THE DECOVALEX III PROJECT:
A SUMMARY OF ACTIVITIES AND LESSONS LEARNED

Chin-Fu Tsang\textsuperscript{1}, Lanru Jing\textsuperscript{2}, Ove Stephansson\textsuperscript{3}, and Fritz Kautsky\textsuperscript{4}

\textsuperscript{1}Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA
\textsuperscript{2}Royal Institute of Technology, SE-10044 Stockholm, Sweden
\textsuperscript{3}GeoForschungsZentrum, Telegrafenberg, D-14473 Potsdam, Germany
\textsuperscript{4}Swedish Nuclear Power Inspectorate, SE-10658 Stockholm, Sweden

ABSTRACT: Initiated in 1992, the DECOVALEX project is an international collaboration for advancing the understanding and modeling of coupled thermo-hydro-mechanical (THM) processes in geologic systems. The project has made important scientific achievements through three stages and is progressing in its fourth stage. It has played a key role in the development of mathematical modeling and \textit{in situ} testing of coupled THM processes in fractured rock and buffer/backfill materials, a subject of importance for performance assessment of radioactive waste geologic repositories. This paper summarizes studies under the most recent stage of the project, DECOVALEX III (2000–2003). These studies include those of two major field experiments: (a) the FEBEX experiment at Grimsel, Switzerland, investigating coupled THM processes in a crystalline rock-bentonite system, and (b) the Drift Scale Test (DST) experiment at Yucca Mountain, Nevada, investigating coupled THM processes in unsaturated tuff. These are two of the largest multiyear heater tests undertaken to date for the study of coupled THM processes in geological systems. In addition, three so-called benchmark tests are also studied to evaluate the impact of coupled THM processes under different scenarios and geometries. Within the DECOVALEX project, multiple research teams participated in each of the studies, using different approaches and computer codes. Comparisons of results have provided insight into coupled THM processes, which in turn has stimulated further development of our modeling capabilities. Lessons learned from these studies are discussed. The scientific advances and enhanced insight gained through this kind of international cooperation illustrate the effectiveness of the DECOVALEX project.
1. Introduction

An international cooperative project entitled DECOVALEX (an acronym for DEvelopment of COupled THM models and their VALidation against EXperiments) was established in 1992 by national regulatory authorities and waste management organizations involved in nuclear waste disposal, to cooperate in developing and testing models capable of simulating coupled THM processes. Under this project, the participating organizations (Table 1) would share results from major field and laboratory experiments, results that would enhance understanding of coupled THM processes and provide data for model validations. Over the last 12 years, more than 15 research teams from nine countries (Table 1) have participated in this joint effort. The project objectives are:

- To support development of computer simulators for THM processes in geological systems
- To investigate and implement suitable algorithms for THM modeling
- To compare model calculations with results from field and laboratory experiments
- To design new experiments to support code and model development
- To study the application of THM modeling to performance and safety assessment of nuclear waste repositories

Table 1. Project funding organizations and research teams

<table>
<thead>
<tr>
<th>Funding Organizations</th>
<th>Acronym</th>
<th>Research teams (Acronyms)</th>
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</thead>
<tbody>
<tr>
<td>National Agency for Radioactive Waste Management, France</td>
<td>ANDRA</td>
<td>INERIS-LAEGO, Ecole des Mines de Nancy (EMN), France; Ecole Polytechnique (EP), G3S, France</td>
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<tr>
<td>Federal Institute for Geosciences and Natural Resources, Germany</td>
<td>BGR</td>
<td>University of Tuebingen, Germany; University of Hannover, Germany; Federal Institute for Geosciences and Natural Resources, Germany</td>
</tr>
<tr>
<td>Commisariat a l’Energi Atomique de Cadarache, France</td>
<td>CEA</td>
<td>CEA/DM25/SEMT, France</td>
</tr>
<tr>
<td>Canadian Nuclear Safety Commission, Canada</td>
<td>CNSC</td>
<td>Canadian Nuclear Safety Commission, Canada</td>
</tr>
<tr>
<td>Department of Energy, USA</td>
<td>DOE</td>
<td>Sandia National Laboratory (SNL), USA; Lawrence Berkeley National Laboratory (LBNL), USA</td>
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<tr>
<td>Funding Organizations</td>
<td>Acronym</td>
<td>Research teams (Acronyms)</td>
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<tr>
<td>Empresa Nacional de Residoos Radioactivds, S. A., Spain</td>
<td>ENRESA</td>
<td>Universidad Politecnica de Catalunya (UPC), Spain</td>
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<tr>
<td></td>
<td></td>
<td>Universidad Politecnica de Valencia (UPV), Spain</td>
</tr>
<tr>
<td>European Commission (through BENCHPAR project)</td>
<td>EU</td>
<td>University of Edinburgh, UK (UEDIN); Royal Institute of Technology (KTH), Sweden</td>
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<td></td>
<td></td>
<td>INERIS-LAEGO, Ecole des Mines de Nancy, France (INERIS); Universidad Politecnica de Valencia, Spain (UPV); CEA/DM25/SEMT, France (CEA) Chalmers University of Technology, Sweden (CTH)</td>
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<tr>
<td>Institute for Protection and Nuclear Safety, France</td>
<td>IRSN</td>
<td>Paris School of Mines, France (PSM)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>CEA/DM25/SEMT, France (CEA)</td>
</tr>
<tr>
<td>Japan Nuclear Cycle Development Institute, Japan</td>
<td>JNC</td>
<td>Tokai Works, JNC, Japan; Hazama Corporation, Japan; Kyoto University, Japan</td>
</tr>
<tr>
<td>Nirex Ltd., United Kingdom</td>
<td>NIREX</td>
<td>University of Birmingham (UoB), UK</td>
</tr>
<tr>
<td>Nuclear Regulatory Commission, USA</td>
<td>NRC</td>
<td>CNWRA, Southwest Research Institute (SWRI), USA</td>
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<td>Ontario Power Generation, Canada</td>
<td>OPG</td>
<td>Atomic Energy of Canada, Ltd (AECL), Canada</td>
</tr>
<tr>
<td>Swedish Nuclear Fuel and Waste Management Co., Sweden</td>
<td>SKB</td>
<td>Chalmers University of Technology, Sweden (CTH)</td>
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<td>Clay technology AB, Sweden (CLAY)</td>
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<tr>
<td>Swedish Nuclear Power Inspectorate, Sweden</td>
<td>SKI</td>
<td>Lawrence Berkeley National Laboratory (LBNL), USA</td>
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<td>Royal Institute of Technology (KTH), Sweden</td>
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<td>Radiation and Nuclear Safety Authority, Finland</td>
<td>STUK</td>
<td>Technical University of Helsinki, Finland (TUH)</td>
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<td>Uppsala University, Sweden (UU)</td>
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A number of benchmark tests (BMT) and test cases (TC) have been studied within the project. The BTMs investigate hypothetical problems in the behavior of individual or coupled THM processes and analyze the extrapolations of results over time and spatial scales of interest to repository performance. As part of the BMTs, sensitivity and scoping analyses are conducted with alternative conceptual and numerical models by
different teams. The TCs are laboratory and field experiments designed to advance our understanding of the THM processes, with numerical modeling helping both to interpret the test results and to test the models. A number of major, large-scale, multiyear experiments have been studied within the project.

In addition to analysis of these BMTs and TCs, particular topics were selected for discussion and review among project participants. These range from the state of the art for constitutive relations of rock fractures, to the current international treatment of THM issues in repository performance assessment.

The activities of the DECOVALEX project are organized around the study and modeling of these BMTs and TCs by multiple research teams. Both BMTs and TCs are carefully developed as initial-boundary value problems with proper thermal, hydraulic, and mechanical initial-boundary conditions and loading sequences. Based on the results from these studies, new experiments are proposed to provide more rational tests of concepts and models, and to advance the state of mathematical modeling for coupled THM processes in fractured rocks and buffer materials. Analytical and semi-analytical solutions to the coupled problems were also developed whenever possible. Representatives of the national regulatory authorities, along with radioactive waste management organizations participating in the project, took an active part in the whole process to ensure that the project was conducted equally from scientific, engineering, and managing points of view. The physical processes studied in the BMTs and TCs are listed in Table 2.

### Table 2. Physical phenomena studied in DECOVALEX

<table>
<thead>
<tr>
<th>Components</th>
<th>Phenomena</th>
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<tr>
<td>Physio-mechanical processes</td>
<td>- Thermal expansion, diffusion, and convection in fractured rocks and buffer materials</td>
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<tr>
<td></td>
<td>- Fluid flow in fractured rocks and buffer materials, including unsaturated flow</td>
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<tr>
<td></td>
<td>- Stress-deformation of fractured rocks and buffer materials</td>
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<td></td>
<td>- Interactions between the processes mentioned above</td>
</tr>
<tr>
<td></td>
<td>- Constitutive laws for rock fractures, fractured rock masses, and buffer materials</td>
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<tr>
<td></td>
<td>- Upscaling/homogenization of fractured-rock properties</td>
</tr>
<tr>
<td>Geometrical factors and properties</td>
<td>- Rock fracture networks and their characterization and representation</td>
</tr>
<tr>
<td></td>
<td>- Rock fracture properties and their effects on upscaling hydraulic parameters of fractured rocks</td>
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</tbody>
</table>
One characteristic of DECOVALEX is that each of the BMTs and TCs is studied by multiple research teams using their own approaches, conceptual models, and computer codes. Through comparisons of results from these teams, much insight could be gained not only on the effects of the coupled THM processes, but also on the strengths, weaknesses, and adequacies of the various approaches and computer codes. It is also an excellent way for all the countries to learn from each other and collaborate to address issues of common interest.

The DECOVALEX project has gone through three stages:

- **DECOVALEX I** 1992–1995
- **DECOVALEX II** 1995–2000
- **DECOVALEX III** 2000–2003

An overview of the project was presented in [1]. The most recent DECOVALEX III program includes two TCs and three BMTs, as well as an additional “Survey and Discussion” task on the role of coupled THM processes in performance assessment. The two TCs are studies of major multiyear field tests concerning THM processes:

- The FEBEX experiment, conducted by ENRESA: Two heaters in crystalline fractured rock at the Grimsel Underground Testing Facility in Switzerland. The heaters are emplaced in bentonite blocks within a drift, and both the bentonite and surrounding rock are monitored continuously through a heating and cooling cycle.
- The Drift Scale Test (DST) experiment, conducted by DOE: A set of 9 large heaters in a test drift and 50 smaller “wing” heaters in boreholes set in unsaturated tuff, with no backfill. Monitoring in the rock includes measurements not only of temperatures and displacement, but also saturation, effective hydraulic conductivity, and water samples for chemical and isotopic studies.
These two field experiments represent two of the largest tests of coupled THM processes in fractured rocks and buffer materials to date for supporting design and performance assessment of nuclear waste repositories. In the following two sections, their study by multiple teams in parallel will be described, and comparisons of their results discussed, followed by descriptions and discussion of three BMT studies within DECOVALEX III. Some details may be found in papers in [2]. The emphasis of the present paper is on lessons learned from these studies. Some general remarks conclude the paper.

2. Studies of the FEBEX Experiment

2.1. Introduction and Task Definition

The international FEBEX (Full-Scale Engineered Barriers Experiment in Crystalline Host Rock) project, conducted by ENRESA with support of the European Commission, has been in operation since 1994. One purpose of the project is the study of the various processes occurring in the near field of a high-activity radioactive waste storage site.

The experiment was installed at the Grimsel Test Site, an underground laboratory in Switzerland, operated by NAGRA. The experiment is based on the Spanish reference concept of deep geological storage in crystalline host rock. In this concept, steel canisters containing conditioned waste are placed along the axis of horizontal galleries drilled in a rock formation, and an engineered barrier is placed in the annular space between them. The engineered barrier is made of high-density compacted bentonite blocks that will swell as a result of water input from the host rock, thus providing a highly impervious seal. In the FEBEX in situ test, the waste canisters were represented by two cylindrical heaters. Figure 1 shows a perspective of the FEBEX drift and associated boreholes.

The FEBEX test is one of the few large-scale tests available that provides an integrated perspective on current concepts for nuclear waste disposal in crystalline rock. The comprehensive instrumentation installed in the rock and in the compacted bentonite buffer has yielded vast amounts of data over the past nine years. Part of this data, corresponding to the first three years of heating, was used in a TC task (Task A) studied under DECOVALEX III. Several papers on this task have been published in the
The modeling exercise under this TC was divided into three parts, as follows:

### 2.1.1. Part A: Hydro-Mechanical (HM) Modeling of the Rock

Based on the available geological, hydraulic, and mechanical characterization of the Grimsel Test Site, as well as on results of hydraulic tests performed in boreholes, a hydro-mechanical model for the surrounding rock of the FEBEX tunnel was prepared. Using this model, changes in water pressure induced by the boring of the FEBEX tunnel, as well as the total water flow rate to the tunnel, were calculated.

Two types of measurements have been selected to develop the modeling exercise: (a) the actual water inflow rates into the FEBEX tunnel, and (b) the rock pore-water pressure response in the vicinity of the tunnel’s outer perimeter during excavation by a tunnel boring machine (TBM).

![Figure 1. Layout of FEBEX test and associated boreholes](image)

The first type of measurement, flow into the tunnel, represents an integrated variable as a function of the problem geometry, rock fracture pattern, fracture anisotropy, rock matrix permeability, and boundary conditions. Water inflow in the test zone (which extends 17.40 m along the tunnel axis) was measured by two techniques (absorbing pads at selected points on the tunnel wall and a small gauge measuring overall leaked water) at different dates within the period January–May 1996, after the tunnel was fully excavated.
The second type of measurement involved the transient changes in water pressure recorded at two borehole intervals in the rock in close proximity to the advancing tunnel during TBM excavation. The pore-water pressure is related to the interaction between rock deformation and water pressure, and provides an interesting record of hydro-mechanical interaction in the saturated granitic rock mass.

2.1.2. Part B: Thermo-Hydro-Mechanical (THM) Analysis of Bentonite Behaviour

Based on the bentonite characterization and on the details of the test-installation process, a thermo-hydro-mechanical model for the bentonite barrier and the heaters was prepared. Using this model, the thermo-hydro-mechanical response of the bentonite barrier as a result of the heat released by the heaters was simulated. Besides local field variables (such as temperature, relative humidity, pore water pressure, stresses, and displacements), integrated variables such as total input power to the heaters were also calculated.

The performance of the test and the comparison among modeling predictions was based on the following variables:

- The evolution of the total heating power of one of the heaters
- The distribution and evolution of the bentonite barrier’s relative humidity (RH)
- Temperature
- Radial stress evolution at some points located at different radial distances in a normal cross section located at the middle of the second heater (Heater 2)

2.1.3. Part C: Thermo-Hydro-Mechanical (THM) Analysis of the Rock

Based on the characterization of the rock mass, and on the details of test installation and performance, the rock response in the immediate vicinity of the buffer was simulated. The rock was subjected to the heat released by heaters and by the swelling pressures resulting from bentonite hydration. The initial hydrological regime was also modified by the presence of the practically impervious bentonite buffer. Temperature, stresses, water pressures, and displacements in selected points of the rock were calculated.
Several instruments were located, at increasing depth, in auxiliary boreholes drilled from the tunnel. Data were available on temperature, rock water pressure, packer water pressure, stress state, and radial displacements. Water pressure was measured in some borehole intervals (each a few meters long) separated by packers.

Three normal components of stress are measured by means of total pressure cells. Four sets of three cells were prepared and grouted in situ in auxiliary boreholes SG1 and SG2 (see Figure 1). It recorded stress increments caused by the subsequent performance of the test (temperature effects, modification of pore water pressures, swelling of the bentonite).

Radial displacements were measured by means of borehole extensometers installed in auxiliary boreholes SI1 and SI2. They were located close to the position of the stress cells.

2.2. Summary of Modeling Approaches and Results

Ten modeling teams participated in this study. They are ANDRA/G3S-EP (denoted as ANG in the discussions below), ANDRA/LAEGO-EMN (denoted as ANN in the discussions below), BGR, CNSC, DOE, IPSN, JNC, SKB, SKI, STUK, with UPC as task coordinators. (Please refer to Table 1 for definitions of the acronyms.)

2.2.1 Results for Part A, HM Processes in the Rock

This part has two objectives: water inflow into the tunnel, and pore-water-pressure changes in rock near the tunnel during excavation. For the former, widely different models for water inflow were used. Some teams (ANN, CNSC, and SKB) used uncoupled hydraulic transient models to solve the first part of the exercise, whereas others (ANG, DOE, SKI) used coupled HM models. Some models describe water circulation in the rock by means of discrete features (tubes and channels such as ANN), some use equivalent porous medium techniques for different zones (such as DOE and SKI), and others combine porous medium and discrete fractures (ANG, CNSC, and SKB). The overall results, however, do not show a particular advantage for any given conceptualisation. Some of the calculations (such as SKI) provide the proportion of flow rates attributed to different origins (matrix, fracture zones). The distribution of
measured water inflow rates along the tunnel axis provides a first approximation to the relative proportions of flow through discrete fractures/shear zones and the matrix or distributed flow.

For the second objective, pore-water pressure changes in the vicinity of the tunnel excavation are initially a direct consequence of changes in the deformation of the surrounding rock mass. The ensuing dissipation of these changes is a consequence of transient flow towards a new hydraulic equilibrium, with a modified boundary condition owing to tunnel excavation. Therefore, fully coupled hydro-mechanical analyses are required to understand these physical processes. Further, it was established that the deformation of the rock in the vicinity of the tunnel depends critically on the orientation and intensity of the in situ stress field, which often shows a large spatial variability and is one of the challenging issues for modeling and interpreting stress measurement data.

2.2.2. Results for Part B, THM Processes in the Bentonite Buffer

Only a few teams participated in the blind prediction of THM behaviour in the bentonite buffer, and only three teams (CNSC, SKB, and SKI) were able to provide predictions for the full task. Some teams (IRSN) used a 1D coupled model to approximate results for those cases that could be approximated by a radial symmetry, such as those in sections normal to the test axis at the center of each of the two heaters. Other teams (BGR, IRSN) used models prepared to solve only the thermo-hydraulic part of the problem. The issues of phase change and vapor transfer were not considered in some models, and this limitation hampered the correct reproduction of measured variables.

The three fully coupled models (CNSC, SKI, and SKB) predicted quite accurately the evolution of relative humidity inside the buffer. Stress prediction, however, proved to be a more difficult task, one potential explanation being a doubt on the actual reliability of measuring procedures.

2.2.3. Results for Part C, THM Behaviour in the Rock

As in Part B, coupled THM models are also required for this part of the task, since temperature has a predominant effect on rock behavior. As is frequently the case,
temperature changes are well reproduced in general terms. Rock water pressures were reasonably well predicted by three of the research teams (IPSN, DOE, and SKI). More limited success was achieved in the prediction of stresses and displacements, with the exception of SKI.

2.3. Scientific Achievements and Lessons Learned

Results of the DECOVALEX study of the FEBEX experiment are discussed above. A few highlights on scientific achievements and lessons learned are given below in two categories, General and Technical:

(A) General Issues

In general, the DECOVALEX study with FEBEX was a learning process for all the involved participants, a process which led to new insights on physical explanations for specific measurements (e.g., the development of pore-water pressures in the granite when the FEBEX tunnel was being excavated) and progressive improvement of THM codes during the project.

The results of the numerical modeling demonstrate that

• success in numerical modeling relies mainly on proper hydrogeological characterization of the rock mass and experimental system, and less on the choice of a particular numerical approach (discrete fractures system or equivalent porous continua).

• demonstrate that fully coupled hydro-mechanical models needs to be applied to simulate/predict the flow and stress/deformation behaviour of fractured rocks—especially when excavation is involved, since the latter presents a significant transient mechanical loading mechanism and change of boundary conditions.

• predicting the behaviour of the bentonite buffer under combined heating and wetting actions requires a fully coupled THM formulation, which incorporates all the necessary physical processes present in the bentonite. Particularly relevant for predicting the early stages of heating was the inclusion of phase changes of water and the vapour transport in the bentonite.

• the hydration of the bentonite buffer was essentially independent of the heterogeneous nature of the hydraulic-conductivity features in the
surrounding rock, when the rock-matrix permeability is much higher than the saturated bentonite permeability.

- heating of the rock had a significant effect on rock stresses in the vicinity of the FEBEX tunnel, but much less on water pressures—a result, perhaps, of the relatively high rock permeability.

(B) Technical Issues

The following physical phenomena have been identified as the most relevant ones for the three parts of this task solved under the FEBEX task. Failure to consider them precludes correct simulation of some or all of the observed features.

*Part A (Especially pore-water-pressure development during excavation)*

- Full hydro-mechanical coupling
- Consideration of a general three-dimensional initial stress field
- Detailed modeling of the rate of geometry changes (progress of tunnelling with time)

*Part B (THM processes in the bentonite)*

- Phase changes between liquid water and water vapour
- Concentration-driven vapour flux
- Saturation-dependent water permeability and thermal conductivity
- Suction-induced deformations

*Part C (THM processes in the rock)*

- Thermal dilation of water and rock skeleton (rock skeleton provides for stress development, and the difference between water and the skeletons’ thermal dilations gives rise to heat-induced pore-water pressures.)
- Full hydro-mechanical coupling

On the other hand, the following aspects were also found to be of interest in the FEBEX case:

- The structure of the granite rock had a negligible influence on hydration of the bentonite buffer at the FEBEX site. This results from the large difference between the saturated permeability of the bentonite and that of the rock matrix.
- The gas pressure may be safely assumed to be constant, because of the high gas permeability.
• Plastic deformation of the bentonite does not seem to be an issue because of
  the high confinement provided by the rigid granite. Simple elastic models
  may suffice, provided that suction effects are incorporated.
• The heat-driven water flow in the rock is not affected by the heterogeneous
  nature of the rock, because the characteristic heating time is larger than the
  characteristic time for dissipations of pore-water pressures.

3. Studies of the DST Test

3.1. Introduction and Task Definition

The Drift Scale Test (DST) at Yucca Mountain, Nevada, USA, is a large-scale,
long-term thermal test being conducted by the United States Department of Energy
(DOE) as an integral part of DOE’s program of site characterization at Yucca Mountain,
to assess whether the mountain is a suitable repository site for the disposal of high-level
nuclear waste and spent nuclear fuel. The heating phase of the DST was initiated in
December 1997 and terminated in January 2002, ushering in a cooling phase of the test
that is expected to continue for four more years. The overarching objective of the DST
is to study coupled thermal, hydrological, mechanical, and chemical processes caused
by the decay heat from nuclear waste emplaced in an underground geologic repository.
The layout of the DST is shown in Figure 2.
Figure 2. Perspective of DST Block Showing Multiple Boreholes to House Heaters and Sensors

The DST consists of a 5-m diameter, 47.5 m long drift heated by nine cylindrical electric heaters placed on the drift floor. Each heater, 1.7 m in diameter and 4.6 m in length, is capable of generating a maximum of 15 kW of heating power. Additional heating is applied by 50 rod heaters, referred to as “wing heaters,” emplaced in horizontal boreholes drilled into either side wall of the drift (Figure 2). The drift’s cross section and the cylindrical heaters have approximately the size of emplacement drifts and waste packages, respectively, being considered for the proposed repository. The wing heaters are employed to simulate the heat that would come from adjoining drifts in the repository, and thus to provide better test boundary conditions. Each wing heater, 10 m long, has two distinct segments capable of generating respectively 1,145 W and 1,719 W of heating power. An Access/Observation Drift (AOD) parallel to the Heated Drift (HD) and an orthogonal Connecting Drift (CD) delineate the periphery of the test block (Figure 2). As shown in Figure 2, numerous boreholes drilled from the drifts into the test block house the heaters, instruments, and sensors for the test.

The DST task under DECOVALEX III had four subtasks: Task 2A, Task 2B, Task 2C, and Task 2D. Task 2A was to mathematically simulate and study the thermal-hydrological (TH) responses of the rock mass in the DST. Tasks 2B and 2C were to
model and analyze the thermal-hydrologic-mechanical (THM) and thermal-mechanical (TM) processes of the rock mass in the test. Task 2C differed from 2B in that measured temperatures were the input in simulating TM response, whereas in 2B, both the TH and the THM responses are predicted or calculated. Task 2D was to study the thermal-hydrologic-chemical (THC) response.

3.2. Summary of Modeling Approaches and Results

The research teams that participated in this task are IRSN/CEA, DOE/LBNL, ENRESA/UPC, JNC, NRC/SWRI and SKI/LBNL. (For definition of the acronyms used, please see Table 1.)

To simulate the thermal-hydrological (TH) response of the DST for Task 2A, the ENRESA/UPC research team employed the finite element code CODE_BRIGHT. To predict TH conditions, this code solves the mass conservation equation (air and water), the energy conservation equation in a nonisothermal state, and the momentum balance equation for mechanical equilibrium. Initially, this model used a single equivalent porosity and permeability structure to represent the fractured tuff in the DST block [12]. Later, the ENRESA/UPC team used a double porosity and double permeability structure to represent the co-located fracture medium and the matrix medium [13].

The NRC/SWRI researchers used the multiphase simulator MULTIFLO to perform Task 2A TH modeling. Their model involved the dual-continuum model (DCM) formulation similar to the dual-permeability model (DKM) used by the DOE researchers [14]. Both the DOE and NRC researchers invoked the active fracture model for unsaturated flow through fractured rock, proposed by Liu [14], to ensure realistic fracture-matrix interaction. The DOE research team used the TOUGH2 code to perform the TH modeling of the DST [15].

For Task 2B, SKI and later DOE teams performed coupled thermal-hydrological-mechanical (THM) analysis of the DST with the combined TOUGH-FLAC code, which is a simulator based on the coupling of two powerful well-established computer codes: TOUGH2 [14] and FLAC3D [16]. TOUGH-FLAC simulation captures the effect of stress changes on hydraulic properties, based on a conceptual model of highly fractured, unsaturated rock mass containing three orthogonal fracture sets. Porosity and permeability correction factors were calculated from the initial and current fracture apertures, assuming equally spaced fractures and adopting the parallel-plate fracture
flow model. The ENRESA/UPC team performed their 2B analysis by using CODE_BRIGHT, which allows permeability changes to be calculated based on changes in porosity resulting from stress changes.

For Task 2C, to predict displacements in the rock, both the IRSN/CEA and NRC/SWRI teams used measured temperature profiles as the thermal input to model the thermal-mechanical process. The NRC/SWRI team performed a continuum analysis using the FLAC code. The CEA team also performed continuum analysis, using the FEM code Castem2000 [17]. The work performed for Task 2B and 2C was reported in Datta et al. [18].

For Task 2D, the JNC team performed coupled THC simulation of the DST employing three codes: the THM code THAMES [19, 20, 21], the mass transport code Dtransu [22] and the geochemical code PHREEQE [23]. These three codes are controlled by a coupling system COUPLYS, which can exchange common data between the three codes and synchronize each code in order. The DOE team used the TOUGHREACT code [24] to model the THC processes in the DST, adopting the dual-permeability method to capture separate yet interacting processes in fractures and the matrix. Simulations of THC processes included coupling among heat, water, and vapor flow; aqueous and gaseous species transport; kinetic and equilibrium mineral-water reactions; and feedback of mineral precipitation and dissolution on porosity, permeability, and capillary pressure. The work performed for Task 2D was reported in Datta et al. [25].

3.3. Scientific Achievements and Lessons Learned

The DST confirmed that the heat-transfer process in the Yucca Mountain fractured tuff was conduction-dominated, although pore water played an important role, especially in the sub-boiling regime. Vaporized water traveled away from the heat via fractures and condensed in cooler regions, thereby filling fractures and lowering the permeability. Various conceptual models were evaluated by comparing simulated and measured temperatures. The dual-continuum or dual-permeability model (fracture and matrix) and the active fracture concept were needed to yield the best agreement under heat load.

The effect of dimensionality (i.e., 2D versus 3D) on temperature was evaluated. A maximum difference in temperature of about 10°C between 2D and 3D results were
found near the wing heaters after four years of heating. The TH calculations indicated that it was possible to choose appropriate hydrological parameters to obtain a distribution of saturation similar to the ones measured in the field.

The good agreement between simulated and measured air permeability indicates that the adopted conceptual model is sound, and that the model coupling stress with permeability is appropriate for predicting TM-induced permeability changes at Yucca Mountain.

Details of task results may be found in [26, 27, 28, 29, 30, 31].

4 BMT1: Flow and Mechanical Integrity in the Near Field

4.1. Introduction and Task Definition

BMT1 was proposed as a scoping calculation to estimate how THM processes can influence the flow pattern as well as the structural integrity of the geological and engineered barriers in the near field of a typical repository. The definition was based on a hypothetical nuclear waste repository in a granitic rock formation at a depth of 1,000 m. The conceptual design of the repository is illustrated in Figure 3a [32]. The centerline distance between adjacent tunnels is 10 m and the centerline distance between adjacent depository holes for the waste is 4.44 m. The depth of each depository hole is 4.13 m and the diameter is 2.22 m. Canisters for radioactive wastes would be emplaced into the depository hole, and a bentonite buffer material would be compacted around the canisters. The tunnels would also be backfilled with a mixture of gravel and clay. The issues being addressed include temperature evolution, buffer resaturation, stresses in buffer and rock, evolution of permeability and flow in rock, mechanical stability of the tunnels, and uncertainties in the above issues and how to model them, considering the spatial homogeneity of rock properties.

The objective of the BMT1 is to study the above issues through THM simulations of the hypothetical repository. The physical processes considered in the BMT1 include mainly (a) water flow in partially and/or fully saturated buffer and rock, in both liquid and vapor states, especially the thermally driven water-moisture diffusion process; (b) heat conduction and convection in buffer and rock; (c) stress, deformation and failure of rock using the Hoek-Brown failure criterion; and (d) variation of swelling pressure,
water content, and relative permeability fields in the buffer caused by coupled THM processes as listed above.

4.2. Summary of Modeling Approaches and Results

Six research teams participated in BMT1, using either finite-element (FEM) or finite-difference (FDM) methods. They are IRSN/CEA, CNSC, ANDRA/INERIS, JNC, BGR/ISEB/ZAG, and SKI/KTH.

All the research teams first conducted a calibration of their computer codes against realistic rock-mass conditions and measured outputs of thermal, hydraulic, and mechanical variables from the Kamaishi in-situ experiment at Kamaishi Mine, Japan, performed at the 550 m level gallery of the experimental site [33]. Then the calibrated codes were used to perform scoping calculations, considering varying degrees of THM couplings. The geometry of the problem, especially regarding the geometry of the fractures, is greatly simplified to regular fracture geometries, to simplify the calculation process and focus on the physics of the problem instead of computational efforts. The rock is studied for three cases: (1) homogeneous, without any explicitly represented fractures, (2) only one horizontal fracture intersecting the repository holes, with a vertical fracture zone from the ground surface down to the repository level, and (3) heavily fractured (Figure 3b, 3c, and 3d). The aim is to identify the coupling mechanisms of importance for construction, performance, and safety of the repository.
The results for the homogeneous rock case indicate that for the typical repository considered, only the full THM analysis predicted some localized rock-mass failure around the deposition holes, which might in turn result in a zone of higher permeability. Other important effects of THM and HM coupling would be the stresses developed in the buffer, which would be transferred to the canister and influence its mechanical integrity. From a safety point of view, engineering measures could be easily carried out to minimize these effects. From these results, it appears that the effect of coupling will be either short lived (several decades to 100 years) and would not have an impact on long-term (thousands to hundreds of thousands of years) safety issues, or could be rectified by adequate design and operation methodology. However, they have a significant impact on design and construction of the repository. Host rock properties (e.g., permeability) seem to have much more influence on long-term safety than the coupling effects. However, a fully coupled approach is necessary to help design the construction strategies and to interpret monitoring data collected in the first few decades after the repository closure. Coupled processes would prevail during that monitoring period, and an adequate interpretation of the monitoring data is essential in building confidence and demonstrating to the stakeholders that the repository is behaving in a predictable manner.

Further calculations assuming the presence of a few fractures (Figure 3c) or many fractures (Figure 3d) led to the following major findings:
• Temperature evolution (T process): no significant effect of HM coupling on heat transfer processes, and heat conduction dominates.

• Resaturation of the buffer (H process): affected by heat transfer process but not significantly by the mechanical process.

• Pressure evolution in the buffer (M process): strongly affected by the hydraulic process and slightly affected by heat transfer.

• Mechanical integrity of the near-field rock (M process): strongly affected by the coupled TH coupling.

The results of the impact of various THM couplings for sparsely fractured rocks are in line with those of a homogeneous rock. The main difference is that the hydraulic conducting fractures provide an additional water supply path that prevents desaturation of the rock and accelerates the buffer resaturation process. Details of work under this task are presented in a number of papers [32, 33, 35, 36, 37, 38, 39, and 40]

4.3 Scientific Achievements and Lessons Learned

In general, the BMT1 is a comprehensive numerical bench-mark-test problem, considering coupled THM processes in the near-field buffer-rock system of a hypothetical repository. Characteristics of buffer resaturation and mechanical integrity of the repository are considered. Through iterative verification against the results from the in situ THM experiments at the Kamaishi Mine, significant progress has been achieved in the development of robust mathematical and numerical models. The computer codes applied to the BMT1 tasks have achieved significant upgrading for the modeling of complex coupled THM processes in buffer materials and rock masses. The codes are thus proven to be reliable tools for the design, construction, performance, and safety assessments of nuclear waste repositories.

From the BMT1 results, it is shown that the evolution of water content, saturation, and permeability change in the buffer have to be simulated with full THM coupling. The thermally driven moisture flow, with the explicit or implicit inclusion of the existence of two phases (liquid and gas), has to be considered to adequately simulate the hydraulic behaviour of the buffer. However, the temperature in both the rock and buffer can be adequately predicted by considering heat conduction alone. The FEM codes used for BMT1 have the required capabilities for simulating the above processes, and thus
produce acceptable results for both hydraulic processes in the buffer and thermal processes in the buffer and the rock. Some other codes, however, lack this important capability and could therefore model the thermal processes only in a generally adequate way.

The finite-element codes applied to BMT1 problems have the capability of simulating fractures as thin-layer continuum elements with equivalent properties. This strategy suffers from the shortcomings of mesh distortion, displacement locking across the fractures, small deformation, and a limited number of fracture elements (to avoid the problem of numerical singularity in the global stiffness matrix). The performances of the codes for BMT1 are acceptable because of the simple fracture size and geometry defined for the problem. However, this may not be the case when more realistic fracture systems need to be represented.

One important issue in repository design, construction, and safety assessments is understanding the effect of a disturbed or damaged zone (DZ) surrounding an excavation. The importance of the DZ is not only in its effect on the mechanical stability of the repository (although it is important to consider this effect in repository design and construction), but also in its effect on coupled THM behaviour of the buffer/backfill, since the EDZ is the interface zone between the buffer/backfill and the undisturbed rock mass. The extent and behaviour of the DZ may also vary during the repository life and therefore continue to exert influence on repository performance and safety after closure.

Although the extent of rock failure was simulated in BMT1 with the Hoek-Brown criterion based on theory of plasticity, the real mechanism of combined damage, microfracturing and plastic deformation, and their effects on the behaviour and evolution of the DZ were not considered.

5 BMT2: Upscaling of THM Processes in Fractured Rock

5.1. Introduction and Task Definition

The Benchmark Test 2 of the DECOVALEX III project concerns the upscaling of the THM properties in a fractured rock mass and its significance for large-scale repository performance assessment. The work is primarily concerned with the extent to which various THM couplings in a fractured rock mass adjacent to a repository are
significant in terms of the solute transport typically calculated in large-scale repository performance assessments. Since the presence of even a few fractures may control the hydraulic, mechanical, and coupled hydro-mechanical behaviour of the rock mass, a key to this work has been to explore the extent to which these can be upscaled and represented by “equivalent” continuum properties appropriate for PA calculations. Given this, the task has two closely integrated aims:

- To understand how an explicit acknowledgement of the need for upscaling of coupled processes alters the approach to performance assessment modeling and the analysis of modeling results
- To understand the uncertainty and bias inherent in the outputs from performance assessment models in which the upscaling of THM parameters is either implicit or explicit

The details of the work performed for BMT2 can be seen in [41, 42, 43, 44, 45, 46].

The reference problem for BMT2 (Figure 4) concerns far-field groundwater flow and solute transport for a situation in which a heat-producing repository is placed in a fractured rock medium. Radionuclides potentially released from the repository may migrate with the groundwater flow and thus reach the biosphere. Specific issues to study are (1) how to assess the far-field hydraulic and transport properties when most data stem from small-scale (borehole) tests, (2) what is the impact of potential mechanical and hydraulic couplings, and (3) if MH or HM couplings are significant, how would they affect the upscaling?

It is assumed that the waste (heat source) is encased within resaturated bentonite that is in turn placed within a repository drift shown as a simple horizontal body. The repository sits within a low-permeability fractured rock unit overlain by a second low permeability fractured rock unit that extends to ground surface. A vertical fracture zone cuts both rock units, but lies beyond the end of the repository tunnel.

The relevant data for the rock formations and fault are based on Sellafield site characterisation data acquired by Nirex [41]. The data are in the form of statistical distributions of properties. Typically, most of the data concern measurements on small scales, whereas the problem to be studied mainly concerns the large scale.

The required work for the teams is to:

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• Derive appropriate conceptual and mathematical models according to provided data on rock-mass fracture and hydraulic, thermal, and mechanical properties from site characterization, using either discrete fracture-network approaches (2D or 3D) or equivalent continuum analyses.

• Derive upscaled equivalent hydraulic, mechanical and coupled hydro-mechanical properties from the small-scale descriptions at properly established representative elementary volume (REV) ranges.

• Model the stress, flow, and transport processes of the large-scale continuum model with values obtained from the above steps, and analyse the importance of the various couplings on solute transport properties at a PA scale.

![Reference problem geometry](image)

*Figure 4. Reference problem geometry*

The overall performance measures defined for BMT2 are the transit time ($\tau$) distributions and the transport resistance ($\beta$) distributions, at two output surfaces: a perimeter surface at 50m outwards from the boundary of the repository, and the land/sea floor surface. Some intermediate performance measures were also compared, including the effective permeability, effective rock mass deformation modulus, or effective
porosity to be used in large-scale numerical models. It turned out that using such intermediate performance measures is more practical than the overall performance measures.

5.2. Summary of Modeling Approaches and Results

Teams participating in these tasks are ANDRA/INERIS, JNC, SKI/KTH, DOE/LBNL, OPG, STUK/UU, NIREX/UoB, and ENRESA/UPV.

5.2.1 Approaches for Calculating Small-Scale Block Properties

Table 3 summarizes the modeling approaches used by the teams for calculating hydromechanical properties of small-scale blocks.

<table>
<thead>
<tr>
<th>Team</th>
<th>Main Features</th>
</tr>
</thead>
<tbody>
<tr>
<td>INERIS</td>
<td>3D DEM with flow in fractures only. Independent block generation, code 3DEC and RESOBLOK</td>
</tr>
<tr>
<td>JNC</td>
<td>2D fracture system generation and fracture density and permeability estimations based on pixels</td>
</tr>
<tr>
<td>KTH</td>
<td>2D DEM with flow in fractures only. Independent fracture system generation using stochastic realizations. Code UDEC</td>
</tr>
<tr>
<td>LBNL</td>
<td>Fractal Levy-motion approach for upscaling heterogeneous porous media, based on a series of short-interval hydraulic test results</td>
</tr>
<tr>
<td>OPG</td>
<td>2D FEM, extension of crack tensor theory to include THM parameters and BB-model of joints, code MOTIF and FRACTUP</td>
</tr>
<tr>
<td>STUK</td>
<td>3D DFN for flow analysis and 2D DEM for thermo-mechanical analysis, code FracMan.Mafic and UDEC</td>
</tr>
<tr>
<td>UoB</td>
<td>2D DEM for HM analysis linked with independent DFN flow analysis, code UDEC-BB and FRAC2D</td>
</tr>
<tr>
<td>UPV</td>
<td>Laplacian upscaling for HM, with effective hydraulic conductivity tensors evaluated at a REV scale of 10 m × 10 m.</td>
</tr>
</tbody>
</table>

In BMT2, the problem definition, on purpose, did not provide a definitive fracture system geometry model, so as to encourage different approaches to be applied to characterizing the equivalent hydraulic and mechanical properties of the rock masses. This naturally leads to quite different interpretations of the data provided. Results suggested that in this case, as defined, the stress is so high at the depth of the repository that fractures are almost completely compressed mechanically, and the permeability is approaching its residual value. Therefore, in general, further stress increase caused by
thermal effects would not significantly reduce the permeability. Results also indicated that in the near field, where temperatures are relatively high, THM coupling through the storage term may be significant. The TH effects, resulting from buoyancy, are relatively limited and would add an uncertainty on the order of a factor of 2.

These observations support the conclusion that the calculations of hydraulic properties are the main sources of uncertainty in a problem of this nature. However, an understanding of the stress/permeability relationship is important for a determination of the permeability field.

5.2.2 Large-Scale Analysis

For the large-scale analysis, the teams used different approaches. INERIS conducted T, TH, TM and THM computations using code FLAC3D, with equivalent properties derived from the upscaling. JNC analyzed the large-scale problem using the FEM code THAMES, with scaling rules obtained from Crack Tensor theory, but using the mean values provided in the Task. Particle tracking was then employed for transport analysis, with 300 particles at different starting times (t=0, t=1,000 years and t=10,000 years). KTH employed the equivalent parameters from a small-scale analysis used for coupled TM analysis of the large-scale problem, using the FEM code ROCMAS.

Multiple realizations of subsurface heterogeneity were generated by LBNL to determine the mean flow and transport properties and the associated uncertainties. Code T2R3D was then used to simulate coupled TH and tracer transport processes—with and without heat. A sensitivity study on the influence of fracture porosity was also performed: OPG used the code MOTIF for large-scale simulations of coupled THM processes and particle migration of radionuclides with three sets of simulations: (1) H, TH (HT), HM (MH) and THM processes with the given rock properties by Nirex; (2) HM (MH) and THM analysis with equivalent properties considering all fractures; and (3) HM (MH) and THM analysis with equivalent properties considering only 1/3 of the active fractures. Six particles were then released from points evenly distributed over the mid-level of the repository block and tracked to the discharge points or model boundary.

On the other hand, STUK used the code TOUGH2 to solve the head and flux fields, with upscaled parameters of effective conductivity and correlation structures. Transport was modeled by particle tracking, with multiple realisations to simulate flow and
transport processes. TM effects were studied as a sensitivity analysis based on input permeability distributions. A particle, released at a nodal point of a random element within the repository area, migrates to the adjacent node in a given direction, following a probability based on the fraction of the total outward directed flux in that same direction. Transit time and transport resistance were then sampled from the probability distributions obtained from the small-scale analysis. UoB used their continuum flow and transport code FAT3D for the far-field studies, with calculations of the median particle travel times for the two considered base cases (H and HM base cases). Finally, UPV developed a detailed description of the hydraulic conductivity field as well as an upscaled description, and compared transport results from the detailed and upscaled fields.

Generally, in the large-scale analyses, all teams used their upscaled small-block properties in various equivalent porous-continuum codes to explore the resulting effects on large-scale flow and transport processes. The impact of the thermal input produced by the decaying waste was calculated. Results are summarized as follows:

- Similar values of the maximum temperature were predicted by different teams.
- The hydraulic process had a negligible effect on stress or displacement variations, with less than 20% difference between TH and THM results. However, mechanical processes had a significant effect on the discharge vectors and pore pressure variations (finding by INERIS).
- TM processes induce relatively small changes in permeability. Thermal loading has a noticeable but insignificant effect on radionuclide transport (finding by LBNL).
- There was a significant thermal effect on flow processes. The average horizontal groundwater velocity in the case of TH processes is about twice the velocity for the isothermal steady-state flow, and the vertical velocity is about 40% to 70%. THM impacts on transit time are more important at the 50 m scale than at the kilometer scale. The fracture density assumed in the modeling and whether upscaling is performed, appear to affect the transit time to final discharge more than THM coupling (finding by OPG).
- Long-term heating affects hydraulic aperture, with a reduction of about 10–15% of apparent aperture during the first 100 years of heating, implying a decrease of fracture transmissivity. TM effects on flow and transport processes are small in
comparison to the intrinsic uncertainties in modeling hydraulic flow in fractured rock (finding by STUK).

- The results for the HM base case show high sensitivity to the chosen mechanical properties (finding by UoB).

5.3. Lessons Learned and Outstanding Issues

Despite the progress made in developing numerical approaches for HM upscaling of fractured rocks, the problem has such a degree of complexity that the current work can only be regarded as a start for understanding both the nature of the problem and the demanding computational skills and resources required for further research. Some highlights of the lessons learned and the outstanding issues that need to be further investigated are summarized below.

If relaxed initial apertures are used as input to models, inclusion of HM coupling is essential for capturing realistic permeability values at depth. It appears that the two-order-of-magnitude decrease, as noted by the KTH team, would account for most of the discrepancy between the modeled block permeabilities (assuming relaxed apertures) and data from borehole measurements. This raises the question concerning the extent to which hydraulic data obtained at one depth can be used in a model at a different depth if not corrected for HM-responses.

A key uncertainty is the relationship between hydraulic residual aperture and maximum mechanical aperture. Evidently this has a strong influence on the impact of HM coupling. Related to this is the significance of an increase of differential stress resulting in localized permeability distribution and channelling of flow paths (caused by fracture shear dilation).

At the outset of the task, it was assumed that the data on fracture geometry was sufficient for the task. However, it turned out that the fractal nature of the fracture lengths and fracture density was poorly constrained, and that markedly different fracture densities could be generated that were consistent with the data. This raises the question, what and how much fracture data are needed for flow and transport modeling?

The teams treated all fractures as formed by the same genetic failure mechanism and did not distinguish joints from veins or from faults, with possible different scaling laws. While it cannot be certain that such considerations are feasible at present or would improve the predictive capability of flow and migration in fractured media, they
nevertheless illustrate the need for a more comprehensive system characterization for more reliable computer simulations.

Considerable uncertainty exists in the interpretation of fracture size. Of particular interest are assumptions made on the correlation between size and hydraulic properties. Such assumptions may have a large impact on upscaling rules.

It is not surprising that the TM processes has very limited impact on the far-field radionuclide transport processes, since their significant sphere of influence are at the near-field of repositories (excavation and EBS performance), which is not considered in BMT2.

6. BMT3: Effects of Glaciation and Permafrost

6.1. Introduction and Task Definition

Bench Mark Test 3 (BMT3) of DECOVALEX III has been designed as a generic numerical study to investigate the coupled THM impacts of a glacial cycle on the long-term (up to 100,000 years) performance of a geosphere in which a repository is located. The results are contained in a series of publications [47-55].

The objectives of this task are:
1. To study, by analytical and/or numerical modeling, the long-term evolution of a fractured rock mass in which a generic repository is located, as it undergoes a glaciation/deglaciation cycle within a time frame of 100,000 years
2. To assess how a glaciation/deglaciation cycle would impact the coupled mechanical and hydraulic responses of the repository system and its ability to isolate waste over the long-term
3. To improve the geoscientific basis for the safety case of a deep geological repository

Although BMT3 is a generic modeling exercise, the simplified data from a specific Canadian research area was utilized to make the simulations realistic. Site attributes have largely been based on those of the Whiteshell Research Area (WRA) in eastern Manitoba, on the western edge of the Canadian Shield.

The model domain encompasses a volume approximately 25 km × 37 km × 4 km (depth) and consists of sparsely fractured rock, moderately fractured rock, and highly fractured rock (uppermost layer and fracture zones). An interconnected 3D network of
fracture zones traverses the rock mass. A generic spent-fuel repository was assumed to be located at 500 m depth. General regional topographic gradient ranges from 0.001 to 0.002; superimposed on this is a higher local topographic gradient. Maximum elevation is 301 masl (metres above mean modern sea level), while the minimum elevation, is 255 masl. For modeling purposes, the topography was smoothed so that elevation lies in the range of 255–290 masl. It was also assumed that the water table coincides with the ground surface.

The network of major fracture zones was idealized so that there were 17 fracture zones, 12 at the vertical boundaries and 5 in the interior of the conceptual model. Of the five interior fracture zones two were vertical, one was horizontal and two were dipping at 45°. In particular, the long horizontal fracture zone was included to study the possibility of glacially induced hydraulic jacking.

Under BMT3, three types of numerical modeling were conducted. The primary purpose of Type 1 modeling was to generate spatially and temporally varying thermal (for permafrost modelling only), mechanical, and hydraulic boundary conditions for the other two types of (site-scale) numerical models. Type 2 modeling focused on simulating the time evolution of subsurface temperature and permafrost at the site scale. The distributions of hydraulic heads and stresses were also calculated. Type 3 modeling focused on the site scale by calculating the subsurface heads, Darcy velocities, displacements, and stresses, which all have a bearing on the safety case of a deep repository.

6.2 Summary of Modeling Approaches and Results

The teams that participated in this task were OPG/AECL, SKB/CTH, STUK/HUT, and UEDIN. The modeling exercise was divided into three phases.

1. Phase I: Enhancing numerical tools for simulations of the climate drive, ice-sheet loading, and basal thermal and hydrological regime (UEDIN); preliminary studies on coupled 1D and 2D processes pertaining to permafrost development (HUT), and 2D site-scale coupled HM subsurface modeling using several sets of generic steady-state boundary conditions (AECL and CTH).

2. Phase II: 3D ice-sheet/drainage modeling averaged over 2D swats to generate transient thermal boundary conditions (UEDIN) for 2D permafrost modelling
(HUT) and transient hydraulic and mechanical boundary conditions for the 2D transient site-scale coupled HM subsurface modeling (AECL and CTH).

3. Phase III: 3D ice-sheet/drainage simulations to generate time-dependent 2D mechanical and hydraulic boundary conditions (UEDIN) for 3D coupled HM site-scale rock-mass modeling (AECL and CTH). In addition, UEDIN and HUT coupled their 2D versions of ice-sheet/dRAINAGE and permafrost models thermodynamically at the ice-bed interface and performed simulations pertinent both to the Äspö Hard Rock Laboratory site, Sweden (assuming that the site is always above the marine line [55]) and to the WRA, Canada [53].

6.3. Scientific Achievements and Lessons Learned

The transient coupled hydro-mechanical modeling in this study represents a major step forward in advancing the state of the science for modeling and understanding geosphere response to glaciation. Although stress/deformation/failure systems for models of glacier-groundwater, glacier-permafrost-groundwater and glacier-groundwater-shallow-rock have been presented previously, this BMT is one of the first attempts to assess the effects at repository depths using site-specific (though simplified) data. Likewise, this study probably represents the first successful attempt at scaling down an ice-sheet/drainage model with 10 km resolution to a 200 m resolution, in order to interface with site-scale subsurface modeling. The results provide insights into the magnitude and rate of change in site-specific hydrogeological and geomechanical responses to external, transient climate forcing. They clearly demonstrate the importance of glaciation scenarios in performance assessments and the effects that result from HM coupling, and underline the need for transient analyses of these coupled phenomena.

Two independent HM rock-mass models have yielded generally similar results, thus enhancing confidence in modeling site-scale subsurface responses to a glacial event. It is no small achievement to demonstrate for the first time a capability to simulate the coupled HM rock-mass response to glaciation, using model-based time-dependent glacial boundary conditions, along with reasonable site-specific (though somewhat simplified) hydraulic and mechanical attributes. The task has provided a systematic and structured framework for assessing the relative importance of coupled HTM effects on
geosphere performance. A few of the outcomes from this assessment are highlighted below.

Coupled HM simulations using transient boundary conditions, obtained from ice-sheet/drainage simulations, to represent a glacial event have yielded a flow field evolution that are markedly different from any simulation using steady-state boundary conditions. This implies that the common practice of assuming a time-invariant flow field in system performance assessment may require serious reconsideration.

During a glacial event, the hydraulic heads, that account for HM effects, increase dramatically throughout the model domain, up to 800 m, equivalent to about 1/3 of the pressure from the weight of the ice sheet. With uncoupled simulations, hydraulic-head distribution below a certain depth remains unchanged from the initial nonglacial conditions.

High residual excess pore pressure (approximately 250 m higher than hydrostatic at 800 m depth) remains 10,000 years after the ice sheet has retreated off the model domain at nominal repository depth or below, resulting from the very low hydraulic diffusivity of the rock. This result suggests that the flow system is currently in a transient state of slow recovery towards equilibrium.

Because of the counterbalancing effects of mechanical stress and hydraulic pressure changes, effective stresses predicted by HM simulations are a small fraction (e.g., 1/8 in the horizontal fracture zone) of the values predicted by uncoupled mechanical modeling. The minimum effective stress in this fracture zone is compressive, with a magnitude of a few MPa, so that no hydraulic jacking is predicted. Neither is shear failure predicted. The principal effective stress ratio and orientation vary during glaciation. Uncoupled stress analysis leads to a significantly higher (i.e., optimistic) safety factor than the coupled HM model.

In a 3D model, the fracture zones are better connected than in 2D models, and consequently, the influence of subglacial channels—the remnants of which are eskers—is stronger. Maximum groundwater velocities are found to be twice as high as those calculated in 2D simulations.

7. Concluding Remarks

The value of the DECOVALEX approach—comparing studies of multiple international research teams, using different approaches and computer codes, to
investigate the same complex site-specific or generic problems—is well demonstrated by achievements obtained during the project. The insight obtained by such cooperative efforts would have been impossible if the teams had worked independently. The understanding of coupled THM processes in different rock formations, along with the development of modeling capabilities for such rock behaviour, has to be considered as work in progress. However, significant progress in understanding crystalline rock-bentonite and unsaturated tuff systems has been made, with a number of valuable new insights, important scientific conclusions, and lessons learned. We believe that the field of coupled THM processes has been much enriched by the results from the DECOVALEX project over the last 12 years.

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