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COUPLED THM PROCESSES IN GEOLOGICAL SYSTEMS AND THE DECOVALEX PROJECT

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ABSTRACT: An overview is given of recent progress in the understanding, monitoring, and modeling of coupled thermo-hydro-mechanical (THM) processes in geologic systems, in the context of major practical applications. The progress has been made possible through individual research efforts, as well as international cooperative research projects. As an example of international cooperation, the DECOVALEX project is described. Initiated in 1992, the project has progressed successfully through three major stages. It has played a key role in the development of the field of mathematical modeling and testing of coupled THM processes in fractured rocks and buffer/backfill materials, a subject of importance for performance assessment of a radioactive waste geologic repository. The DECOVALEX project has been supported by a large number of radioactive waste management organizations and regulatory authorities, including those in Canada, Finland, France, Japan, Germany, Spain, Sweden, UK, USA, and EU. This paper presents a summary of the project, including the objectives, scope, problems investigated, scientific achievements and major outstanding issues, with emphasis on the science of the coupled THM processes.

1. INTRODUCTION

The last fifteen years have seen substantial progress in experimental and theoretical studies regarding the effects of coupling temperature gradient (T), hydrologic flow (H), and mechanical deformation (M) in fractured rocks. Much of the impetus behind these efforts is the concern over the role of such couplings in the performance and safety assessment of a heat-releasing nuclear waste repository in the subsurface (Tsang, 1987). However, the problem is of wider interest, ranging from coupled THM processes associated with geothermal energy extraction, gas production from coal beds, seismicity induced by fluid injection and the construction of underground openings, to guidelines on injection pressures needed for stimulating deep petroleum reservoirs with water colder than *in situ* fluids.

To understand and predict the effects of coupled processes in all these practical problems, models are being developed that are capable of simulating coupled thermo-hydro-mechanical (THM) processes. The term “coupled processes” implies that one process affects the initiation and progress of another. Thus, the rock mass behavior cannot be predicted with confidence by considering each process individually or in simple succession. Previously, binary TM and TH couplings have been studied in the context of, for example, rock mechanics and geothermal reservoir engineering.

For many current applications, however, we must study the full triply-coupled THM processes. In some cases, the introduction of chemical processes (C) into the study of THMC couplings and its impact are also of important. Work has been initiated by different researchers, in various countries

The coupling of THM processes is a major challenge to the geoscience community, since the three processes have widely different characteristic time and spatial scales. The thermal effect in rock material has relatively long time and spatial scales. Mechanical effects, on the other hand, have a short time scale, since changes in the mechanical response can propagate through the rock mass with the speed of elastic waves, and deformability is often dominated by the presence of fractures of various size scales, such as joints, faults and fracture zones. Finally, groundwater flow and transport are sensitive to both small-scale heterogeneities and fracture system characteristics, but are characterized by longer flow and solute transport times.

Numerically, these processes can be modeled by different techniques, such as finite-difference methods (FDM), finite-element methods (FEM), and discrete-element methods (DEM), as well as discrete fracture network (DFN) methods. In addition, many of the coupled processes are nonlinear, and the constitutive equations typically contain certain parameter sets. Combining all these processes into

an efficient model for the simulation of coupled THM processes in fractured rocks is a challenging task.

A key element in the study of coupled THM processes is the verification of numerical codes and validation of model results against well-conditioned field and laboratory experiments. Here, the challenge lies in providing a set of well-defined conditions for the boundaries, the rates of thermal and mechanical loading, the initial state (of stress, temperature and flow), and constitutive equations for coupling and material properties. Coupled THM experiments in the field require well-considered test designs, robust instrumentation, careful result interpretation, and often have durations of months and years.

In the next section, recent progress in the understanding of the various coupled THM processes in geo-systems for a wide range of problems is briefly reviewed, with references to other chapters in this volume. In the following section, we turn from a general discussion to one particular international cooperative project involving research teams from about ten countries to develop and study a set of coupled THM problems and data sets devoted to nuclear waste isolation. This is the so-called DECOVALEX project, within which significant advances on modeling THM processes related to nuclear waste repositories have been made over the past 12 years. The paper then concludes with some general remarks.

2. PROGRESS IN RESEARCH OF COUPLED THM PROCESSES IN GEOLOGICAL SYSTEMS

The progress made over the last decade in our understanding, monitoring, and modeling of coupled THM processes in geo-systems has been on many fronts, such as on problems related to nuclear waste geological disposal, development of geothermal and hot dry/wet rock systems, coal bed gas production and underground coal gasification, petroleum production and reservoir dynamics, and stability of large-scale civil constructions. Research in these fields is presented in the various chapters in this volume. The present section briefly describes a number of highlights and points out the potentials for cooperation and cross-fertilization among these fields.

In the study of coupled THM processes related to nuclear waste geological isolation, many laboratory experiments to investigate the constitutive

relationships and individual processes have been performed, and a number of large-scale (~10–100m), long-term (1–8 years) field experiments have been conducted (see, for example, Alonso and Alcoverro, 2004; Datta et al., 2004; Chijimatsu et al., 2004). Modeling capability has advanced from studies of THM-induced permeability changes caused by fracture opening and closing, shear displacement and dilation in hard rocks, to simulation of flow and transport under coupled THM processes in fractured rocks accounting for complex geologic structures and heterogeneity. A number of attempts for homogenization of the discrete fracture network for simulation of coupled THM effects have been made (Liu H. et al., 2004; Guvanasen and Chan, 2004; Gomez-Hernandez and Cassiraga, 2004). Significant progress has also been made in coupled THM processes in bentonite, which is used as a buffer around a nuclear waste canister emplaced in a geologic repository, and in its interaction with neighboring rock (Thomas et al., 2004; Rutqvist et al., 2004). Increasingly, work has now turned to detailed studies of the role of gases (air from tunnel ventilation or gas produced from canister corrosion) and of coupled processes for softer rocks (Alonso and Olivella, 2004; Shao et al., 2004; Su et al., 2004). Soft rocks, such as clays and shales, are also being considered as potential host rocks for nuclear waste repositories. These rocks can experience large deformation, and their behavior is particularly sensitive to changes in moisture level or humidity in their environment, e.g., in the tunnels and boreholes. These cases under coupled THM processes represent challenging and exciting areas of continued research.

In the field of geothermal hot dry rock or hot wet rock (HDR/HWR) reservoirs, considerable progress in detecting and mapping of hydraulically created permeable structures has been made (Niitsuma, 2004). Much of the progress has been in the improved analysis of microseismic monitoring, which is currently the best available method for obtaining three-dimensional structural information away from boreholes. The maps of seismic clouds produced through conventional analysis of seismic events due to hydrofracturing involve significant location inaccuracy. Such errors can be much reduced through a suite of integrated methods, such as collapsing, doublet/multiplet analysis, clustering analysis and multiplet-clustering analysis. These methods are able to reveal, from the conventional seismic clouds, the macro- and microstructures, and these structures can be correlated with geologic and hydraulic structures identified from well logs. The

method has been successfully applied to data from the cooperative European HDR research program at Soultz-sous-Forêts site in France. Besides this work, significant progress has also been made in modeling of coupled THM processes as well as their interaction with chemical processes in geothermal systems (see for example, Fomin et al., 2004b; Hosni et al., 2004).

In contrast to nuclear waste geologic isolation, in which disturbance to the geological formation is to expected to be minimized, petroleum exploration aims at maximizing production and large changes in pressure, temperature, stresses, deformation, flow rates and chemistry are expected. These have stimulated studies of mechanical-chemical coupling, quasi-static solid-liquid coupling, and dynamic solid-liquid coupling (Dusseault, 2004). Both the fundamental processes and practical implications of these couplings are investigated. Borehole integrity is an important issue in petroleum exploitation, often controlled by coupled THMC processes in shales present around the borehole (where the C in THMC refers to chemical effects). Shale expansion or contraction changes the stress states, causing potential for damage. Another issue is sand production, creating stress changes and the potential for further yield, channeling and dilation. Improved analysis and modeling of these types of problems have been conducted (e.g., Choi et al., 2004; Guimaraes et al., 2004; Han and Dusseault, 2004).

Underground coal gasification involves even more drastic coupled THM processes than petroleum exploitation. The high heat energy released in in-situ coal seam burning and the creation of new cavities in the coal seam dramatically modified the local permeability field, which in turn affects the gasification process. Such cavity evolution has been accounted for in a coupled THM model of the system (Liu J. et al., 2004). For the more moderate processes of coal mining and methane production from coal seams, there are the problems of gas pressure changes, opening or closing of coal cleats, and gas sorption or desorption from the coal matrix. These affect gas production and, in some cases, cause coal and gas outbursts. Modeling of these processes has made significant progress (Choi and Wold, 2004; Sun, 2004).

Advances in coupled processes research have also been made in the context of construction of major dams (Guo et al., 2004; Zhu et al., 2004), the best researchers from a number of countries and serves both to encourage and stimulate development and also to peer review each others' work. Two

development of cold storage caverns (Lee and Lee, 2004), and grouting boreholes in permafrost (Fomin et al., 2004a).

The discussion above has centered on geological systems impacted by human activities. Much work has also been done on natural geological systems, in which coupled THMC processes play a key role in understanding the natural evolution of the systems. Such research includes modeling of sediment compaction during burial in sedimentary basins (Bjørlykke et al., 2004), lava dome collapse triggered by rainfall infiltration (Elsworth et al., 2004), and state of earth crust structure as a result of rock fracturing under high pressure-temperature conditions (Nikolaevskiy and Garagash, 2004).

It is interesting to note some of the common problems connecting the different fields. The reasons for such connections are the basic physics and the need to account for geological structures common to all these fields. For example, identification of faults and fractures away from boreholes is an important problem in nuclear waste geologic isolation, since faults or fractures may be the main conduits for leakage from the repository. In a recent multi-year heater test (Datta et al., 2004), microseismic events have been measured. The advances in methodology in analyzing these events made by HDR researchers can be applied to such data to great advantage. Another example is the interest of coupled processes in shales related to stability in petroleum boreholes. This interest is shared by researchers who are studying tunnel stability where shales are present, and by researchers considering the potential of storage of nuclear waste in shales. There are also overlaps between research on gas processes in coal seams and on gas transport in petroleum reservoirs. Often a computer code and model developed and tested in one field can be modified and applied to another. Then those computer codes and models, that have been successfully applied and tested in more than one field, will command a much higher confidence level.

A significant part of the progress would have been much delayed without major international cooperative programs. Cooperation brings together

examples are the Soultz HDR project, supported by the European Commission, and the DECOVALEX project. To illustrate the importance and

effectiveness of cooperative research, the rest of this paper will be devoted to an overview of the DECOVALEX project, and the major results pertaining to coupled THM processes that have emerged from this international cooperative project will be summarized.

3. THE DECOVALEX PROJECT

An international cooperative project DECOVALEX (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. The participating organizations would share results from major field and laboratory experiments, results that would enhance understanding of coupled processes and provide data for model validations. Over the last twelve years, more than 15 research teams from 10 countries have participated in this joint effort. The project objectives include:

- To support development of computer simulators for THM modeling
- 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 development
- To study the application of THM modeling to performance and safety assessment of nuclear waste repositories.

A large number of benchmark tests (BMT) and test cases (TC) have been studied within the project. The former are hypothetical problems used for investigating the behavior of individual or coupled THM processes with general complexity in processes, properties and parameters, and evaluating the extrapolations of results into time and spatial

scales of interest to repository performance (which cannot be performed by experiments). As part of

BMTs, sensitivity and scoping analysis will be conducted with alternative conceptual and numerical models by different teams. The TCs are laboratory and field experiments that were designed to advance our understanding of the THM processes, and numerical modeling was applied to both test the models and to help interpret the test results. 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 of 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 BMTs and TCs by multiple research teams using different mathematical models and computer codes. 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 were 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 and 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 1.

The next section describes the activities of the three stages of DECOVALEX I, II, and III, covering the years 1992–1995, 1995–2000 and 2000–2003, respectively. Following this, two specific examples are presented to illustrate, in different depths, the work of one BMT and one TC performed under the project.

Table 1. Physical phenomena studied in DECOVALEX	
Components	Phenomena
Physio-mechanical processes	<p>Thermal expansion, diffusion, and convection in fractured rocks and buffer materials</p> <p>Fluid flow in fractured rocks and buffer materials</p> <p>Deformation of fractured rocks and buffer materials</p> <p>Constitutive laws for rock fractures, fractured rock masses, and buffer materials</p> <p>Swelling pressure and suction potential of the buffer materials</p>
Geometrical factors and properties	<p>Rock fracture networks and their characterization and representation</p> <p>Rock fracture properties (aperture, roughness, gouge production, filling, conductivity, storativity)</p> <p>Variability and representability of network connectivity</p>

4. SUMMARY OF DECOVALEX STAGES I, II, AND III

(a) DECOVALEX I

In the DECOVALEX I project, modeling was conducted on three hypothetical BMTs and six TCs, involving three small laboratory tests of rock samples and fractures, and three large field tests. Details may be found in Jing et al. (1995). One of the BMTs simulated a Swedish KBS-3 disposal concept in a fractured granitic rock with a fracture network system and properties similar to those of the Stripa granite. This case will be presented in more detail in section 5.

(b) DECOVALEX II

In the second phase of the project, DECOVALEX II, studies were focused on two major large-scale *in situ* experiments, and also on evaluating how the studies conducted in the project could be applied to the performance and safety assessment of a potential repository. The following studies were undertaken:

- Task 1: Numerical study of NIREX's Rock Characterization Facility at Sellafield
- Task 2: Numerical study of the in-situ THM experiment in the Kamaishi Mine, Japan
- Task 3: Review of the state-of-the-art in constitutive relations of rock fractures
- Task 4: Current understanding on the coupled THM processes related to design and performance assessment of radioactive waste repositories.

Results of Task 1, 2, and 4 are presented in Stephansson et al. (2001). Of particular note is Task 1, under which an extensive data package on the geology, hydrology, and rock mechanics was distributed to the research teams, who were then free to select, develop, and parameterize their own conceptual models of the local site within the Sellafield system. One lesson learned from this procedure is the recognition of the significance of calibration procedures in predicting the response to pumping and shaft sinking. Another lesson learned is the importance, and also the difficulty, of performing the simulations assuming fully coupled processes. The simulations of the Kamaishi Mine heater experiment, Task 2, have also provided valuable experience in analyzing coupled THM processes in the near field of a waste canister-bentonite-rock system. Some details of this study are given in section 6.

(c) DECOVALEX III

In the third phase of the project, DECOVALEX III, the following tasks have been performed:

- Task 1: FEBEX experiment conducted by ENRESA in Grimsel Mines in Switzerland
- Task 2: The Drift Scale Test (DST) in the Exploratory Studies Facility (ESF) at Yucca Mountain, USA
- Task 3: Three benchmark tests about, (a) near-field repository performance (BMT1), (b) Material property homogenization and far-field repository performance (BMT2), and (c) Glaciation process effects on far-field repository performance (BMT3)

- Task 4: Survey and discussion of THM processes in performance assessment.

Below we shall give a brief description of these tasks, and detailed results are presented in some of the other chapters in this volume.

In the FEBEX experiment, a full-scale *in situ* experiment is being performed on a heater-buffer-rock system in the Grimsel Test Site in Switzerland, with a long period of heating followed by cooling. The aim of the project is to demonstrate the present capabilities for building bentonite barriers in conditions similar to actual repository design and providing monitoring data to understand coupled THM processes in the near field. A large quantity of monitoring data on stress, deformation, water content, water pressure, and temperature distributions and their histories were recorded at a large number of monitoring places *in situ*. Also, a large number of rock/buffer property parameters were measured in laboratory tests. Three subtasks are conducted within DECOVALEX III: (1) simulation of hydro-mechanical behavior in the fractured rock mass with respect to the tunnel excavation; (2) simulation of the THM processes of the heater-buffer system; and (3) simulation of coupled THM responses of the complete rock-buffer-heater system during the heating period. Ten research teams supported by nine national organizations participated in this task.

The second task, the Drift Scale Test (DST) in the Exploratory Studies Facility (ESF) at Yucca Mountain, is a large-scale thermal test conducted by the Yucca Mountain Site Characterization Office of the U. S. Department of Energy (DOE). It is part of DOE's program of characterizing the Yucca Mountain site to evaluate its suitability for a potential nuclear waste repository. The heating phase of the test started on December 3, 1997, and lasted for about four years, ending on January 14, 2002. The objective of the test is to help increase confidence in models of coupled THMC processes in the rock mass. These models will be employed to quantitatively assess the long-term performance of the potential repository. Heating is effected through nine cylindrical heaters placed on the floor of a 47.5 m drift and 50 wing heaters, each 10 m long, inserted into horizontal boreholes on either side of the drift. The purpose of this arrangement is to: (a) simulate the thermal field that an emplacement drift will experience from neighboring drifts, and (b) heat a large volume of rock mass to boiling temperatures within the experimental heating period of four years.

Processes occurring in the DST include heat and fluid flow in unsaturated fractured rocks; heat-pipe effects and other heat transfer mechanisms; effects of temperature on permeability and conductivity; THM changes in concrete lining; THM processes in unsaturated fractured rocks with the presence of drifts; effects of thermo-mechanical processes on hydrologic characteristics; chemical changes under air-water-vapor flow in fractured rock; changes in Eh and pH chemical reactions under phase change; and effects of dissolution and precipitation on hydrologic characteristics. Six research teams supported by six national organizations participated in this task.

Task 3 consists of three benchmark tests: BMT1, BMT2, and BMT3. BMT1 focuses on near-field behaviour of a hypothetical repository in fractured hard rock from excavation to post closure. Databases developed at the Kamaishi experiment were used for the detailed technical definition of the BMT, with repository geometry similar to that of the Kamaishi mine experiment. The main performance assessment (PA) measures were the resaturation progress in buffer and rock, the mechanical effects on buffer and waste form, and the mechanical stability of the repository. The thermo-hydro-mechanical evolution of the whole configuration is simulated over a period of 1000 years. Comparison of the results predicted by fully coupled THM analysis with those from partially coupled TH, TM, and HM analysis (in terms of several predefined indicators) identifies the couplings that play a crucial role with respect to safety issues. Six research teams supported by six national organizations participated in this study.

The BMT2 is on homogenization (originally proposed as an upscaling problem) concerns the relationship between an equivalent continuum (which could be heterogeneous) and detailed discrete representations of fractured rocks. A key issue is the extrapolation of rock properties obtained from small-scale tests and observations to a large repository scale, with analysis for uncertainties. The main focus is on the method of deriving flow and deformation properties of the fractured rocks as equivalent continua, and its impact on prediction of large-scale changes in flow and deformability fields. The database developed at Sellafield for Task 1 of DECOVALEX II is used for the detailed technical definition of the BMT2. Eight research teams supported by eight national organizations participated in this study.

Finally, the glaciation test, BMT3, concerns mainly the hydro-mechanical processes during a

cycle of glaciation and deglaciation for assessing the long-term performance (up to 100,000 years) of a hypothetical post-closure repository, without considering thermal effects. Many different alternative scenarios are included in the task, such as permafrost, different ice-rock interface conditions, 2D–3D transition, inland/coastal repository locations, or sea level changes. The main PA measures are the maximum deformation, changes in permeability fields, flow patterns and formation of critical flow paths, and groundwater pressure. Only long-lasting and large-scale changes in PA measures are significant. Four research teams supported by four national organizations participated in this study.

To better understand the relevance of THM coupling to PA and the associated uncertainties and the applicability ranges, Task 4 of DECOVALEX III was established as a platform for presentation, discussion, and documentation of the treatment of THM issues in the framework of PA analyses. The task contains two subtasks: (1) a state-of-the-art review on the current and past international treatment of THM issues in PA and (2) a forum on and documentation of THM treatment in the PA.

5. AN EXAMPLE OF A BMT STUDY

In this and next sections, we shall illustrate the type of research under DECOVALEX by two examples from DECOVALEX I and II, respectively. The first example is a BMT and the second example, a TC.

The nature of a BMT study is well demonstrated with BMT3 of the DECOVALEX I project. It was a problem associated with a near-field repository model, set up as a two-dimensional plane-strain problem in which a tunnel with a deposition hole was located in a fractured rock mass. The model is 50×50 m in size, and situated at 500 m below the ground level (Figure 1). The fracture network is a two-dimensional realization of 6,580 fractures from a realistic three-dimensional fracture network model of the Stripa Mine, Sweden (Figure 2). The problem is set up as a fully coupled THM near-field repository problem, with thermal effects caused by heat release from radioactive waste in the deposition hole (the heater). Heat output decreases exponentially with time. The rock matrix is assumed to be isotropic and linearly elastic, and its mechanical properties do not change with temperature variations. Its thermal conductivity and expansion are also assumed to be isotropic. The fractures are assumed to consist of parallel, planar,

smooth surfaces at the macroscopic level, with an effective hydraulic aperture.

The initial and boundary conditions for the mechanical, thermal, and hydraulic effects are shown in Figure 1, with heating maintained for 100 years. (See Table 2 for the research teams and codes applied to this study). Figure 3 shows the different representations and simplifications in the models used by the various teams. This BMT was regarded as an excellent model for testing the capabilities of many alternative mathematical models and computer codes (Stephansson et al., 1996).

The major findings from this BMT study include the following:

- This BMT was a well-defined near-field problem, with both a realistic fracture network (which may likely be encountered in practice) and complete aspects of coupled THM processes.
- Agreement in temperature results from all research teams was remarkable.
- Heat convection had negligible effects on the temperature results.

Figure 1. Definition of BMT3(DECVALEX I): Model geometry and boundary conditions

Figure 2. Reference fracture network from Stripa Mine for BMT3 (DECOVALEX I)

- Displacement results agreed reasonably well among the research teams and between discrete and continuum approaches. Large discrepancies occurred only when monitoring points are located on loose blocks with large movements, close to the boundary of the tunnel and the deposition hole.
- Stress results agree less well among the teams than the displacement results, especially at points closer to the heat source and tunnel boundary, although a consistent general trend in the stress results can be observed.
- The flow rate results were highly divergent, both between the discrete and continuum approaches and among models in the same approach group.

AEA (NAPSAC code, DFN model)
Complete and explicit representation of 6580 fractures by DFN method, without heat and rock deformation, but with analytical model for stress approximation	
CEA/DMT (CASTEM 2000 code, FEM model)
Equivalent continuum approach with FEM method (1344 elements, 4216 nodes), homogenization (scale 25 x 25 meters) by Crack Tensor theory (Oda, 1986)	
CNWRA (UDEC code, DEM model)
Vertical symmetry and simplified fracture network with 295 fractures, 337 blocks, 1540 finite difference elements, and 10853 nodes. A small inner region with random fractures and larger outer region with regular artificial fractures	
ITASCA (FLAC code, FDM model)
Equivalent continuum approach with FDM (735 finite difference elements and 792 nodes) without formal homogenization. Vertical symmetry and inhomogeneous permeability	
INERIS (UDEC code, DEM model)
Simplified fracture network with inner region of random fractures and outer regions of regular artificial fractures (564 fractures, 677 blocks, 24391 finite difference elements, and 16791 nodes)	
KPH (THAMES code, FEM model)
Equivalent continuum approach with FEM method (674 elements, 2127 nodes). Homogenization (scale 10 x 10 meters) by Crack Tensor theory (Oda, 1986). Heat convection considered	
NGI (UDEC code, DEM model)
Two models of vertical symmetry (one left half and one right half) with simplified fracture network without heating, about 512 fractures, 510 blocks, and 1580 finite difference elements	
VTT (UDEC code, DEM model)
Vertical symmetry (left half) with simplified fracture network, 814 fractures, 496 blocks, 1308 finite difference elements, and 2222 nodes.	

Figure 3. Different model representations and simplifications for BMT3 (DECOVALEX I)

Table 2. Research teams and codes applied to study BMT3 (the acronyms for the organizations are defined in Jing et al., 1995)		
Research team (Sponsor)	Code	Method
AEA (NIREX, UK)	NAPSAC	DFN – fracture flow only
CEA/DMT (ANDRA, France; CEC)	CASTEM 2000	FEM – homogenization scale 25 m
CNWRA (NRC, USA)	UDEC	Dem with simplified fracture network
INERIS (ANDRA, France; CEC)	UDEC	DEM with simplified fracture network
ITASCA (SKB, Sweden)	FLAC	FDM without homogenization
KPH (PNC, Japan)	THAMES	FEM – homogenization scale 10 m
NGI (NIREX, UK)	UDEC	DEM with simplified fracture network
VTT (STUK, Finland)	UDEC	DEM with simplified fracture network

- Two homogenization scales were obtained by two teams using the same Crack Tensor theory, and the validity of representative elementary volume (REV) and its relationship to the size of finite element are unresolved, and remain an open problem.

6. AN EXAMPLE OF A TEST CASE STUDY

In this section, we present an example of a test case study to illustrate DECOVALEX activities. Task 2 of the DECOVALEX II project was the numerical modeling of the *in situ* THM experiment of a fractured rock-buffer-heater system at Kamaishi Mine, Japan (Figure 4). The Kamaishi Heater Test was an experiment conducted in a $5 \times 7 \text{ m}^2$ alcove excavated from an existing drift, located at a depth of about 250 m. In 1995, a vertical test pit, 1.7 m in diameter and 5 m in depth, was drilled into the floor of the alcove (Figure 5). The hole was drilled with a gentle shot boring method, using a large-diameter boring machine to avoid mechanical disturbance of the rock. In 1996, an electric heater was installed into the test pit and surrounded by a buffer of bentonite clay. Bentonite was placed into the test pit in layers of 0.1 m, with compaction of each layer to a dry density of about 1.6 ton/m^3 . After the entire test pit was filled with bentonite, a watertight concrete lid was placed on the drift floor, which in turn was supported by steel bars from the ceiling of the drift. Because the rock was not fully saturated

immediately around the test pit, a flooding pool was set up on the drift floor above the test pit. At the end of 1996, the heater was turned on and the temperature was set to 100°C for 8.5 months, followed by a 6-month cooling period. System responses, including temperature, moisture content, fluid pressure, stress, strain and displacement, were measured in both the bentonite and surrounding rock mass. The experiment was completed in early 1998, and thereafter the monitoring sensors were recovered and recalibrated.

The task for the DECOVALEX research teams was to predict the THM effects in the buffer material inside the test pit and in the surrounding rock, both during excavation of the test pit and the heater testing. The test case was divided into three main tasks: Tasks 2A, 2B, and 2C. Task 2A was to predict the HM effects in the rock caused by the excavation of the test pit. Geometrical, mechanical and hydraulic rock properties, as well as hydraulic conditions before excavation, were given to the research teams, and they were asked to predict water inflow distribution in the test pit. Task 2B was a model calibration of rock and fracture properties and the hydromechanical boundary conditions, based on actual measured results predicted in Task 2A. Task 2C was to predict the THM effects in the rock and buffer during the heating experiment. The rock model was presumed to have properties based on the calibration in Task 2B, with the calibrated permeability distribution in the near-field rock. At

Figure 4. Location of the Kamaishi Main in Japan (a) and a 3D view of the test site in Kamaishi Main (b)

they are highly conductive and dominated the flow of water into the open test pit. The rock in between the main fractures is highly fractured (spacing 0.1 to 0.3 m) but has a much smaller hydraulic conductivity and was represented by an equivalent continuum. AECB, CLAY and KPIH teams reduced the size of their models and the drift system. One reason for doing this was the computer-intensive nature of the problem, which includes a year of simulation time and coupling of highly nonlinear processes in five degrees of freedom per nodal point

A smaller model can also be justified if interest is limited to the behavior of the clay-buffer, and if the effect of the far-field rock mass can be represented by the boundary conditions on the near-field model. The axisymmetric geometry used in AECB and KPIH models was motivated through an exploratory two-dimensional modeling, with results showing that the resaturation of the bentonite buffer by wetting from the surrounding rock was uniform and axisymmetric, thus making it unnecessary to include discrete fractures in the model. The CLAY model is one-quarter symmetric.

There are many challenges facing the research teams for the study of this task, such as limitations in the different “effective stress” principles for the bentonite material under complex loading conditions; the uncertainty of the hydraulic boundary and the *in situ* conditions; and the complex and largely unknown *in situ* fracture properties (both geometrical and hydromechanical).

There were many scientific and operative lessons learned from the study, including the following:

- First of all, an in-depth understanding of THM processes in the heater-bentonite-rock system was obtained through the study of the Kamaishi experiment. Model results, when compared with test data, show that all the major THM processes involved in the system have been identified and their behavior described.
- The main limitations of current capability of modeling coupled HM processes in fractured rocks are a lack of knowledge about fracture geometry and uncertainty in *in situ* properties.
- Despite great progress in characterization and parameterization of bentonite, models and knowledge of the physical behavior of partially saturated swelling clays still need improvement in areas such as the effective stress behavior, vapor flow, and water retention.

- Our current knowledge of the rock-buffer interaction, especially the hydraulic interactions with the presence of rock fractures is limited and requires more study.
- In the Kamaishi experiment, very limited effect on the hydraulic behavior of the buffer from the surrounding rock and fractures could be observed. This may have resulted from the following:
 - a) The *in situ* experiment was not maintained long enough such that possible larger hydro-mechanical interaction between the rock and buffer at the longer period could be observed.
 - b) The hydraulic conductivity of the rock is much higher than that of the buffer, so that whether or not fractures in the rock were considered did not result in much difference in the hydraulic behavior of the buffer.
 - c) The rock fractures near the buffer might have been sealed by buffer material during installation of the buffer material.
- Also in the Kamaishi experiment, very limited mechanical effect on the buffer from the surrounding rock was observed, which may have resulted from
 - a) The low stress magnitudes in the test area, which make the rock and rock fractures mechanically inactive, besides the fact that thermal expansion and stresses induced by heating have also only a limited effect due to low power input and small magnitudes of the temperature gradient
 - b) Point-wise measurement of mechanical behavior, which may not be nearly enough to capture essential aspects and patterns of the mechanical responses.

7. CONCLUDING REMARKS

The DECOVALEX project has played a key role in advancing coupled THM models of geomaterials and their testing against field experiments over the last ten years or so. New and sophisticated models have been developed to simulate coupled THM processes in heater-bentonite-rock systems. Their intercomparison through BMT studies, as well as their testing against major field tests in Europe, Japan and the U.S., has provided substantial insight into the effects and impacts on the coupled THM processes of a geological nuclear waste repository. It

also gives us an understanding of our modeling capabilities, i.e., what we can and cannot predict well. The international cooperation under the DECOVALEX organizational framework has been very effective and profitable to all participants. Research teams have been able to share the results of very expensive major field experiments, as well as continually provide detailed ideas, technical suggestions, and peer review to each other's work. Such unique in-depth cooperation among multiple national teams has proved to be beneficial to all involved.

On a more general level, it can be seen from all the chapters of this volume, that substantial progress has been made in coupled THM processes in many related fields in the geosciences, ranging from nuclear waste isolation, to geothermal HDR energy extraction, civil engineering, mining projects, and petroleum reservoir dynamics. On the one hand, many challenging and important research issues remain, and interactions and discussions across

these fields will be most useful. On the other hand, significant advances already made over the last decade have enabled us to model the relevant basic physics behind the coupled processes, and have allowed us to simulate these processes in realistic complex geologic systems. Now we are in a good position to study and evaluate the behavior of such complex systems under various THM scenarios relevant to practical applications.

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