations performed to meet the defined task aims in the 1st and 2nd stages (see Chapter 4.1). These results are outputs from the final 3D model created by the IGN team. The results were sent to the Task Leader in the required extent. They are also located in the data repository and were made available to SÚRAO (electronic annex).

Further details on the design of the model and the results were obtained are given in Annex 2 with 34 pages written in English. This will form a contribution to the summary report prepared by the Task Leader.

4.1 Summary of the task description and evaluation of the data provided

The INBEB task was divided into individual stages, which refer to the in-situ experiments mentioned above, and the presented report concerns two of the stages:

1. Stage 1: Modelling of the EB experiments during hydration (10.5 years) and a comparison of the results with the data from the monitoring system.
2. Stage 2: Calculation of the final state of the saturation of the barrier and comparison of the results with the data from dismantling.

The task description is formulated in the corresponding documents, Stage 1 (Gens, 2016b) and Stage 2 (Gens, 2016c), which are also included as electronic annexes to this report. The data for these phases were partly provided in documents prepared by the Task Leader A. Gens made available at the web repository

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see (Gens 2016b) and (Gens 2016c) and were supplemented by literature sources (Alonso et al., 2010), (Villar et al., 2014).

The task description for the model solution is in fact defined by the experiment itself and supplemented by data on the materials used. This explains the structuring of the following text

4.1.1 EB Experiment

The EB experiment is characterized by the use of a combination of pellets and bentonite blocks, artificial hydration (the barrier is almost entirely saturated at the end of the test) and isothermal conditions, i.e. the existence of only hydro-mechanical interactions.

The overall layout of the EB experiment is included in Fig. 57 and Fig. 58. There were several objectives of the experiment. Firstly, from a technological point of view, the objective was to verify the seal design for a repository of the spent nuclear fuel and high level radioactive waste in horizontal galleries with a combination of a bed made from compacted bentonite blocks and a buffer in the upper part made from granular material (bentonite pellets). Secondly, the aim was to understand the ongoing processes and causes of inhomogeneities in the engineering barrier at the end of the saturation period. This inhomogeneity (heterogeneity) develops from the initial heterogeneity of the structure (bentonite blocks, uneven pellet bedding, gap between the blocks, backfill and rock, fractures in the surrounding rock, etc.) depending on the saturation and deformation processes. The maximum permeability will not be described only by the average dry density but also by the zones of reduced density. Heat phenomena can then contribute to the development of heterogeneity.

The EB experiment was equipped with sensors for monitoring displacements in the dummy canister, the relative humidity in the barrier, pore pressure in the rock environment, and total stress at the interface of the canister and the barriers and the rock environment and the barrier. Observations from the monitoring system are available for the duration of the test (10.5 years) until almost complete saturation.

Fig. 57 Installation of the EB experiment (Mont Terri) (Gens, 2016b)
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**Fig. 58 Diagram of the EB experiment (Gens, 2016)**

**Geometry of the experiment** - see the task documentation (Gens, 2016b, from page 57). The prescribed height of the corridor is 2.65 m, on the floor there is concrete at a height of 10 cm, the clearance height of the corridor is 2.65 - 0.1 = 2.55 m. The prescribed width of the corridor is 2.9 m, the cross-section consists of a rectangle of 2.65 x 1.2 m, on which there is a semicircle with a radius of 1.45 m (the height of the corridor is 1.2 + 1.45 = 2.65 m). The length of the corridor is 6 m, the length of the cylinder, the bentonite blocks and the concrete bed is 4.5 m, the diameter of the steel canister is 0.97 m and the weight is 11 000 kg (the weight of 1 m of the canister in the 2D model is 11 000/4.5 = 2 444 kg). At the end of the experiment, after 10.5 years, a pressure of 2 MPa is applied to the canister. The effect of the weight of the cylinder on the calculation is minimal (in the program, the weight of the canister is 23.98 kN). The three series of bentonite blocks have an initial dry density of 1.69 Mg/m³, height of approximately 21.4 cm and width of 12.5 cm (i.e. 4.5 m length equals 450/12.5 = 36 blocks). There are many fractures between the blocks.

**Hydration system**

Natural saturation of the EB experiment through the rock mass would take a too long time, so it was decided to install irrigation tubes with holes wrapped in a saturation mat. According to the task documentation (Gens, 2016b), only 22 hydration tubes of approximately 6 m in length were placed, located only in the pellets. According to the photo documentation and literature, the hydration was achieved using 37 hydration tubes, see Fig. 59.

**Fig. 59 Hydration system - placement of the hydration tubes, see (Gens 2016b).**
An additional 15 “tubes” (2 times 15 injectors) were installed to the level of the first and last bentonite blocks only (Fig. 59) so that they mainly injected the hydration geotextile (Fig. 60 “Mat”).

The hydration tubes were supplied from a common Pearson water tank and were interconnected at the beginning and at the end of the corridor in order to form three horizontal injection levels (Fig. 61) from the bottom to the top of the corridor.

Pearson water containing 19 g/l of sodium chloride has a similar composition to the surrounding rock (Opalinus clay). The chemical composition of the water is shown in Tab. 8. The salt content of the water significantly influences the input physical parameters - swelling pressure, permeability, saturation curve (osmotic pressure).

<table>
<thead>
<tr>
<th>Ion</th>
<th>Concentration (mg/l)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cl⁻</td>
<td>10635.90</td>
</tr>
<tr>
<td>SO₄²⁻</td>
<td>1354.41</td>
</tr>
<tr>
<td>HCO₃⁻</td>
<td>25.75</td>
</tr>
<tr>
<td>Mg²⁺</td>
<td>413.19</td>
</tr>
<tr>
<td>Ca²⁺</td>
<td>1034.06</td>
</tr>
<tr>
<td>Na⁺</td>
<td>5550.01</td>
</tr>
<tr>
<td>K⁺</td>
<td>62.95</td>
</tr>
<tr>
<td>Sr⁺</td>
<td>44.69</td>
</tr>
<tr>
<td>pH</td>
<td>7.6</td>
</tr>
</tbody>
</table>
Artificial hydration began on 5 May 2002 and the volume of the injected water was measured for all time, until 18 June 2007. The pressure in the water tank was measured from 2 November 2003, see Fig. 62.

Hydration took place in four phases over a period of 10.5 years (3827 days), and these phases correspond to the phases of the solution using the created model.

- **Phase 1**: 05/05 – 07/05/2002. Artificial hydration of 6.7 m³ over two days. The high volume of injected water was caused by very high permeability (low pellet resistance) in the initial phase when water could freely flow between the pellets in the direction of gravity. Hydration was stopped due to observed water leakage through the concrete plug.

- **Phase 2**: 08/05 – 11/09/2002. Artificial hydration stopped. Natural hydration took place from the surrounding rock mass only.


- **Phase 4**: 18/06/2007 – 22/10/2012. Natural hydration from the surrounding rock mass. End of continuous measurement 22/10/2012

Fig. 62 Artificial hydration-measurement of the volume of injected water and storage pressure, see (Gens 2016b). Development over time – injection pressure in blue, quantity in litres per hour in red.
The development of the total volume of artificially injected water in time is shown in Fig. 63. The total free space in pellets and bentonite blocks, including gaps, is approximately 14 m³, but the total volume of the injected water is 18.9 m³. A partial explanation can be found in the fact that in the initial period a certain volume of water drained from the experimental space, and another may have escaped via diffusion through the concrete plug. The main reason is that bentonite has the ability to bind more water than the pore volume (at a water density of 1 Mg/m³). At an initial suction pressure in the pellets of 300-400 MPa, the water is first deposited into micropores with a density higher than 1 Mg/m³, and with complete saturation we can see that more water is contained in the bentonite (up to 60% extra water for high density dry bentonite) than the free space defined by the porosity. It should be emphasized that the developed hydro-mechanical model includes this physical phenomenon, which is moreover related to changes in the dry density during deformation of the bentonite. This effect is very difficult to model mathematically and is one of the main achievements of the model construction.

As discussed in the previous interim report (Maryška et al., 2017, available on Sievert server of SÚRAO), the experiment involves a number of uncertainties. An example is the uneven flow of water from the individual hydration tubes.

From the point of view of hydration, only the total volume of injected water (or the pressure in the water tank) is known but the volume of water injected from the individual hydration bars is unknown. In addition, the situation is complicated by the fact that, in addition to the 22 main hydration tubes, another 2x15 injectors-hydration sources were added to the experiment in order to hydrate the geotextile. Hydration irregularities can be documented from the relative humidity measurements in the pellets in cross-sections B1 and B2 (Fig. 64), where the same hydration conditions are theoretically created, and the measured relative humidity curves should be almost the same. According to the relative humidity in cross-section B2, it appears that in the first phase of intensive injection (2 days - 6.7 m³ of injected water) no water flowed in the given location.
Decommissioning began in October 2012 and ended in January 2013. A range of high-quality data on the final state of the barrier (especially water content, density and saturation, hydraulic conductivity) were obtained. EDZ information is also available from before and after decommissioning. An example of the information obtained is given in Fig. 65.
4.1.2 Data for the EB experiment

Below is a brief summary of the data used to construct the model used for the modelling of the EB hydro-mechanical experiment.

- **Flow**
  - Initial dry density, \( \rho_d \)
  - Initial porosity \( \phi \)
  - Permeability
  - Volume of water for complete saturation \( w_{max} \)
  - Residual water volume \( w_{res} \)
  - Parameters for construction of retention/saturation curves \( \lambda, P_0, \lambda_1, P_{00} \) (the last only for the bentonite blocks and pellets)
  - Initial suction potential
  - Parameter (exponent) for expressing the relative permeability (generalized Irmay’s equation)

- **Mechanics**
  - Non-linear elasticity (dependent on \( \rho_d \))
  - Constant Poisson ratio

Saturation curve for the pellets (see Annex 2)

\[
w = \left( 0.08 + \frac{\phi}{\rho_d} \right) \cdot \left( 1 + \left( \frac{1}{\left( 2.4 \times 10^{-5} \times e^{(6.9592 \times \rho_d)} \right) \times \text{suction}} \right)^{1-0.14} \right)^{-0.14} \cdot \left( 1 - \frac{\text{suction}}{1100} \right)^{3}
\]

and for the blocks

\[
w = \left( 0.04 + \frac{\phi}{\rho_d} \right) \cdot \left( 1 + \left( \frac{1}{10^{-5} \times e^{(4.2 \times \rho_d)}} \times \text{suction} \right)^{1-0.14} \right)^{-0.14} \cdot \left( 1 - \frac{\text{suction}}{1000} \right)^{1.5}
\]

where suction is a value in [MPa] and porosity \( \phi = 1 - \frac{\rho_d}{\rho_s} = \frac{2.7-\rho_d}{2.7} \).

For the elasticity module we use the expression

\[E = E(w, \rho_d) = E(\text{suction}, \rho_d) = \begin{cases} E_{sat} + \frac{s}{50} (E_{max} - E_{sat}) & \text{if } s \leq 50 \text{ MPa}, \\ E_{max} & \text{if } s > 50 \text{ MPa}, \end{cases}\]

where \( s = \text{suction pressure} \) [MPa], whereby we use

\( E_{max} = 150 \text{ MPa} \) for the pellets and \( E_{max} = 300 \text{ MPa} \) for the blocks.

The specific parameter values are given in Tab. 9. A more detailed description and explanation of the constitutional relations used is given in Annex 2.
Tab. 9 Overview of the main parameters used in the hydro-mechanical model (see Schneider et al., 2012 - properties similar to the Belgian repository).

<table>
<thead>
<tr>
<th></th>
<th>Bentonite</th>
<th>Rock</th>
<th>Hydration</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Blocks</td>
<td>Pellets</td>
<td>Opalinus</td>
</tr>
<tr>
<td>Initial ( \rho_d ) [Mg/m(^3)]</td>
<td>1.69</td>
<td>1.26-1.46</td>
<td>2.45</td>
</tr>
<tr>
<td>Initial ( \phi )-porosity (-)</td>
<td>0.374</td>
<td>0.46-0.53</td>
<td>0.15</td>
</tr>
<tr>
<td>permeability [m(^2)]</td>
<td>=f((\rho_d))</td>
<td>=f((\rho_d))</td>
<td>5.0( \times )10(^{-20})</td>
</tr>
<tr>
<td>(w_{\text{max}}) (kg/kg(\text{bentonite}))</td>
<td>=0.04+(\phi /\rho_d)</td>
<td>=0.08+(\phi /\rho_d)</td>
<td>0.061</td>
</tr>
<tr>
<td>(w_{\text{res}}) (kg/kg(\text{bentonite}))</td>
<td>0.001</td>
<td>0.001</td>
<td>0.001</td>
</tr>
<tr>
<td>(\lambda ) (van Genuchten)</td>
<td>0.14</td>
<td>0.14</td>
<td>0.4</td>
</tr>
<tr>
<td>(P_0) [MPa]</td>
<td>=f((\rho_d))</td>
<td>=f((\rho_d))</td>
<td>18</td>
</tr>
<tr>
<td>(\lambda_1) (van Genuchten)</td>
<td>1000</td>
<td>1100</td>
<td></td>
</tr>
<tr>
<td>(P_{\text{oo}}) [MPa]</td>
<td>1.5</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>Initial suction pressure [MPa]</td>
<td>120</td>
<td>400</td>
<td>0</td>
</tr>
<tr>
<td>exponent (n) Se(^{\text{n}})</td>
<td>3</td>
<td>1.9</td>
<td>3</td>
</tr>
<tr>
<td>elast. modul. [GPa]</td>
<td>=f((\rho_d, \text{suction}))</td>
<td>=f((\rho_d, \text{suction}))</td>
<td>30</td>
</tr>
<tr>
<td>Poisson ratio</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
</tr>
</tbody>
</table>

4.2 Summary of the solution between 7/2016-6/2018

4.2.1 The model

A combined hydro-mechanical model was developed and implemented in COMSOL Multiphysics, which includes:

- A description of the saturation development using pore pressure, mass water content and dry density (\(p_w, w, \rho_d\)).
- Richards equation with water vapour diffusion for flow in variable saturated/unsaturated bentonite blocks and pellets, rock and concrete.
- Parameters for permeability in a saturated state and a function for relative permeability depending on the volume of saturated water.
- Construction of retention curves for bentonite blocks and pellets, i.e. the dependence between pressure variables, mass water content and dry density (\(p_w, w, \rho_d\)).
- Swelling of bentonite blocks and pellets.
- Non-linear elasticity for the behaviour of bentonite with a variable tangential module \(E = E(w, \rho_d)\).
- Flow model for gaps between bentonite blocks and a model of permeable layers for gaps in the pressure saturation phase.
• Simulation of the presence of injection tubes using liner sources that allow for description using a pressure source or mass flow.

The processes were first modelled as a 2D model (perpendicular to the canister) and consequently as a 3D model using vertical symmetry, see Fig. 66. The overall model is described in detail in Annex 2.

![Fig. 66 Mesh for the final 3D model discretized by finite element method (FEM).](image)

**4.2.1 Required outputs from Stage 1**

The aim of the first stage was to create a complex hydro-mechanical model of the buffer and surrounding rock that allows time monitoring of canister displacement, total pressure and relative humidity in the bentonite for the entire duration of the EB experiment - over 10.5 years. The model outputs were compared to the required measured variables (displacement, total pressure and relative humidity) that were monitored in the experiment, see Fig. 67.

A comparison of the outputs from the final 3D model with the measurements is included in the Fig. 68 to Fig. 75. It is clear from the outputs that the model produces qualitatively correct results, an exact agreement with the measurements can also be difficult to achieve due to the considerable uncertainties in the model input (outflow of an unknown volume water, inaccurate measurement of canister displacement, heterogeneity of the properties of the used pellets, difference in the properties of the bentonite using Pearson water for the experiment and pure water in the laboratory experiments). These uncertainties are discussed in more detail in the English text in Annex 2. The following figures show that the calculated values, unlike the measurements, often reflect the expected behaviour. This is commented on, for example, in the case of horizontal pressure. When calculating the relative humidity, the calculation gives a logical (averaged) result, while the measurements are only localized and are apparently influenced by the location of the sensor in the vicinity of the water injectors. Further comment is given in the descriptions of several of the graphs.
Fig. 67 Required values of measured displacement variables, relative humidity and total pressure, see (Gens2016b).
Fig. 68 Measured and calculated time course of the total pressure in pressure sensors PE1 and PE2 located in pellets in section E (Fig. 67).

Fig. 69 Measured and calculated time course of the total pressure in pressure sensors PE3, PE7, PE4, and PE8 located in pellets in section E (Fig. 67). The measurement shows unexpected asymmetry, especially in the pressure on the left and right side when the plug is in contact with the rock. The calculated pressures are symmetrical, with a smaller difference between the measurements near the rock and the canister, both calculated pressures seem more natural.
Fig. 70 Measured and calculated time course of the total pressure in pressure sensors PE5 and PE6 located in bentonite blocks in section E (Fig. 67)

Fig. 71 Measured and calculated time course of the relative humidity in points WB13 and WB14 located in bentonite blocks in section B1 (Fig. 67).
Fig. 72 Measured and calculated time course of the relative humidity in points WB23 and WB24 located in bentonite blocks in section B2 (Fig. 67).

Fig. 73 Measured and calculated time course of the relative humidity in points WB11 and WB21 located in the pellets in section B1 (Fig. 67).
Fig. 74 The measured and calculated time course of relative humidity at points WB21 and WB22 located in the pellets in section B2 (Fig. 67).
Fig. 75 The measured and calculated time course of the vertical (in points EA12, EA22) and the horizontal (in points EA11, EA21) displacement of the front and rear parts of the canister in sections A1 and A2 (Fig. 67). The measurement has an unexpectedly large difference between A1 and A2, the behaviour of EA22_V is probably influenced by the measurement issue. The calculated behaviour is logical but reaches somewhat high values. The comparison is further discussed in Annex 2 of the report.
4.2.2 Required outputs of Stage 2

The aim of the second stage was to extend the complex hydro-mechanical model of the buffer and the surrounding rock, which follows on from the solution of the first stage and allows the calculation of dry density, mass water content and saturation after the EB experiment was decommissioned (after 10.5 years). The required output was a comparison of the measured (evaluated) and calculated variables (dry density, water content and saturation degree) along selected radial segments (orthogonal to the canister) on three of the decommissioned sections (Fig. 76). For comparison, the investigators did not have a description of the measured quantities but only their graphic processing. A description of the decommissioning of the experiment and the sampling including the measurements is given in (Villar et al., 2014).

Fig. 76 Selected sections in which the results are required: distribution of dry density, water content and level of saturation. For a comparison with the state after dismantling, see (Gens 2016c)

A comparison of the outputs from the final 3D model and with the measurements are given from Fig. 78 to Fig. 94. For visualization with an odd number order, the left scale represents the value in the blocks and the right scale represents the value in the pellets. The results show good agreement taking into account the measurement error, the method of decommissioning and the uncertainty with the amount of injected water during the experiment.
Fig. 77 Measured effective saturation [%] in the experiment from the in-situ data analysis in section A1-25.

SECTION A1-25

Fig. 78 Course of calculated effective saturation [%] in section A1-25 after 3827 days.

Fig. 79 Measured effective saturation [%] in the experiment from the in-situ data analysis in section E.

SECTION E

Fig. 80 Course of calculated effective saturation [%] in section E after 3827 days.
Fig. 81 Course of calculated effective saturation [%] in section B2 after 3827 days.

Fig. 82 Measured effective saturation [%] in the experiment from the in-situ data analysis in section B2.

Fig. 83 Course of calculated dry density of the bentonite [kg·m⁻³] in section A1-25 after 3827 days.

Fig. 84 Measured dry density of the bentonite [kg·m⁻³] in the experiment from the in-situ data analysis in section A1-25.
**SECTION E**

Fig. 86 Measured dry density of the bentonite [kg · m\(^{-3}\)] in the experiment from the in-situ data analysis in section E.

**SECTION B2**

Fig. 88 Measured dry density of the bentonite [kg · m\(^{-3}\)] in the experiment from the in-situ data analysis in section B2.
Fig. 89 Course of calculated mass water content of the bentonite $[kg \cdot kg^{-1}]$ in section A1-25 after 3827 days.

Fig. 90 Measured mass water content of the bentonite $[kg \cdot kg^{-1}]$ in the experiment from the in-situ data analysis in section A1-25.

Fig. 91 Course of calculated mass water content of the bentonite $[kg \cdot kg^{-1}]$ in section E after 3827 days.

Fig. 92 Measured mass water content of the bentonite $[kg \cdot kg^{-1}]$ in the experiment from the in-situ data analysis in section E.
4.2.3 Results of the numeric model – discussion

A detailed description of the HM model and the settings of the boundary and initial conditions is given in Annex 2, which was submitted to the INBEB Task Leader A. Gens. It describes in detail the calculation procedure and the interim results. The conclusions include an analysis of the large uncertainties in the interpretation of the measured quantities. Therefore, in this chapter we will only briefly describe the basic calculation procedure and assess the comparison of the calculated and measured quantities presented in the previous two chapters - the required outputs for Stage 1 and Stage 2.

In the calculations of the 3D HM model, we use two saturation level indicators - Se corresponds to the real filling of the free space with water and its maximum value is 100% and Se_ef represents the saturation, which corresponds to the pore space, is evaluated experimentally after the decommissioning of the experiment and is based on a water volume of 1000 kg · m⁻³ and may reach values greater than 100% (Villar et al., 2014).

The calculation, which is based on the 3D HM model, began with the excavation of the corridor and its ventilation for a period of 160 days. Subsequently, from a mathematical point of view, the one-off installation of the EB experiment (container, bentonite pellets and blocks, concrete plugs, hydration tubes) and the calculation of the individual hydration phases followed.

- Phase 1: 05/05 – 07/05/2002. Artificial hydration of 6.7 m³ over two days. The high volume of injected water was caused by very high permeability (low pellet resistance) in the initial phase when water could freely flow between the pellets in the direction of gravity. Hydration was stopped due to observed water leakage through the concrete plug.
In the 3D model, water injection is included using tubes embedded at the start and end of the bentonite blocks saturating water through the geotextile located longitudinally between each bentonite block (Fig. 60). For a detailed description, see Annex 2.

The calculation of experimental effective saturation Se_ef [%] is shown in Fig. 95, which shows that it was possible to simulate the initial free flow of water between the pellets and their placement in the lower part of the corridor,

- Phase 2: 08/05 – 11/09/2002. Artificial hydration stopped. Natural hydration took place from the surrounding rock mass only.

  Fig. 96 shows the calculation of experimental effective saturation Se_ef [%] at the end of Stage 2, when the pellets are homogenized as a result of their expansion and filling of the macro pores. There was a significant decrease in the permeability of the pellets and the water from the surrounding rock mass accumulated in the pellets near the surface of the corridor.

- Phase 3: 11/09/2002 – 18/06/2007 Slow continuous hydration by means of tubes in the pellets and injectors in the bentonite blocks with measurements of the total water injection and from 02/11/2003 the pressure in the tank. End of artificial hydration 18/06/2007

  Fig. 97 shows the calculation of the experimental effective saturation Se_ef [%] at the end of Stage 3, when there was a significant increase in the volume of water in the pellets and the bentonite blocks. The bentonite blocks and pellets around the hydration tubes were almost fully saturated and Se_ef > 100%.

- Phase 4 – 18.6. 2007 – 22/10/2012. Natural hydration from the surrounding rock mass. End of continuous measurement on 22 October 2012 after 3827 days.

  Fig. 98 shows the calculation of experimental effective saturation Se_ef [%] at the end of the continuous measurement on 22 October 2012. The bentonite blocks and pellets near the wall of the corridor were almost fully saturated and Se_ef > 100%. The real saturation Se [%] Fig. 99 and suction pressure [MPa] Fig. 100 are displayed at the end of the continuous measurement on 22 October 2012 and show that the pellets were not yet fully saturated, as confirmed by the exact measurement of relative humidity in the pellets during the decommissioning of the experiment - see the enclosed English supplementary report.
Fig. 95 Effective saturation $Se_{ef}$ [%] in the area of the pellets and blocks after completion of the first phase of the experiment after 7 days of intensive injection of 6.7 m$^3$.

Fig. 96 Effective saturation $Se_{ef}$ [%] in the area of the pellets and blocks after completion of the second phase of the experiment after 133 days.

Fig. 97 Effective saturation $Se_{ef}$ [%] in the area of the pellets and blocks after completion of the third phase of the experiment after 1896 days.
Fig. 98 Effective saturation $S_{e_{f}}$ [%] in the area of the pellets and blocks after completion of the phase of the experiment after 3827 days.

Fig. 99 Effective saturation $S_{e}$ [%] in the area of the pellets and blocks after completion of the experiment after 3827 days.

Fig. 100 Dry density of the bentonite $\rho_{d}$ [g·cm$^{-3}$] in the area of the pellets and blocks after completion of the experiment after 3827 days.
The end of the continuous measurement on 22 October 2012 after 3827 was also the time when the EB experiment was decommissioned in the 3D HM model. At 3827 days the distribution of mass water content $w \ [kg \cdot kg^{-1}]$ (Fig. 101) and the dry density of the bentonite $\rho_d \ [g \cdot cm^{-3}]$ were evaluated.

The calculated and measured (evaluated) quantities presented in Stage 1 and Stage 2 according to the requirements of the Task Leader can only be compared in terms of qualitative indicators. This is due to the large uncertainties in the interpretation of the measured variables, which are described in detail in Annex 2.

The development of the total pressure (Fig. 68 - Fig. 70) in time - the measured values in all sensors reached approximately 2 MPa after approximately 6 years (almost full saturation) and remained with only slight changes until the end of the experiment. The calculated total pressure qualitatively reached the measured values of 2 MPa only in the pressure sensors in the vertical direction (Fig. 68 and Fig. 70). In the horizontal direction, the calculated pressure values were roughly half at 1 MPa (Fig. 69), which corresponds to the maximum swelling pressure for the average dry density of the pellets in this area.

The development of the relative humidity in the pellets (Fig. 71 - Fig. 74) and the blocks in time shows full saturation within 2 years. In addition, the measurements by more accurate relative humidity sensors after decommissioning did not show 100% humidity (see Annex 2). A gradual increase in the measured relative humidity values should follow the gradual increase in total
pressure (6 years). The outflow of water from the injection tubes is apparently very uneven (Fig. 6). Calculation of the time course of the relative humidity only corresponds to the measurement qualitatively and copies the calculated increase in swelling pressure.

Measurement of the time development of the vertical displacement (Fig. 71) reach a maximum of 2cm and is completely inconsistent with the change in measured dry density of bentonite blocks at the start ($\rho_d = 1.69 \, g \cdot cm^{-3}$) and after decommissioning of the experiment (Fig. 84, Fig. 86, Fig. 88 ($\rho_d = 1.36 \, g \cdot cm^{-3}$)), where the dry density of the pellets and blocks is almost the same. This change in the bentonite blocks is so marked by the "measurement" that it would move the canister vertically by 6-7 cm (see Annex 2). There is a big assumption that the sample will expand even when the experiment is decommissioned and sampling for laboratory evaluation of water content and dry density. The minimal calculated mean dry density of the bentonite blocks reaches $1.58 \, g \cdot cm^{-3}$, the vertical displacement of the canister is 2.5 cm (Fig. 75). Homogenization - a pronounced stretch in bentonite is an extremely complex mathematical problem in terms of setting the model, optimal physical parameters, and achieving convergence. Of all the teams of investigators in the INBEB Task, IGN achieved the most visible extension of the bentonite blocks.

The measured and calculated mass water content (Fig. 89 - Fig. 94) is highest in the corners of the lower part of the corridor, which corresponds to the reduction of the dry density of the pellets (Fig. 83 - Fig. 88).

The measured and calculated experimentally evaluated saturation $S_{e_ef}$ (Fig. 77 - Fig. 82), which is evaluated after the experiment is decommissioned and is based on the density of the water of $1000 \, kg \cdot m^{-3}$, is greater than 100% when the experiment is decommissioned. Experimental saturation values are somewhat lower due to the partial drying of the bentonite during decommissioned and also by laboratory drying of the sample at 110 °C not possible to completely dry the sample.
4.2.4 Interaction between the pellets and the bentonite blocks

During the discussions with the Team Leader A. Gens, there was uncertainty about the assessment of the models and approaches of the individual project teams of DECOVALEX - Task D. Therefore, an artificial benchmarking task was developed to test the interaction of the pellets and the bentonite blocks. This involved the saturation of a cylindrical shaped sample, which appears cross-section according to Fig. 103.

![Diagram of the model task for simulation of interactions between the pellets and the bentonite blocks used to test the numerical models](image)

A 2D axially symmetric model was created with a vertical axis of symmetry in the centre of the area, 5 cm in diameter, 10 cm in height, the lower part of the block was 5 cm in height, and the upper part was also 5 cm in height. The input parameters are identical to the 3D EB model, i.e. the initial suction of the blocks was 120 MPa, and of the pellets was 400 MPa, and the initial pressure was 0.1 MPa, dry density of the pellets was 1.36 g/cm$^3$ and of the blocks was 1.69 g/cm$^3$.

Boundary conditions on the cylinder were applied so that the saturation was allowed to occur from the top and bottom, while the model did not allow any inflow through the casing. Mechanical boundary conditions allow for a displacement in the direction perpendicular to the wall.

The model ran until full saturation Fig. 105, which occurred on day 400. The aim was to compare the state at the start and at the end of the experiment. This made it possible to better predict the interaction between the bentonite blocks and the pellets.

The distribution of the dry density of bentonite in Fig. 104 shows that the swelling forces of the blocks are larger than the pellets. The blocks pushed into the pellet space to a distance of 0.35 cm.

Fig. 106 shows a comparison of the mass content of water $w$ [%] at the start and at the end of the experiment.
Fig. 104 Comparison of the dry density distribution $\rho_d [g \cdot cm^{-3}]$ at the beginning of the experiment (left) and at the end of the experiment (right).

Fig. 105 Comparison of the effective saturation $S_e [%]$ at the beginning of the experiment (left) and at the end of the experiment (right) - saturated state with differences in numerical accuracy.
Fig. 106 Comparison of the mass water content \( w \) [%] at the beginning of the experiment (left) and at the end of the experiment (right)

Fig. 107 Comparison of the porosity \( \phi \) [%] at the beginning of the experiment (left) and at the end of the experiment (right)

Fig. 109 shows a comparison of the deformation \( \varepsilon_v \) [%] and the total pressure \( \sigma \) [MPa] at the end of the experiment. It is possible to observe the expansion of the blocks and the compression of the pellets in a vertical direction, which is due to the equalization of the total pressure in the vertical direction. In the horizontal direction, there is still a different overall pressure at the level of pellets and blocks.

Overall, this seemingly simple case shows the changes in homogenization of the bentonite blocks and the pellets that occur in the presence of water.

An important factor is the approximation of the porosity value \( \phi \) [%] in Fig. 107. This corresponds to the saturable permeability value \( k_s \) \( [m^2] \) shown in Fig. 108.
Fig. 108 Comparison of saturation permeability $k_s [m^2]$ at the beginning of the experiment (left) and at the end of the experiment (right).

Fig. 109 Comparison of deformation $\varepsilon_v [%]$ (left), total pressure $\sigma [MPa]$ in the vertical direction (center) and in the horizontal direction (right). All of the results represent the end of the experiment—full saturation.
4.3 Discussion of the results

The main results of the project relate to the formulation of hydro-mechanical models, the implementation of these models in the COMSOL software and the solution of selected tasks for validation of the models. This is visible from the above-mentioned text as well as from the contents of the accompanying interim report (Annex 2), which was also submitted to the INBEB Task Leader, who will use it to produce a summary report, which will be made available to the Steering Committee of the DECOVALEX-2019 project. More details on the modelling are described in the accompanying DECOVALEX Interim Report (Annex 2), which has already been read by the INBEB Task Leader Prof. A. Gens and other members of the Task D investigation teams. From the presentations available to members of the Steering Committee, in which SÚRAO is represented, a good agreement can be found between the presented IGN model, the data obtained during the decommissioning of the experiment and other foreign teams that worked on the project.

Data from the EB experiment are used to validate the model, whose main objective is to understand the process of homogenization of the sealing material, which in particular means homogenization of the filled pellet space in contact with water, see Fig. 100. Furthermore, the interaction of the bentonite pellets, bentonite blocks and concrete (forming a plug and bed for the bentonite blocks) is investigated. These aspects represent the contribution of the modelling even in an international scale. The other objectives of the EB experiment were to assess the quality of the proposed solution as an engineering barrier (the Spanish concept of nuclear waste disposal), measure the canister displacement, assess the functionality of the concrete plug, measure the saturation of all of the materials over time, measure the pressure, the effect of Pearson water on the engineering barrier and many others, see the task documentation (Gens 2016b).

During the project solution, the numerical model was greatly improved, and is now able to model combined hydro-mechanical processes with the following specifics:

- 3D simulation with full interaction between the hydration tubes, bentonite pellets, bentonite blocks, geotextiles, bentonite plugs, concrete beds, the surrounding rock mass, injectors and the open corridor.
- Artificial saturation using hydration tubes and injectors. Natural saturation through the surrounding rock mass.
- Higher saturation of bentonite than its pore space.
- Variable saturation curves for the pellets and blocks depending on dry density and porosity.
- Gaps between the blocks and their gradual closure over time.
- Flow of water between the pellets due to gravity, swelling of the pellets to fill the space between them, work with an inhomogeneous distribution of the pellets due to the technology used to place them, work with different pellet permeabilities depending on their distribution.
- Filling of the pore space of the geotextile with bentonite.
- Use of the H, M or HM models where needed, for example, the hydration bars are impermeable, so we only use the M model.
- The open model is implemented in the COMSOL software, which allows for additional phenomena such as thermal processes.
The implementation of all these specifics is unique even in the DECOVALEX-2019 project. Over the project solution, it has been shown that all of the above-mentioned specifics are important for constructing the model which is able to simulate the behaviour of the seal installed in the EB experiment. The experience gained can be transferred to the environment of the development of deep geological repository in the Czech Republic.

For collaboration with experimental research, based on the experience gained, it is possible to determine which material parameters are critical for modelling the behaviour of the bentonite barrier for storing nuclear waste using bentonite blocks as well as pellets and blocks. On the contrary, knowledge of these parameters can be used to model the proposed designs. Experience with the model can also help in designing experiments related to the considered topics, and avoid possible problems in interpreting the data obtained.

Participation in the INBEB Task has received a good response (invitations to lectures and the organization of a special section at the EGU 2018 conference) and the experience and contacts gained will allow a better understanding of the problems related to the construction of a nuclear repository in the Czech Republic. Hence, the following requirements formulated in the SÚRAO material (Pospíšková et al., 2015) were met:

- Increase the knowledge and understanding of processes in the repository,
- Create a sufficient knowledge base for DGR safety assessments,
- Facilitate the transfer of knowledge from advanced repository preparation programmes (Sweden, Finland, France, etc.),
- Educate experts in this area.
5 Task G – EDZ

In a wider context, the objective of Task G was to understand changes in the permeability of the rock, in relation to the creation of EDZ in the vicinity of the underground structures. In a narrower context, it was to validate approaches that use the different simulation software of the individual teams of investigators. Another objective was to understand the measured data from the hydraulic tests in a fracture environment and to use them correctly in numerical simulations (both during preparation of the model and interpretation of its results).

The designer of the Task was the Swedish Radiation Safety Authority (SSM) and the Task Leader is Tobias Backers as an external collaborator of SSM, with the support of other consultants Joel Geier (Clearwater Hardrock Consulting), Erik Eberhard (Fisher Rock Engineering) and Tobias Meier. SSM is represented by Carl-Henrik Pettersson. Teams from three countries also participated in the Task, in addition to the joint TUL and IGN team, Geomecon GmbH (Germany) and the Seoul National University (South Korea). The Geomecon team also includes the Task Leaders (Backers and Meier).

5.1 Summary of the task description and evaluation of the data provided

In the first task “work package 1.3.3” (named by the authors of the Task), comparable 2D problems with simple tunnel geometry were provided (Backers, 2016, Backers et al., 2017a). In the first case (WP1_A), homogeneous rocks without fractures were considered, in the second case (WP1_B) a discreet fracture network (DFN) with several DTMs was added. In addition, detailed tables were provided with uniquely specified material parameters and boundary conditions and other inputs into the models.

The task was solved in parallel by both participating institutions (TUL, IGN). Since the same software tool was used at this stage, the results below should be seen as common but independently verified, with both institutions working separately.

The follow-up task within “work packages 2.1 and 2.2” is used to describe hydro-mechanical behaviour through the 3D model of the TAS04 tunnel located in the Swedish Underground Laboratory at Äspö (Backers et al, 2017a, 2018). In the simulations, discontinuities and EDZs were considered in the vicinity of the tunnel, as well as the irregular inner surface of the tunnel, for which several input data was provided by the Task Leader. In Task 2.1, a qualified estimate of hydromechanical behaviour was made with the models using the maximum amount of provided data. In Task 2.2, further specifications of the area were provided (more detailed fracture networks at various scales) and then three injection tests were simulated and the impacts of differing shapes of the tunnel on the model results were compared.

5.2 Modelling poroelasticity in COMSOL Multiphysics

The “Subsurface flow” module, specifically the built-in interface for the calculation of poroelasticity in COMSOL Multiphysics, COMSOL (2017), was used for the simulations in WP1_A and WP1_B in two versions: TUL v. 5.0.1 and IGN v 5.2. Biot’s poroelasticity (1962), which combines Darcy flow in a saturated porous environment with a linear equation (5.1) with
linear elasticity, was implemented in the interface, which was solved in a 2D approximation as the role of plane deformation (5.2)

\[-\nabla \cdot \left( \frac{\kappa}{\mu} \nabla p \right) = 0 \tag{5.1}\]

\[
\begin{bmatrix}
\sigma_{xx} \\
\sigma_{yy} \\
\sigma_{xy}
\end{bmatrix}
= \frac{E}{(1 + \nu)(1 - 2\nu)} \begin{bmatrix}
1 - \nu & \nu & 0 \\
\nu & 1 - \nu & 0 \\
0 & 0 & 1 - 2\nu
\end{bmatrix}
\begin{bmatrix}
\varepsilon_{xx} \\
\varepsilon_{yy} \\
\varepsilon_{xy}
\end{bmatrix}
- \begin{bmatrix}
\alpha_B p & 0 & 0 \\
0 & \alpha_B p & 0 \\
0 & 0 & \alpha_B p
\end{bmatrix}, \tag{5.2}
\]

where \(\kappa\) is the permeability of the material, \(\mu\) is the dynamic viscosity of the liquid, and \(p\) is the fluid pressure, \(\sigma_{ij}\) are stress tensor components, \(\varepsilon_{ij}\) deformation tensor components, \(\nu\) is Poisson’s constant, \(E\) is Young’s modulus of elasticity, and \(\alpha_B\) is Biot’s coefficient.

In the case of an alternative with a fracture network, so-called fracture flow is also used in the model, which considers tangential derivations to define the flow along the lines representing the fractures, according to the following equation

\[-\nabla_T \cdot \left( \frac{\kappa_f}{\mu} \nabla_T p \right) = 0, \tag{5.3}\]

where \(\kappa_f\) indicates the permeability of the fracture and \(\nabla_T\) is the gradient operator limited to the tangential direction towards the fracture.

The grouping of hydraulic and mechanical problems is considered unidirectional based on the description of task 1.3.3. It addressed the effect of a steady flow of water through a porous medium on the change in stress fields and deformation (i.e. stationary models).

Tasks 2.1 and 2.2 were solved using newer versions of COMSOL Multiphysics (5.2.0.166 and 5.3.0.316, respectively). The problems are defined as time-dependent – bidirectionally coupled in 3D, for which the following governing equations are considered, generalizing the description given for the 2D problems.

\[\nabla \cdot \sigma = F_v \tag{5.4}\]

\[\sigma = C : (\varepsilon - \varepsilon_0) - \alpha_B p I \tag{5.5}\]

\[\varepsilon = \frac{1}{2} \left[ (\nabla u)^T + \nabla u \right] \tag{5.6}\]

\[\rho S \frac{\partial p}{\partial t} + \nabla \cdot (\rho u) = Q_m - \rho \alpha_B \frac{\partial e_{vol}}{\partial t} \tag{5.7}\]

\[u = -\frac{\kappa}{\mu} \nabla p \tag{5.8}\]
\[
S = \varepsilon_p \chi_f + \frac{(\alpha_B - \varepsilon_p)(1 - \alpha_B)}{K},
\]

where \(\sigma\) is the stress tensor, \(F_v\) is the volumetric force, \(C\) is the coefficient of elasticity tensor, \(\varepsilon\) is the deformation tensor, \(\varepsilon_0\) is the initial value of the deformation tensor, \(u\) is the stress vector, \(\rho\) is the density of the liquid, \(S\) the coefficient of storativity, \(Q_m\) is a member expressing the source, \(t\) is time, \(\chi_f\) is the compressibility of the liquid, \(\varepsilon_p\) is porosity, \(K\) is hydraulic conductivity and \(\varepsilon_{vol}\) volumetric deformation.

5.3 Task WP1_A: 2D model with homogeneous rock

The first task was the 2D model with simple geometry (a tunnel placed in the middle of homogeneous rock with dimensions of 100 \(\times\) 100 m). The mechanical and hydraulic boundary conditions are given in Fig. 110.

Applied pore pressure:
- External boundaries of the model: 5 MPa,
- Tunnel edge: 0 MPa.

Mechanical boundary conditions:
- Upper boundary: 12.5 MPa,
- Right boundary: 29 MPa,
- Tunnel edge: 0 MPa,
- Left and lower boundaries: "roller" (zero normal displacement).

At the geometry level there were three monitoring lines according to Fig. 110 (one horizontal line leading from half the height of the tunnel to the right edge of the model, one vertical line leading from the centre of the top edge of the model to the tunnel and a final horizontal line leading 15 cm below the lower edge of the tunnel). The lines serve to output the required variables. All of the material parameters needed for the simulations were entered (and are summarized in Tab. 10).

![Fig. 110 Geometry of the model problem, monitoring lines and the applied boundary conditions](image-url)
Tab. 10 Material parameters of the rock and water for tasks WP1_A and WP1_B

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young's module of elasticity</td>
<td>76</td>
<td>GPa</td>
</tr>
<tr>
<td>Poisson's constant</td>
<td>0.25</td>
<td>1</td>
</tr>
<tr>
<td>Density</td>
<td>2750</td>
<td>kg·m⁻³</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.01</td>
<td>%</td>
</tr>
<tr>
<td>Permeability</td>
<td>5·10⁻¹⁸</td>
<td>m²</td>
</tr>
<tr>
<td>Biot's coefficient</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Dynamic viscosity (water)</td>
<td>10⁻³</td>
<td>Pa·s</td>
</tr>
<tr>
<td>Compressibility (water)</td>
<td>4.4·10⁻¹⁰</td>
<td>Pa⁻¹</td>
</tr>
<tr>
<td>Density (water)</td>
<td>1000</td>
<td>kg·m⁻³</td>
</tr>
</tbody>
</table>

5.4 Task WP1_B: 2D model with a discrete fracture network

In task WP1_B, a discreet fracture network was added in two alternatives to define the task with homogeneous rock. In the first case, an alternative with a stochastic fracture network was selected composed of smaller fractures (hereinafter referred to as the DFN alternative, see Fig. 111 on the left). In the second case, both the smaller fractures and seven deterministically determined larger fractures were included (Fig. 111 on the right), referred to as the DFN+DTM alternative. Both types of fractures were assigned different opening and permeability values according to the task description, see the summary of the material characteristics for the fractures in Tab. 11 and Tab. 12.

The geometry and computational mesh were defined directly in the COMSOL Multiphysics environment based on the geometry from task WP1_A, to which the specified fracture network was added. Fractures represented by lines were imported using a .dxf file, which had to be retrieved from the provided data (in .prn format) using external modifications. Specifications of the stochastic fracture network are described in detail in Backers et al. (2017a), only one selected alternative provided by the Task organizers was used to construct the geometry. The computational mesh defined based on the described geometry contained 247,000 triangular elements and 18,000 linear elements in the DFN alternative and 303,000 triangular elements and 23,000 linear elements in the DFN+DTM alternative (Fig. 112).
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Fig. 111 Fracture network for the geometry of task WP1_A (DFN on the left, DTM on the right)

Tab. 11 Material parameters of the applied discrete fracture network

<table>
<thead>
<tr>
<th>Parameter (DFN)</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Permeability</td>
<td>2.8 $\cdot$ 10$^{-11}$</td>
<td>m$^2$</td>
</tr>
<tr>
<td>Opening</td>
<td>1.8 $\cdot$ 10$^{-5}$</td>
<td>m</td>
</tr>
<tr>
<td>Porosity</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Storativity</td>
<td>3 $\cdot$ 10$^{-8}$</td>
<td>1</td>
</tr>
<tr>
<td>Transmissivity</td>
<td>5 $\cdot$ 10$^{-9}$</td>
<td>m$^2$ s$^{-1}$</td>
</tr>
</tbody>
</table>

Tab. 12 Material parameters of the applied deterministic fracture network

<table>
<thead>
<tr>
<th>Parameter (DFN)</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Permeability</td>
<td>2.8 $\cdot$ 10$^{-10}$</td>
<td>m$^2$</td>
</tr>
<tr>
<td>Opening</td>
<td>3 $\cdot$ 10$^{-5}$</td>
<td>m</td>
</tr>
<tr>
<td>Porosity</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Storativity</td>
<td>3 $\cdot$ 10$^{-8}$</td>
<td>1</td>
</tr>
<tr>
<td>Transmissivity</td>
<td>5 $\cdot$ 10$^{-8}$</td>
<td>m$^2$ s$^{-1}$</td>
</tr>
</tbody>
</table>
Fig. 112 Computational network with a close up of the tunnel surroundings for the DFN+DTM alternative with 303,000 elements

5.5 Results of the WP_A and WP1_B modelling

The results of all of the alternatives are summarized in a single chapter, because the results of the models with the fracture network alternatives are compared with the basic model with homogeneous rock. In addition to the required outputs in the form of dependence graphs of the variables along the monitoring lines mentioned below, we also provide graphical representations of the selected values on the coloured maps.

By comparing the pressure fields shown in Fig. 113, the effect of both fracture network alternatives on changes in the pressure fields in the models (and subsequently the direction and velocity of the water flow)

Without fractures  DFN  DFN+DTM without fractures

) is clear: evenly distributed pressure Fig. 113 in the alternative with the homogeneous rock changes only to a limited extent in the case of the DFN alternative, but for the DFN+DTM
alternative the change is much more pronounced and the distribution considerably uneven. The pressure field is most affected by the deterministic fractures that have a similar direction as the flow, whereas the fractures close to perpendicular to the flow affect the pressure field a lesser extent (e.g., the two highest placed fractures in the model).

The changes in the mechanical variables are small and the images in the colour scale are usually unable to representatively describe them; however, in the case of the \( y \)-component of the vector, differences in displacement are evident (Fig. 115). The differences are not only in size, but also in direction. The DFN alternative is almost identical to the model with homogeneous rock, whereas the DFN+DTM alternative strongly differs and is almost entirely shifted downward (in the lower part of the model the displacement is significantly lower than in the upper part, which

![Without fractures](image1)
![DFN](image2)
![DFN+DTM without fractures](image3)

with a normalized size of arrows does not capture. In the model with homogeneous rock, the \( y \)-component of the displacement vector reaches a maximum absolute value of \( 4.67 \times 10^{-4} \) m (in the \( \uparrow \) direction), in the DFN model it reaches \( 4.21 \times 10^{-4} \) m (in the \( \downarrow \) direction) and in the DTM+DFN model it reaches \( 1.93 \times 10^{-3} \) m (in the \( \downarrow \) direction). The \( x \)-component of the displacement vector is similar in all alternatives and thanks to the more pronounced specified boundary conditions (maximum \( 3 \times 10^{-2} \) m in the \( \leftarrow \) direction) the differences in the \( y \)-component do not have a major effect on the overall displacement.
Fig. 113 Pressure field (MPa) for the WP1_A model and both alternatives WP1_B

Fig. 114 Normalized flow velocity vector shown using arrows for the WP1_A model and both of the WP1_B alternatives
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Fig. 115 Displacement vector components in the y-direction for WP1_A and both WP1_B alternatives are shown by arrows and colour maps (the size of the arrows is normalized in all cases, and for illustration the x-component of the displacement vector is reduced by factor of 1000.)

Fig. 116 to Fig. 122 show selected variables depending on the position on the given monitoring line (we include the graphs for lines 1, 2, 3 and the courses along the edge of the tunnel where the start is considered in the lower left corner of the tunnel and the edge is monitored in a clockwise direction, x-coordinates in the graphs marked “Tunnel” mean: 0 – 3.6 m: the left vertical wall of the tunnel, 3.6 – 8.9 m: the ceiling of the tunnel, 8.9 – 12.5 m: the right vertical wall, 12.5 – 16.7 m: the tunnel floor). The required outputs from the organizers are:

- Pore pressure, water flow rates in the direction of the x- and y-axis, and the xx and yy stress and deformation tensor components along the monitoring lines 1, 2 and 3,
- Pore pressure, water flow rates in the direction of the x- and y-axis, and the xx and yy stress and deformation tensor components along the entire edge of the tunnel,
- Pore pressure, water flow rates in the direction of the y-axis, and the yy stress and deformation tensor components along the lower layer of the edge of the tunnel (which is part of the graphs in the previous point, so the results in this report will not be shown separately).

The course of the pore pressure in Fig. 116 confirms the differences in the pressure fields described above. Along line 1 and 2, the DFN alternative is no different from the model with the homogeneous rock. Along line 3, the differences are greater and are caused by a higher number of smaller fractures intersecting this line and pointing in a direction corresponding to the direction of flow. The DFN+DTM alternative shows significant differences. Along line 3, the pressure on the extreme points of the line is significantly lower than the other alternatives due to the overall pressure distribution.
The flow velocity components plotted along the monitoring lines are shown in Fig. 117 and Fig. 118. The courses highly fluctuate for the alternatives with fractures and are discontinuous in many cases. An exception is the dependence along line 3 (immediately below the tunnel) in the DFN + DTM model, which corresponds more closely to the alternative without the fractures, and the pressure distribution on Fig. 116.

The stress tensor plotted along the monitoring lines and along the tunnel in Fig. Fig. 119 and Fig. 120 shows similar values for the xx-component and the yy-component (deviations from the model without the fractures are higher for the DFN+DTM alternative and reach a maximum of tenths of MPa). Differences in the components of the strain tensor on Fig. 121 and Fig. 122 are similar (we draw attention to the scale of the axes, which in some cases distorts the significance of the difference). The difference between the DFN+DTM alternative and the model with homogeneous rock is approximately 2-3 mm for both components of the strain tensor for line 1, for line 2 it is roughly half and for line 3 it is in the order of $10^{-4}$ m.

Fig. 116 Course of the pore pressure in relation to the position on the monitoring line for the model alternatives with homogeneous rock and rock with DFN and DFN+DTM
Fig. 117 Course of the fluid velocity in the x-direction in relation to the position on the monitoring line for the model alternatives with homogeneous rock and rock with DFN and DFN+DTM
Fig. 118 Course of the fluid velocity in the y-direction in relation to the position on the monitoring line for the model alternatives with homogeneous rock and rock with DFN and DFN+DTM
Fig. 119 Course of the xx-component of the stress tensor in relation to the position on the monitoring line for the model alternatives with homogeneous rock and rock with DFN and DFN+DTM.
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Fig. 120 Course of the yy-component of the stress tensor in relation to the position on the monitoring line for the model alternatives with homogeneous rock and rock with DFN and DFN+DTM
Fig. 121 Course of the xx-component of the strain tensor in relation to the position on the monitoring line for the model alternatives with homogeneous rock and rock with DFN and DFN+DTM
5.6 Data processing for solution in Flow123d

The plan during the solution was to use the Flow123d simulation software developed at TUL where possible. This would help verify the solution even in the case of more complicated connections between the discrete fractures and the continua, even though the solution is limited to hydraulics for the time being. For the purposes of the software, it was necessary to process the geometry using a single-purpose algorithm.

In the framework of the task of the DECOVALEX project, a list of nearly 1,000 fractures randomly distributed in the 2D area was provided. To calculate the flow in Flow123d, it was necessary to insert a fictitious line into the geometry so that each end of the fracture has a peak degree of at least two (the 2D lines formed by the fractures and fictitious lines form an uninterrupted region). The addition of these fictitious lines will not cause a change in the task description because they will be assigned the same conditions (such as hydraulic conductivity) as the rock matrix.

The procedure for the algorithm used to create a network in a msh format is as follows:

1) Upload the fracture network in the area and save the list of peaks (the peak with the end fracture) and list of fractures.

---

**Fig. 122** Course of the yy-component of the strain tensor in relation to the position on the monitoring line for the model alternatives with homogeneous rock and rock with DFN and DFN+DTM
2) Determine the intersections of the fractures, add intersections to the list of peaks. This creates a set of all peaks to which fictitious fractures are added.

3) Divide the fractures according to the calculated intersections of the peaks.

4) Determine the degrees of the peaks.

5) Join peaks with degree 1 to the nearest peak meeting the minimum angle conditions. The matrix of distances between all peaks is determined using Pythagoras theorem. At the same time, it is necessary to ensure that the angle between the inserted fracture and the already defined edge is greater, ideally to create equilateral elements in the computational mesh (at minimum angle of 40° was selected for the calculation). Angle minimization is necessary due to the creation of a geometry network of the area, because very small angles create small elements, significantly prolonging computational difficulties, and worsening the convergence of the calculation. The result is a flat graph consisting of fractures.

6) Create a list of peaks and fractures in the file.

7) Search for circles in the area. Create a list of edges (fractures) from each peak. Find all of the circles in the area by browsing the list of edges. Other edges in circles, are considered those, which form the smallest angle in a clockwise direction. These edges are removed from the list and added to the circle. The unambiguity of the solution is ensured by the flatness of the graph and the formation of the smallest angles in a clockwise direction. The resulting circles formed by the fracture numbers are added to the list of circles. The circles are then used to define contiguous 2D regions representing the rock.

8) Check each circle to see if there is a bridge on it (the same edge repeats twice within a single circle, but in the opposite direction) or articulation (the same peaks repeat several times within a single circle). Bridges or articulation cause the GMSH SW to report an error in these 2D areas while creating a mesh, and the area of the mesh is not created. If a bridge or articulation has been found, the circle is divided into two areas by adding an edge (even in a file) and then checking whether the added edge crosses another edge and whether there are no bridges or articulations on the circles.

9) Determine the direction of the edge orientation for each circle. In the case of reversed orientation, replace the fracture with a negative sign.

10) Create a list of circles in the area geometry file.

The computational mesh of the area was created using GMSH SW.

5.7 Work package 2.1: 3D model with the tunnel and fractures

Work package 2.1 was solved in 3D geometry with a tunnel and some of the most important fractures in the surroundings of the tunnel. Preparation of the geometry required considerable effort, and some operations had to be performed outside the COMSOL environment. The data were entered in a *.stl format and modified using the Meshmixer tool (simplification of input data describing the inner surface of the tunnel) and GMSH (calculation of intersections of individual fractures, which can also be done in COMSOL but for the entered data the operation did not work properly and returned an empty set as a result).
The geometry contains a rock block with horizontal dimensions of 40×40 m and a height of 15 m with an inserted tunnel, which is represented by a cavity inside the block. In the initial phase, geometry with a regular-shaped tunnel was created, and the version with an irregular tunnel surface was also tested, a close-up of the tunnels for both versions is shown in Fig. 124. The fractures located in the space surrounding the test wells below the invert of the tunnel (Fig. 123 – extended into the free space of the tunnel for illustration) are represented by the 2D planes with the orientation shown in Tab. 13. In COMSOL, the predefined “Fracture Flow” tool was used to calculate the flow through the fractures – as in the case of the 2D problem (Task 1.3.3, chapter 5.4), i.e. the set of comparative 2D studies with schematized geometry. Unfortunately, the tool only works for hydraulics, while the mechanical changes (e.g., changes in the opening) due to flow are not considered for the fractures.

At the geometry level, boreholes were added during the phase of task 2.1. The injection boreholes (K04017G02, K04018G01, K04020G01) are represented by cuboid-shaped cavities (height and location corresponding to the depth range of the borehole section where the injection was performed, see Backers et al., 2017b). Observation wells are represented by lines because they only serve to display the results. For a more detailed description of the injection tests, see Chapter 5.8.

For the initial calculations in Task 2.1, the data specified in the task description that matches the parameters for the 2D models (Tab. 10) were used. The material parameters of the fractures are also based on the task description of the 2D problem (only their hydraulic conductivity was recalculated by a cubic law according to the opening of the fractures described in Tab. 13).

**Tab. 13 Fractures defined in the 3D model**

<table>
<thead>
<tr>
<th>Fracture</th>
<th>Fracture No.</th>
<th>Strike (°)</th>
<th>Dip (°)</th>
<th>Opening (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>K04023G03</td>
<td>99</td>
<td>135</td>
<td>66</td>
<td>0.5</td>
</tr>
<tr>
<td>K04023G03</td>
<td>94</td>
<td>315</td>
<td>50</td>
<td>-0.1</td>
</tr>
<tr>
<td>K04021G02</td>
<td>137</td>
<td>300</td>
<td>70</td>
<td>0-0.5</td>
</tr>
<tr>
<td>K04019G02</td>
<td>144-c</td>
<td>120</td>
<td>55</td>
<td>0-0.2</td>
</tr>
<tr>
<td>K04017G01</td>
<td>143</td>
<td>120</td>
<td>10</td>
<td>0.3</td>
</tr>
<tr>
<td>K04017G02</td>
<td>150</td>
<td>170</td>
<td>40</td>
<td>0.2</td>
</tr>
</tbody>
</table>
Fig. 123 Detail of the applied fractures that intersect the tunnel invert (Backers et al, 2017b).

Fig. 124 Detail of the updated alternatives of the computational meshes for models with regularly and irregularly shaped tunnels

The following hydraulic and mechanical boundary conditions were applied in the models (their definition is again based on Backers et al. (2017b)), whereby injection boreholes were not considered in the geometry during this phase:

Hydraulic boundary conditions:
- Outer boundary of the model: pressure 5 MPa,
- Inner boundary of the model: pressure 0 MPa.

Mechanical boundary conditions:
- Upper outer boundary of the model: vertical stress: 12 MPa,
- Right outer boundary of the model: horizontal stress: 12 MPa,
- Front outer boundary of the model: horizontal stress: 24 MPa,
- Left, lower and back outer boundaries of the tunnel: zero normal displacement,
- Inner boundaries of the tunnel: stress: 0 MPa.

A steady-state problem (regular tunnel shape) was solved first, where the pressure distribution was obtained in the model, which served as the initial condition for the time-dependent injection tests in Chapter 5.8. The behaviour of the steady-state model is based on assumptions and experience gained from the 2D geometry models. Fig. 125 and Fig. 126 show the pressure distribution and the vertical component of the stress tensor in a longitudinal section and in a section perpendicular to the axis of the tunnel. The pressure field is visibly affected by the fractures; on the contrary, when comparing the results with the irregular tunnel surface model in Fig. 127, significant differences are not apparent. For a more detailed description of
differences in the use of a differently defined tunnel surfaces, see Chapter 5.8.1. From the simulations, it is also possible to determine the total value of the inflow to the tunnel, which is $5.2959 \times 10^{-6}$ m$^3$·s$^{-1}$, when converted to a unit of the tunnel surface (the total surface area of the tunnel is 625.4 m$^2$) its value is $8.4680 \times 10^{-9}$ m·s$^{-1}$.

Fig. 125 Pressure distribution in the section through the tunnel axis and in the direction perpendicular to the tunnel axis near the fractures
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Fig. 126 Distribution of the vertical component of the stress tensor in the section through the tunnel axis and in the direction perpendicular to the tunnel axis near the fractures

Fig. 127 Pressure distribution in a longitudinal and cross section for the model with an irregular tunnel surface
5.8 Work package 2.2: 3D model with a tunnel and fractures with updated input data

Task 2.1 closely follows on from the previous simulations in Task 2.1, starting from the same concept. The first pilot injection tests were performed on the geometry described in Chapter 5.7. These are time-dependent simulations, where water is injected under a defined pressure into one of the three selected boreholes for 20 minutes. The initial distribution of variables was obtained from a steady-state problem and discontinuous simulations are defined as follows:

1) Injection borehole: K04017G02 (depth range 0.4 – 0.6 m, injection pressure: 442 kPa), observation boreholes: K04016G01, K04017G01, K04017G03, K04018G01,
2) Injection borehole: K04018G01 (depth range 0.1 – 0.2 m, injected pressure 92 kPa), observation boreholes: K04017G01, K04017G02,
3) Injection borehole: K04020G01 (depth range 0.2 – 0.4 m, injection pressure: 80 kPa), observation boreholes: K04019G03, K04021G02.

The boundary conditions used in the simulations are based on Chapter 5.7, in addition to the corresponding injected water pressure on the inner surface of the injection borehole and the zero pressure on the surface of the remaining two injection boreholes. Each injection test was designed as a separate model with and without fractures. The responses to the injection tests are summarized in Tab. 14, from which two conclusions are apparent at first sight: The results of the injection tests are not greatly influenced by the presence of fractures (the injection response to borehole K04017G02 differs, but only in the order of tenths to single units of kPa). Furthermore, it is clear from the table that the evaluated injection response to boreholes K04018G01 and K04020G01 is minimal and is in the order of tenths of kPa (for both alternatives with and without fractures). Fig. 128 shows the distribution of the individual injection boreholes together with the positions of the observation boreholes and the nearby fractures (e.g. K04020G01 does not intersect any of the fractures, which can mean a low influence of pressure on the respective observation boreholes. On the contrary, boreholes K04017G02 and K04018G01 are crossed by one common fracture, so we can expect a greater influence).
Several changes were made to the model based on these results and the newly provided data for work package 2.2 (Backers et al., 2018). Changes were made at a geometry level – firstly, the overall dimensions of the model were increased to 60×60×50 m. Two new sub-horizontal fractures leading below the bottom of the tunnel (located based on the data supplied) and a simple EDZ surrounding the tunnel were added. These two additions were made to ensure better connectivity between the existing fractures and to improve the responses to the injection tests in the observation boreholes (analysed in chapter 5). In addition, a new functional version of the geometry with fractures and an irregularly shaped tunnel (with the inner surface described in detail) was created, but for the calculations and based on the results of the comparison from chapter 5.8.1, it was more beneficial to use geometry with a regular tunnel shape, due to demands on the discretization of the model domain and the related computational complexities.
5.8.1 Comparison of the model with regular and irregular geometry

A comparison of the effect of the tunnel surface shape on the simulation results was also made using the newly prepared geometries (Fig. 124). The geometry of a tunnel with an irregular surface uses approximately 3,000 points to describe it, and the computational mesh includes approximately 158,000 four-sided elements (a regular-shaped tunnel with approximately 160,000 elements). Comparisons were made between the steady-state simulations and injection tests. In the case of the steady-state simulations, an IGN with an irregular tunnel shape (with a more detailed description of the tunnel surface with 215,000 elements), which does not include wells, was made available. Comparisons were also made between several variables plotted along predefined lines (two horizontal lines and one vertical line in a section along the tunnel axis and an analogically defined line in a section perpendicular to the tunnel axis, at approximately half its length).

When comparing the pore pressure along the longitudinal and transverse sections (Fig. 130 and Fig. 131 on the left), the differences are only minimal and are caused by a differently defined tunnel position in the geometry between TUL and IGN, which displaces the results plotted along the lines. The differences in the vertical component of the stress tensor (Fig. 130 and Fig. 131 on the right) are more evident, more is reflected in the local oscillations of the courses due to the differently defined surfaces, but there is also a displacement caused by the different tunnel positions.

When comparing the courses of the geometry with the same tunnel positions but with different surfaces (both TUL geometries) in Fig. 132, the differences are more obvious (especially for the two courses along the horizontal lines immediately above the tunnel ceiling where the unevenness results in a slightly more pronounced difference - the maximum difference is approximately 0.1 mm).

Comparisons were also made in the case of the discontinuous problems – injection tests on the TUL geometries with the material parameters set based on chapter 5.7. The results of the comparison of responses to the injected pressure in the observation wells are shown in Tab. 15, where comparable values for both model alternatives are observed, with differences in most cases being up to 10%. In the case of injection into borehole K04017G02 there was a higher response in observation well K04017G01 (with a difference of 17.6 %), which based on Fig. 128 is located in the immediate vicinity of the injection borehole and is intersected by the same fracture.

Because the effect of irregularities is concerned, it is not possible to analyze exact physical reasons for individual minor changes. The practical conclusion for further calculations is that
by simplifying the shape of the surface there is no significant error beyond the other uncertainties in the data.

Fig. 130 Comparison of the effect of tunnel geometry on the pressure and the vertical component of the stress tensor plotted on the lines in the traverse section through the tunnel

Fig. 131 Comparison of the effect of tunnel geometry on the pressure and the vertical component of the stress tensor plotted on the lines in the longitudinal section through the tunnel
Fig. 132 Comparison of the effect of the tunnel geometry on the vertical component of the displacement vector plotted on the lines in the longitudinal and transverse sections of the tunnel

Tab. 15 Results of a comparison of the injection tests for regular and irregular tunnel geometry

<table>
<thead>
<tr>
<th>Injection borehole</th>
<th>Injection pressure (kPa)</th>
<th>Observation borehole</th>
<th>Measured response (kPa)</th>
<th>Regular tunnel</th>
<th>Irregular tunnel</th>
<th>Difference (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>K04017G02</td>
<td>442</td>
<td>K04016G01</td>
<td>1.4</td>
<td>3.91</td>
<td>4.29</td>
<td>9.00</td>
</tr>
<tr>
<td></td>
<td></td>
<td>K04017G01</td>
<td>0.3</td>
<td>6.95</td>
<td>8.44</td>
<td>17.62</td>
</tr>
<tr>
<td></td>
<td></td>
<td>K04017G03</td>
<td>3</td>
<td>3.51</td>
<td>3.77</td>
<td>6.69</td>
</tr>
<tr>
<td></td>
<td></td>
<td>K04018G01</td>
<td>0.4</td>
<td>3.78</td>
<td>4.17</td>
<td>9.38</td>
</tr>
<tr>
<td>K04018G01</td>
<td>92</td>
<td>K04017G01</td>
<td>88</td>
<td>0.13</td>
<td>0.11</td>
<td>-9.49</td>
</tr>
<tr>
<td></td>
<td></td>
<td>K04017G02</td>
<td>4</td>
<td>0.14</td>
<td>0.14</td>
<td>3.24</td>
</tr>
<tr>
<td>K04020G01</td>
<td>80</td>
<td>K04019G03</td>
<td>4</td>
<td>0.17</td>
<td>0.17</td>
<td>-1.69</td>
</tr>
<tr>
<td></td>
<td></td>
<td>K04021G02</td>
<td>21</td>
<td>0.13</td>
<td>0.15</td>
<td>10.62</td>
</tr>
</tbody>
</table>
5.8.2 Sensitivity study

With the newly defined geometry, models with different hydraulic conductivity of fractures were solved in the form of a simple sensitivity study. The material parameters of the rock and fractures correspond to Tab. 10, except for the hydraulic conductivity of the rock, which on the basis of the test model was reduced to $5 \cdot 10^{-12}$ m·s$^{-1}$. EDZ is not considered in the basic alternative “0” and all of the used hydraulic conductivity values of the fractures are listed in the corresponding column labelled “0” in Tab. 16. Each additional column indicates an alternative model where one parameter was changed. Simplified numerical designation refers to fractures whose hydraulic conductivity has been modified ($10^\times$ increase in all cases, except for fracture K04021G01 where the was a $100^\times$ increase). In all of the alternatives except “0” there is an EDZ around the tunnel. Alternatives “hor1” and “hor2” refer to models with altered parameters of sub-horizontal fractures, in the alternative “rock” the hydraulic conductivity of the rock was modified, and in the alternative “EDZ2” the hydraulic conductivity of the EDZ was modified.

The results of the sensitivity study in relation to the described model alternatives are summarized in Tab. 17. All three injection tests for each alternative, together with the responses in the observation boreholes and the measured values, are also included in this figure. When comparing the results with the basic alternative, or with the measured data, we can come to several conclusions:

- The response to the injection to borehole K04017G02 changed only when the permeability of the EDZ was changed (but at the same time the results were not affected by injection into boreholes K04018G01 and K04020G01);
- A $10^\times$ increase in the hydraulic conductivity of fractures K04017G02 and K04023G01 was not reflected in the pressure in any of the observation boreholes,
- The additional sub-horizontal fractures positively affected the observed results - response to injection to boreholes K04018G01 and K04020G01 may be affected by changes in the parameters of the fractures, which were not possible in the test alternative without the sub-horizontal fractures,
- The test models fail to capture a different response within the individual observation boreholes – the values correlate after injection into a single borehole (e.g. this is evident for injection into borehole K04018G01, which caused different responses for the different alternatives in boreholes K04017G01 and K04017G02 but the response values always mutually correlated).
### Tab. 16 Hydraulic conductivity (m·s⁻¹) for alternatives of the sensitivity study model (the basic alternative is marked “0”, the hydraulic conductivity of the fracture is increased by 10× in each additional column). The hydraulic conductivity of fracture K04021G01 is increased 100×, the basic alternative does not consider the EDZ, the EDZ is included in the others, hor1 and hor2 denote sub-horizontal fractures – the numbers with a background indicate changes.

<table>
<thead>
<tr>
<th>Fracture/ model subdomain</th>
<th>Notation of alternatives</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0</td>
</tr>
<tr>
<td>1701</td>
<td>7.4E-02</td>
</tr>
<tr>
<td>1702</td>
<td>3.3E-02</td>
</tr>
<tr>
<td>1902</td>
<td>8.2E-03</td>
</tr>
<tr>
<td>2101</td>
<td>5.1E-02</td>
</tr>
<tr>
<td>2301</td>
<td>2.0E-01</td>
</tr>
<tr>
<td>hor1</td>
<td>2.0E-01</td>
</tr>
<tr>
<td>hor2</td>
<td>2.0E-01</td>
</tr>
<tr>
<td>k_rock</td>
<td>5.0E-12</td>
</tr>
<tr>
<td>k_edz</td>
<td>bez EDZ</td>
</tr>
</tbody>
</table>

### Tab. 17 Results of the sensitivity study – values of response to the injected pressure (for varied hydraulic conductivity values of individual fractures based on Tab. 16), grey numbers were without effect, red backgrounds indicate changes.

| Injection borehole | Injecti on pressure (kPa) | Observatio n borehole | Measur ed respons e (kPa) | 0 | EDZ | 1701 | 1702 | 1902 | 2101 | 2301 | hor1 | hor2 | rock | EDZ2 |
|--------------------|---------------------------|-----------------------|---------------------------|---|-----|------|------|------|------|------|------|------|------|------|------|
| K04017G02          | 442                       | K04016G01             | 1.4                       | 0.21 | 1.35 | 1.35 | 1.35 | 1.35 | 1.35 | 1.35 | 1.35 | 1.35 | 5.26 |
|                    |                           | K04017G01             | 0.3                       | 0.34 | 3.48 | 3.48 | 3.48 | 3.48 | 3.48 | 3.48 | 3.48 | 3.48 | 8.38 |
|                    |                           | K04017G03             | 3                         | 0.20 | 1.25 | 1.25 | 1.25 | 1.25 | 1.25 | 1.25 | 1.25 | 1.25 | 3.33 |
|                    |                           | K04018G01             | 0.4                       | 0.25 | 1.38 | 1.38 | 1.38 | 1.38 | 1.38 | 1.38 | 1.38 | 3.98 |
| K04018G01          | 92                        | K04017G01             | 88                        | 65.70 | 65.70 | 30.58 | 65.70 | 55.65 | 56.12 | 65.70 | 87.67 | 64.13 | 65.70 | 65.69 |
|                    |                           | K04017G02             | 4                         | 67.59 | 67.59 | 39.90 | 67.59 | 55.54 | 57.35 | 67.59 | 87.91 | 65.91 | 67.59 | 67.59 |
| K04020G01          | 80                        | K04019G03             | 4                         | 55.34 | 55.33 | 55.09 | 55.33 | 39.93 | 25.16 | 55.33 | 51.60 | 76.29 | 55.33 | 55.33 |
|                    |                           | K04021G02             | 21                        | 54.14 | 54.14 | 54.03 | 54.14 | 46.89 | 15.87 | 54.14 | 52.40 | 76.23 | 54.14 | 54.14 |
A similar study was carried out for cases where the material parameters were retained for the basic alternative “EDZ”, but one fracture was always a neglected (closed). These models provided the injection responses given in Tab. 18, from which we can draw the following conclusions:

- According to estimates and previous results, the addition of the sub-horizontal fractures improved the response to injection into boreholes K04018G01 and K04020G01 (when they are neglected in alternatives “hor1” and “hor2” there is an almost complete loss of a response)

- In the other cases, closing the fractures led to only minor changes in the response to injection (and, as in the previous cases, these responses correlated in the observation wells).

Three alternatives of the final models that best affect the behaviour of the injection tests (Tab. 19) were defined based on both sensitivity studies. In alternative “var1”, the hydraulic conductivity of the fracture K04021G01 changed to 0.031 m·s⁻¹ and the hydraulic conductivity of the sub-horizontal fracture No.1 to 10 m·s⁻¹. Alternative “var2” followed on from “var1”, but hydraulic conductivity of the EDZ was reduced by half and “var3” also followed on from “var1” but the hydraulic conductivity of the rock and the EDZ zone was increased by 10. However, the results for these alternatives did not provide sufficient agreement in all the observed responses and the pressure values corresponded to the given alternatives only in three of the eight observed pressures (Tab. 20, cells marked in green). The other responses failed to capture the changes in the considered parameters.

**Tab. 18 Results of the sensitivity study – values of the response to the injection (when individual fractures are neglected)**

<table>
<thead>
<tr>
<th>Injection borehole</th>
<th>Injection pressure (kPa)</th>
<th>Observation borehole</th>
<th>Measured response (kPa)</th>
<th>EDZ</th>
<th>Closed fracture</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0</td>
<td>1701 1702 1902 2101 2301 hor1 hor2</td>
</tr>
<tr>
<td>K04017G02</td>
<td>442</td>
<td>K04016G01</td>
<td>1.4</td>
<td>0.21</td>
<td>1.35 1.31 1.31 1.31 1.31 1.52 1.31</td>
</tr>
<tr>
<td></td>
<td></td>
<td>K04017G01</td>
<td>0.3</td>
<td>0.34</td>
<td>3.48 3.49 3.45 3.45 3.45 3.45 3.72 3.45</td>
</tr>
<tr>
<td></td>
<td></td>
<td>K04017G03</td>
<td>3</td>
<td>0.20</td>
<td>1.25 1.24 1.34 1.24 1.24 1.24 1.61 1.24</td>
</tr>
<tr>
<td></td>
<td></td>
<td>K04018G01</td>
<td>0.4</td>
<td>0.25</td>
<td>1.38 1.41 1.43 1.41 1.41 1.41 1.62 1.43</td>
</tr>
<tr>
<td>K04018G01</td>
<td>92</td>
<td>K04017G01</td>
<td>88</td>
<td>65.70</td>
<td>65.70 65.67 65.16 76.21 65.67 0.01 69.12</td>
</tr>
<tr>
<td></td>
<td></td>
<td>K04017G02</td>
<td>4</td>
<td>67.59</td>
<td>67.59 67.57 68.16 78.57 67.57 0.01 71.28</td>
</tr>
<tr>
<td>K04020G01</td>
<td>80</td>
<td>K04019G03</td>
<td>4</td>
<td>55.34</td>
<td>55.33 55.34 55.28 55.85 77.72 55.28 60.29 0.05</td>
</tr>
<tr>
<td></td>
<td></td>
<td>K04021G02</td>
<td>21</td>
<td>54.14</td>
<td>54.14 53.91 53.88 54.14 78.78 53.88 56.18 0.09</td>
</tr>
</tbody>
</table>
Tab. 19 Resulting three alternatives where the best agreement with the measured data was found (orange values changes in hydraulic conductivity of the fractures, blue are rocks and EDZ)

<table>
<thead>
<tr>
<th>Model area</th>
<th>Hydraulic conductivity (m·s$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>var_1</td>
</tr>
<tr>
<td>1701</td>
<td>7.4E-02</td>
</tr>
<tr>
<td>1702</td>
<td>3.3E-02</td>
</tr>
<tr>
<td>1902</td>
<td>8.2E-03</td>
</tr>
<tr>
<td>2101</td>
<td>3.1E-01</td>
</tr>
<tr>
<td>2301</td>
<td>2.0E-01</td>
</tr>
<tr>
<td>hor1</td>
<td>1.0E+01</td>
</tr>
<tr>
<td>hor2</td>
<td>2.0E-01</td>
</tr>
<tr>
<td>k_rock</td>
<td>5.0E-12</td>
</tr>
<tr>
<td>k_edz</td>
<td>5.0E-11</td>
</tr>
</tbody>
</table>

Tab. 20 The resulting responses for the three selected model alternatives based on Tab. 19, green values are in agreement with the measurements.

<table>
<thead>
<tr>
<th>Injection borehole</th>
<th>Inject. Pressure (kPa)</th>
<th>Observation borehole</th>
<th>Measured response (kPa)</th>
<th>var_1</th>
<th>var_2</th>
<th>var_3</th>
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5.9 Summary and discussion of the results

This chapter describes the results of the 2D and 3D simulations, in relation to understanding the changes in the permeability of the rock after creating EDZ, which was solved in “WP 1.3.3”, “WP 2.1” and “WP 2.2” of Task G.

Task 1.3.3 includes a basic model with homogeneous rock (WP1_A) and a simulation with specified versions of the fracture network (stochastic discrete fracture network and combinations of the stochastic fracture network with larger deterministic fractures - WP1_B).

The simulations were solved as unidirectional coupled steady-state problems where the stress and deformation field are affected by a steady flow of water. The simulations show a more pronounced influence of deterministic fractures on the pressure field, the flow velocity, and hence the changes in stress and deformation. Whereby, the pressure field and the flow velocity are affected by the fractures quite significantly. Changes in mechanical quantities (along the monitoring lines, compared to the model with the homogeneous rock matrix) are in the order of tenths of MPa for stress and at most in the order of mm for deformations. The procedure for creating the computational mesh for Flow123d is also described. This constitutes preparatory work for future calculations within this task.

In work packages 2.1 and 2.2, the task was to create a 3D model of the tunnel with fractures under the real conditions found at the Åspö underground laboratory (based on the data provided in the form of the positions of the individual large-scale fractures and stochastic fracture networks as well as data describing the uneven inner surface of the tunnel). The related task was to use the simulation to capture a set of injection tests and real conditions in the rock. Due to considerable delays in the provision of the task description and the data, it was not possible to use all of the data provided, so only the large-scale fractures and, in some cases, irregular tunnel surfaces were used in the models.

The effect of the shape of the surface of the tunnel (both regular geometry and geometry with an irregular tunnel) was compared in both the steady-state and the time-dependent simulations. In the steady-state problems, the course of several variables was plotted along lines in the longitudinal and transverse sections and the results did not show any significant differences (only local effects). The effect of tunnel shape was also verified during the injection tests, where the response was monitored in several observation boreholes. Here, the response changes varied to a maximum of 10% (with one exception where the difference was 17.6%).

On the basis of these comparisons, the geometry with a regular-shaped tunnel was selected to solve the injection tests and was subjected to simple sensitivity studies. The hydraulic conductivity of individual fractures, rocks and EDZ was first altered, and the individual fractures were also neglected in the next phase. The results of these studies showed, in particular, the correlation of the responses in the different boreholes during the injection into the borehole – this geometry is not likely to correctly capture the complete response to all injection tests. For example, it was not possible to modify the response by simply changing the parameters of the EDZ (again correlating to the individual responses) during injection into borehole K04017G02.

Nevertheless, three alternatives were selected where at least partial agreement was reached (corresponding to three out of eight injection responses). In order to improve the results, it would be necessary to review the currently used fractures and consider adding or neglecting them based on the data provided, or include the anisotropy into the model. Such adjustments exceeded the project participation period described in this report.
6 Conclusion – use of the findings from DECOVALEX-2019 for the safety assessment of the DGR

The participation of the Czech team in the international project DECOVALEX has shown that it is fully comparable to other teams in terms of its professional level and computer equipment. The investigators achieved similar results to the other participants, and in many cases using original methods better capturing the control processes. Minor differences in the results were discussed and explained at joint workshops. These differences were appropriate to differences in the models and uncertainties in the data. The investigators actively contributed to improvements of the provided data interpretation in their Task groups.

During the course of the project and discussion of the results, experience with the creation of models and interpretation of the results was gained, which can be subsequently used during the preparation of DGR in the Czech Republic. In addition to the international experience, the benefits of obtaining experimental data of very costly and long-term projects, the equivalent of which will undoubtedly be dealt with by the Bukov underground laboratory, should also be emphasized. Experience gained in the data structuring and their collection can be used in the planning of experiments in the Czech Republic.

For example, Task C involved the unique application of a multidimensional model, which at this scale and with the selected deterministic fractures has not yet been experienced, but compromises had to be made in the pre-processing. TUL’s suggestions for possible reasons for differences in chloride concentrations led to the Task Leader supplementing the task specification in the task description. The geochemical analysis of J. Zeman (TUL’s external consultant) brought a new viewpoint to the spatial and temporal distribution of groundwater composition in the surroundings of the laboratory, as a mixture of two water types (analysed samples) at various ratios. During the Task D solution, a model was developed that systematically represents the saturation of bentonite outside a classical pore space. By this approach, the developed model, as the only one in Task D, predicts changes in dry density. The IGN research team was the only team in the framework of Task D to use a 3D model of the entire EB experiment. It also led a discussion on the uncertainties of different aspects of the model, which was highly appreciated by the Task Leader.

In addition, the preparation and creation of the models inspired the investigators in the context of further development of the Flow123d software, both in the development of new functionalities, and in the pre-processing of data and their interpretation and evaluation. We can also mention the experience gained with the implementation of complex hydromechanical processes in the COMSOL Multiphysics environment. Participation in international projects of this nature can rapidly increase the experience of teams involved in the preparation of the DGR project.

In order to correctly understand the context of the conclusions below and the recommendations for the use of knowledge for safety assessment of the DGR, it is necessary to explain their relativity. The acquired knowledge cannot always be explicitly transformed and applied to the safety assessment performed by the project investigators. This is mainly due to the fact that the tasks (whose investigators did not have a direct influence upon) are not constructed and there is no room for the calculation of e.g. “superstructure” tasks representing the state/conditions that are the subject of safety assessment. Some of the suggestions for use of the findings are therefore formulated more generally, and in some cases, they are not only
taken from the solution of the DECOVALEX Tasks. It should also be noted that, in terms of the Tasks in DECOVALEX-2019, the conclusions are only partial, given that their solution will continue until the end of 2019.

The uses also need to be understood in such a way that specific numerical values of parameters for safety models cannot be given now, but conditionally in the future in the context of further experimental research. In order to specify the planning and evaluation of the experiments, it is possible to draw on the results and procedures of the DECOVALEX project in the context of known conditions (locations, materials). The tasks and models can be considered as “templates” for application in the safety assessment with the specific parameters of the planned repository – for systems of physical phenomena that have been verified in the project to be able to predict behaviour under the given initial conditions.

**Finding 1.** The DECOVALEX project and its Tasks are based on (field and laboratory) experimental data obtained through, often long-term, monitoring. Input data and the results of the modelling are subject to uncertainties, which are being further reduced through concurrent solutions.

Usage: Such experiments were not carried out in the SÚRAO research program. In the project “Research support for the safety assessment of the deep repository”, some were in the final stages of planning, and are expected to be implemented in the near future. The finding counts on the need for concurrent monitoring and modelling calculations with continuous calibration. Changing the calibrated parameters from different stages of the monitoring indicates uncertainty in their determination or an erroneous conceptual model. At the same time, according to the model data, it is possible to determine the scope of the monitoring during its planning, but also to obtain feedback on the benefits of the measured data. Without this, doubts about the correct quantification of uncertainties cannot be ruled out in the future.

**Finding 2.** The approach of more than one team to the tasks of modelling hydrogeological processes and transport of RN also indicates the main strengths/weaknesses of the SW, in addition to the influence of the conceptual approach used, which may subsequently lead to their modifications or modifications to the input data of the models so that the results of the various approaches to the same task get closer to each other.

Usage: Even though the simulation software is currently at a very high level, the conditions and phenomena studied in the context of the construction, operation and safety of the DGR, and in the context of large field experiments, often deviate from the routine use, and this should be taken into account when planning the modelling calculations. The model implementation of an experiment does not only mean the interpretation of a specific case study, but also the extension, refinement, or greater effectiveness of future calculations, e.g. for conditions of safety calculations (i.e. with similar processes but with different parameters).

**Finding 3.** Task C solved/solves the dynamic problem of drainage and flooding of galleries, and the related geomechanical and geochemical changes. The results of the experiment show that the state after closure of the repository will not reflect the original state. This result does not arise from simple hydraulic considerations. A more accurate model may be able to predict the resulting state, but with the inclusion of detailed data over a certain monitoring period.

Usage: The results and experience of this Task will help determine the initial conditions of the DGR post-closure for its subsequent long-term development. Errors and inaccuracies in determining the initial conditions of DGR will lead to changes in its development in terms of hydraulic conditions and transport, which will directly influence the input data for the safety
assessment model in the long-term. For a sufficiently accurate prediction of these conditions, it is necessary to have detailed spatial data, especially on rock permeability; on the contrary, in the event they are not available, it is necessary to consider greater uncertainties in the estimation of water movement and chemistry after closure of the repository.

**Finding 4.** Task D solved/solves the coupled problem of saturation of the bentonite sealing layer around the container in the storage system in a horizontal concept. The sealing barrier is made of bentonite blocks and pellets, and is therefore heterogeneous. The model of the EB experiment explained most of the observed phenomena based on generally valid hydro-mechanical equations and constitutional relationships, even under complicated 3D conditions. Although the results of this Task primarily determined the hydro-mechanical conditions and changes in the initial stage – up to full saturation of the seal, these changes directly affect not only the behaviour of the adjacent EDZ but also the pressure on the container and the lifespan of the container against corrosion.

Usage: The prediction of the state of the bentonite after the period of saturation and homogenization allows for more accurate determination of the insulation properties of the bentonite at the time when it fulfils the function of a barrier, i.e. distribution of dry density, saturation and swelling pressure, with consequences on the migration parameters of radionuclides. The form of the model created for the Task facilitates the inclusion of the critical elements considered so far (technological gaps, artificial elements). The properties of the bentonite layer and their changes over time will also influence the process of corrosion of the container and thus also the leakage of radionuclides from the area of the DGR, and will also significantly affect the safety assessment. It will also be necessary to study the degradation of the bentonite liners due to thermal and pH effects, which will lead to the loss of the elastic properties of the liners and thus speed up the breakage of the container due to changes in geomechanical stresses in the rock environment. This should also be studied in the future, including experimental verification, as the bentonite properties will directly affect the lifespan of the container and hence the model of the DGR safety assessment in a long-term perspective.

**Finding 5.** Task G solved/solves the hydraulic and hydro-mechanical phenomena in relation to the packer permeability tests in the area of the EDZ in close proximity to the wall of the tunnel. The values, otherwise commonly interpreted by a simple formula for an “infinite” environment, are evaluated in the model in the context of the surrounding boreholes and the tunnel, which does not always lead to unambiguous results and confirms the uncertainty of determining the transmissivity of the fractures (it is not a homogeneous area, affecting communication with other fractures).

Usage: The procedure used in the Task shows how to obtain EDZ parameters more accurately, especially permeability, with the effect to the radionuclide migration in close proximity of the storage area.

**Finding 6.** It is necessary to prepare complex models for the transport of RN and base the safety assessment on them. A complex transport model will determine the influence of geophysical and geochemical conditions on the speed and amount of the RN transfer at the geo-biosphere interface without the need to speculatively determine the significance of the individual effects on the transport.
Further intermediate results, experience and findings gained through the involvement of the Czech team in the DECOVALEX-2019 project are presented in the introductions and conclusions of the chapters of each Task. Hence, for Task C, these findings are dealt with in Chapter 2.7 in close connection with the results achieved in this Task. For Task D, these findings are described in Chapter 4.3 and finally for Task G they are described in Chapter 0. These conclusions are formulated with a view to their possible use in the future safety assessment of the DGR, as explained in the introductory paragraph.
7 List of literature


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