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February 2005

Foreword

DECOVALEX is an international consortium of governmental agencies associated with the disposal of high-level nuclear waste in a number of countries. The consortium's mission is the DEvelopment of COupled models and their VALidation against EXperiments. Hence theacronym/name DECOVALEX. Currently, agencies from Canada, Finland, France, Germany, Japan, Spain, Switzerland, Sweden, United Kingdom, and the United States are in DECOVALEX. Emplacement of nuclear waste in a repository in geologic media causes a number of physical processes to be intensified in the surrounding rock mass due to the decay heat from the waste. The four main processes of concern are thermal, hydrological, mechanical and chemical. Interactions or coupling between these heat-driven processes must be taken into account in modeling the performance of the repository for such modeling to be meaningful and reliable.

The first DECOVALEX project, begun in 1992 and completed in 1996 was aimed at modeling benchmark problems and validation by laboratory experiments. DECOVALEX II, started in 1996, built on the experience gained in DECOVALEX I by modeling larger tests conducted in the field. DECOVALEX III, started in 1999 following the completion of DECOVALEX II, is organized around four tasks. The FEBEX (Full-scale Engineered Barriers EXperiment) in situ experiment being conducted at the Grimsel site in Switzerland is to be simulated and analyzed in Task 1. Task 2, centered around the Drift Scale Test (DST) at Yucca Mountain in Nevada, USA, has several sub-tasks (Task 2A, Task 2B, Task 2C and Task 2D) to investigate a number of the coupled processes in the DST. Task 3 studies three benchmark problems: a) the effects of thermal-hydrologic-mechanical (THM) coupling on the performance of the near-field of a nuclear waste repository (BMT1); b) the effect of upscaling THM processes on the results of performance assessment (BMT2); and c) the effect of glaciation on rock mass behavior (BMT3). Task 4 is on the direct application of THM coupled process modeling in the performance assessment of nuclear waste repositories in geologic media.

This executive summary presents the motivation, structure, objectives, approaches, and the highlights of the main achievements and outstanding issues of the tasks studied in the DECOVALEX III project. The main sources of the materials came from summaries of the individual tasks prepared by the respective task force group leaders. They are:

Task 1 (Chapter 2): E. Alonso and J. Alcoverro
Task 2 (Chapter 3): R. Data and D. Barr
Task 3-BMT1 (Chapter 4): T. S. Nguyen and L. Jing
Task 3-BMT2 (Chapter 5): J. Andersson and J. L. Knight
Task 3-BMT3 (Chapter 6): T. Chan and R. Christiansson
Task 4 (Chapter 7): J. Andersson

The editors of this summary, together with the Steering Committee of the DECOVALEX III project, feel very encouraged by the progresses which have been made during the project time and very positive about the usefulness of the achievements reached by the project to the larger international community of scientific research and management of radioactive wastes in different countries. A new phase of the DECOVALEX project, DECOVALEX-THMC, is under preparation and we sincerely hope that the continued efforts will advance the science and improve the numerical tools so that the disposal of radioactive waste could be managed on a more reliable scientific basis.

L. Jing, F. Kautsky, J.-C. Mayor, O. Stephansson and C.-F. Tsang

Stockholm
January 2005

Summary

This report is an executive summary of the works performed for the international co-operative research project DECOVALEX III (1999-2002). The report is divided into seven chapters. Chapter 1 provides a brief introduction to the project's goals, organizations, task definitions, implementation steps, overall achievements and lessons learned. The rest of the chapters are devoted to executive summaries of individual tasks covering mainly the case definitions, objectives, participating organizations and research teams, the tools and approaches applied, main achievements and the lessons learned with outstanding issues for future studies.

Content

1. Introduction

The DECOVALEX III project is the third stage of an ongoing international co-operative project to support the development of mathematical models of coupled Thermal (T), Hydrological (H) and Mechanical (M) processes in fractured geological media for potential nuclear fuel waste repositories. During the first stage (May 1992 to March 1995), called DECOVALEX I, the main objective was to develop computer codes for coupled T-H-M processes and their verification against small-scale laboratory or field experiments. In the second stage, called DECOVALEX II, the main objective was to further develop and verify the computer codes developed in DECOVALEX I against two large-scale field tests with multiple prediction-calibration cycles, the pump test at the Sellafiled, UK, with a hypothetical shaft excavation and the in-situ THM experiment at the Kamaishi Mine, Japan. The DECOVALEX III project is the third phase of the DECOVALEX project series and was run through the period of 1999-2003.

The DECOVALEX III project is initiated with two main objectives. The first is the further verification of computer codes by simulating two additional large scale in-situ experiments: the FEBEX T-H-M experiment performed in Grimsel, Switzerland, designated as Task 1, and the drift scale heater test at Yucca Mountain, Nevada, USA, designated as Task 2. The second objective is to determine the relevance of THM processes on the safety of a repository.

To achieve the second objective of DECOVALEX III project, three benchmark tests (BMT) are proposed to examine the relevance of THM processes to performance and safety assessments: 1) BMT1: the impact of THM processes in the near-field of a hypothetical repository in fractured hard rocks; 2) BMT2: homogenisation and upscaling of hydro-mechanical properties of fractured rocks and their impact on far-field performance and safety assessments; and 3) BMT3: Impact of glaciation process on far-field performance and safety assessments. These three BMTs are designated as Task 3.

An additional Task 4 was also organized to present the states of the current understandings on the impacts and treatments of the THM issues on PA and SA of nuclear waste repositories, from the views of the Funding organizations of the project, through compilation of answers to a questionnaire prepared for this purpose.

On September 25, 2000 the European Commission (EC) signed a contract of FIKW-CT2000-00066 "BENCHPAR" project with a group of European members of the DECOVALEX III project. The BENCHPAR project stands for ´Benchmark Tests and Guidance on Coupled Processes for Performance Assessment of Nuclear Waste Repositories´ and is aimed at improving the understanding to the impact of the thermo-hydro-mechanical (THM) coupled processes on the radioactive waste repository performance and safety assessment. The project has eight principal contractors, all members of the DECOVALEX III project, and four assistant contractors from universities and research organisations.The project is designed to advance the state-of-the-art via five Work Packages (WP). In WP 1 is establishing a technical auditing methodology for overseeing the modeling work. WP´s 2-4 are identical with the three bench mark tests (BMT1 - BMT3) in DECOVALEX III project. A guidance document outlining how to include the THM processes in performance assessment (PA) studies will be developed in WP 5 which explains the issues and the technical methodology, presents the three demonstration PA modeling studies, and provides guidance for inclusion of the THM components in PA modeling.

Tables 1.1 and1.2 list the Funding Organizations and their research teams of the Project. Figure 1.1 shows the organization of the project.

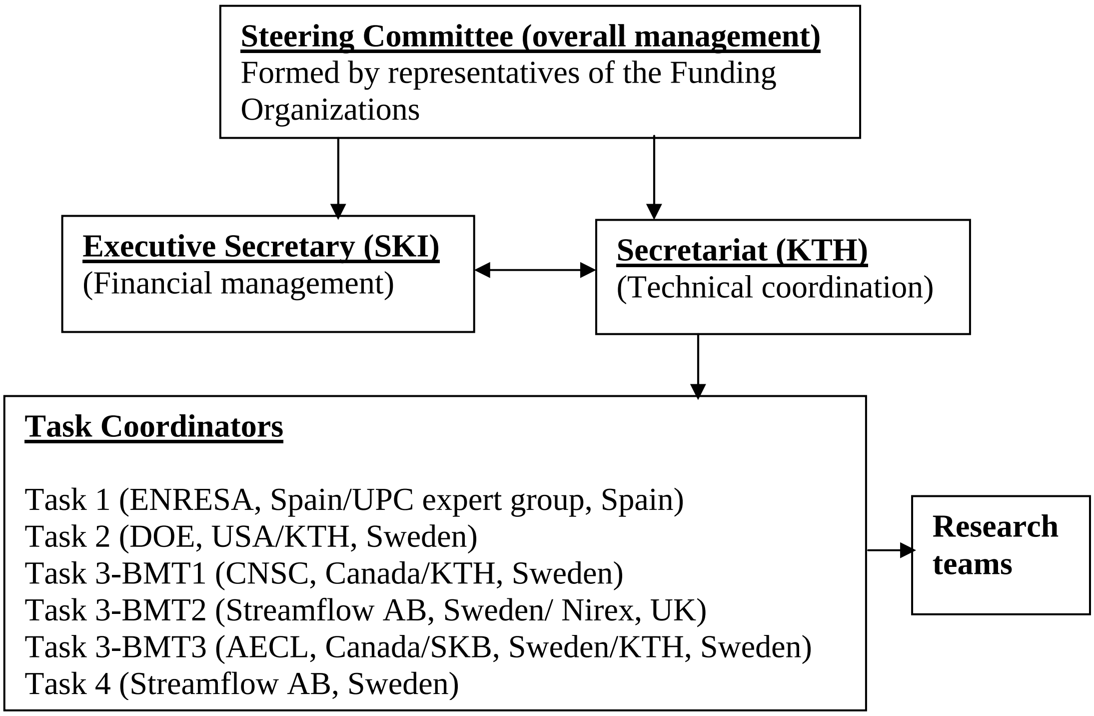


Figure 1.1: Organization of the DECOVALEX III Project. See Tables 1.1 and 1.2 for the acronyms of the organizations.

Table 1.1. Funding organizations of the project

Funding Organizations (Acronyms)	**Acronym**
National Agency for Radioactive Waste Management, France	ANDRA
Federal Institute for Geosciences and Natural Resources, Germany	BGR
Commisariat a l'Energi Atomique de Cadarache, France	CEA
Canadian Nuclear Safety Commission, Canada	CNSC
US Department of Energy, USA	DOE
Empresa Nacional de Residoos Radioactivds, S. A., Spain	ENRESA
European Commission (through BENCHPAR project)	EU
Institute for Protection and Nuclear Safety, France	IRSN
Japan Nuclear Cycle Development Institute, Japan	JNC
United Kingdom Nirex Ltd., UK	NIREX
Nuclear Regulatory Commission, USA	NRC
Ontario Power Generation, Canada	OPG
Swedish Nuclear Fuel and Waste Management Co., Sweden	SKB
Swedish Nuclear Power Inspectorate, Sweden	SKI
Radiation and Nuclear Safety Authority, Finland	STU

Table 1.2. Research Teams of the project

F.O.	**Research team**	**Tasks studied**
ANDRA	INERIS-LAEGO, Ecole des Mines de Nancy, France; Ecole Polytechnique, G3S, France	Task 1; BMT2 Task 1
BGR	University of Tuebingen, Germany; University of Hannover, Germany; Federal Institute for Geosciences and Natural Resources, Germany	BMT2; BMT2; Task 1
CEA	CEA/DM25/SEMT, France	Task 2
CNSC	Canadian Nuclear Safety Commission, Canada	Task1, BMT2
DOE	Sandia National Laboratory, USA; Lawrence Berkeley National Laboratory, USA	Task 1; BMT2
ENRESA	Universidad Politecnica de Catalunya, Spain Universidad Politecnica de Valencia, Spain	Task 2; BMT2
EU (through the BENCHPAR Project)	University of Edinburgh, UK; Royal Institute of Technology, Sweden; INERIS-LAEGO, Ecole des Mines de Nancy, France; Universidad Politecnica de Valencia, Spain; CEA/DM25/SEMT, France Chalmers University of Technology, Swedeb	BMT3; BMT1; BMT2 BMT2; BMT1; BMT1; BMT3
IRSN	Paris School of Mines, France CEA/DM25/SEMT, France	Task 1; BMT1
JNC	Tokai Works, JNC, Japan; Hazama Corporation, Japan; Kyoto University, Japan	Task 1, Task 2, BMT1, BMT2 BMT1, BMT2
NIREX	University of Birmingham, UK	BMT2
NRC	CNWRA, Southwest Research Institute, USA	Task 2
OPG	Atomic Energy of Canada, Ltd., Canada	BMT2, BMT3
SKB	Chalmers University of Technology, Sweden Clay technology AB, Sweden	BMT3; Task 1
SKI	Lawrence Berkeley National Laboratory, USA Royal Institute of Technology (KTH), Sweden	Task 1; BMT1, BMT2
STUK	Technical University of Helsinki, Finland Uppsala University, Sweden	Task 1, BMT3; BMT2

During the project time six workshops and many task force meetings were held and numerous reports were generated reporting progresses in research. Near the end of the project an international conference on coupled THMC processes in geological systems, GeoProc 2003, at Royal Institute of Technology (KTH), Stockholm, Sweden, on Oct.

13-15, 2003 (Stephansson et al., 2003). Besides the presentations of research results from the teams of the DECOVALEX III and BENCHPAR projects, a large number of high quality papers in the fields of numerical modelling of nuclear waste disposal, oil/gas reservoirs, geothermal energy extraction, geological systems, coal mining, geotechnical engineering, environmental engineering and, fundamental researches about coupled THMC processes in different geo-materials and geo-systems. The conference is the first of such academic gatherings in the specific field of coupled THMC processes in geo-systems that would be continued in 2005 in China.

This executive summary is a presentation of the overall activities of the project, the scientific achievements and the outstanding issues as needs for further scientific investigations, one chapter for each task or BMT.

2 Executive summary-Task 1

This summary presents a general view of the contents, objectives, scientific achievements and outstanding issues of the Task 1 of the DECOVALEX III Project, based on the reports and papers listed in the references at the end of this chapter. The technical details of the modelling approaches, governing equations, material models and main features in results can be found in the progress reports (Alonso and Alcoverro, 2003a, b & c), and papers published on the international Conference of GeoProc 2003 (Alonso & Alcoverro, 2003d; Jussila, 2003; Merrien-Soukatchoff et al., 2003; Nguyen et al., 2003; Nowak et al., 2003; Rutqvist et al., 2003; Rutqvist & Tsang, 2003; Sobolik et al., 2003 and Sugita et al., 2003).

2.1. Case definition and objectives

The international FEBEX (Full-scale Engineered Barriers Experiment in Crystalline Host Rock) project, co-financed by ENRESA and the European Commission has been in operation from 1994 to 2003. The purpose of the project is the study of the various processes occurring in the near field of a high activity radioactive waste storage.

The experiment is 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 the 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 left between them. The engineered barrier is made of high density compacted bentonite blocks that will swell due to water input from the host rock, providing thus a very impervious sealing. In the FEBEX "in situ" test, the waste canisters were replaced with two cylindrical heaters.

Due to the detailed geological and hydrogeological characterization of the Grimsel Test Site, the comprehensive characterization of the bentonite used to fabricate the engineered barrier and the monitoring performed during the drilling of the FEBEX tunnel as well as during the test, the FEBEX "in situ" test was selected as a modelling exercise for DECOVALEX III. Figure 2.1 shows a perspective of the FEBEX drift and associated boreholes.

The modelling exercise was divided into three parts: Part A – hydro-mechanical modelling of the rock; Part B – thermo-hydro-mechanical modelling of the bentonite; and Part C – thermo-hydro-mechanical modelling of the rock, as described bellow.

2.1.1. Part A: Hydro-Mechanical modelling 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 on boreholes, a hydro-mechanical model for the zone around the FEBEX tunnel will be 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 excavated tunnel will be required.

Two types of measurements have been selected to develop the modelling exercise: the actual water inflow rates into the FEBEX tunnel and the water pressure response in the vicinity of the tunnel outer perimeter against the tunnel excavation by a Tunnel Boring Machine

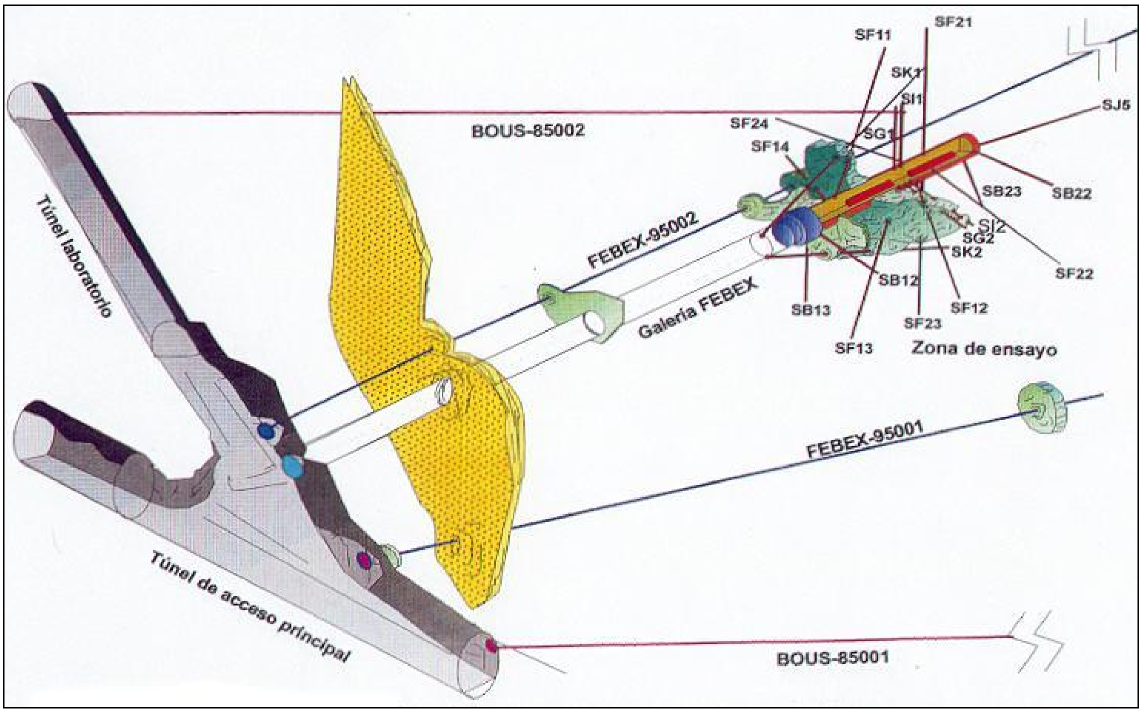


Figure 2.1: Layout of FEBEX test and associated boreholes.

Flow measurements into the tunnel provide an integrated variable, controlled by the problem geometry, rock mass fracture pattern, fracture anisotropy, rock matrix permeability and boundary conditions.

The second part asked for a prediction of the transient changes in water pressure recorded at two borehole intervals in the close proximity of the advancing tunnel. The pore water pressure record exhibited a marked transient behaviour when the tunnel face was close to the measuring section of the borehole. This transient behaviour was characterized (in one of the measuring segments) by a rather sharp increase in pressure followed by a slow decay as the tunnel moved away from the measuring section.

This behavior 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. Total water inflow in the test zone (which extends along 17.40 m along tunnel axis) was measured by two techniques (absorbing pads on selected points of the tunnel wall and small gauge measuring of overall leaked water) at different dates in the period January-May 1996, once the tunnel was fully excavated. With this information, it was possible to know the distribution of water input flow on the wall of the FEBEX tunnel.

2.1.2. Part B: Thermo-Hydro-Mechanical Analysis of the Bentonite Behaviour

Based on the characterization of the bentonite and on the process of test installation, a T-H-M model for the bentonite barrier and the heaters will be prepared. Using this model, the thermo-hydro-mechanical response of the bentonite barrier as a result of the heat released by the heaters will be required. Besides local field variables such as temperature, relative humidity, pore water pressure, stresses and displacements and global variables such as total input power to the heaters will also be required.

The performance of the test and the comparison with modeler's predictions was based on the following variables:

- The evolution of the total heating power of one of the heaters. The starting time will be the "day 53" which corresponds to the beginning of the automatic control, once the hottest point at the contact between the heater and the bentonite has reached 100ºC. The heating power is a global performance variable which integrates the changing thermal conduction coefficient of the bentonite as the barrier experiences water content changes
- The distribution and evolution of relative humidity of the bentonite barrier. This is a key variable of the experiment since it shows the effects of inner heating and outer hydration from a host rock in a direct manner. Relative humidity variations are the result of water transport processes in liquid and vapour form. Two locations have been selected to show the radial distribution of RH: Section E1 which affects the heater directly, and section H that is a centered section located between the two heaters. The evolution in time of RH is examined in three points at increasing radial distance (in both sections E1 and H): a point close to the heater, "H", a mid point, "C" and a point close to the granite wall, "G".
- Temperature. Field information on temperature is vast but it offers limited information on other relevant physical processes and it is essentially controlled by conduction phenomena. Couplings do not affect temperature in a significant way and experience indicates that predictions with most models lead to accurate results. Therefore, the comparison between measurements and temperature predictions will be made in one section (D1) in radial direction.
- Radial stress evolution at some points located at different radial distances in section E2. Measurement errors are often likely in the case of (normal) stresses. In addition, heterogeneous stress distributions and large variations over short distances are possible. Nevertheless the cells installed offered also an interesting field information to the development of swelling-induced stresses inside the barrier

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

Based on the characterization of the rock massif and on the details of the process of test installation and performance, the rock response in the immediate vicinity of the buffer will be required. The rock is now subjected to the heat released by heaters and by swelling pressures resulting from bentonite hydration. The initial hydrological regime (Part A) is also modified by the presence of the impervious barrier. Temperature, stresses, water pressures and displacements in selected points of the rock will be required.

Several instruments were located, at increasing depth, in the auxiliary boreholes. The length of these radial boreholes does not exceed 15m. Typically, readings are available in three or four positions: close to the tunnel wall (say at 1-3m distance from the origin of the boring, one or two intermediate distances and a distant position (13-14m deep))

Data is available on the following variables: temperature, water pressure in rock, water pressure in packers, stress state and radial displacements.

Water pressure was measured in some boring intervals (a few meters long) separated by packers. The rubber packers were also filled with water and their pressure was maintained and measured externally. Water pressure gauges are located in the measuring area of the FEBEX tunnel. They are connected with the measuring intervals by means of steel tubing.

Three normal components of stress are measured by means of total pressure cells. Four sets of 3 cells were prepared and grouted "in situ" in boreholes SG1 and SG2. Each cell had five sensors oriented in different directions and fixed on a common support 2 m long. Each one of the sensors was a circular steel flat cell. An interpretation of the five readings provides the normal stress components in three directions: radial (with respect to the tunnel axis) (σr), axial (along the direction of tunnel axis) (σx) and circumferential (normal to the radial direction (σθ). Once the sets were in position the borehole was filled with a slightly expansive mortar. Once the mortar was cured, cells were pressurized against the mass of surrounding mortar to guarantee a good initial contact. Note that this procedure provides increments of stress over the moment of cell installation. It will record therefore stress increments due to the 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 borings SI1 and SI2. They were located close to the position of the stress cells. Each extensometer consists of graphite rods with independent anchoring points located at a depth of 1.0, 3.0 and 7.0 m into the borehole.

2.2. Participating organizations and research teams

Ten modelling teams, as detailed in Table 2.1, have participated in Task 1 of DECOVALEX III. The acronym of the Founding Organization (F.O.) is also indicated.

In order to organize presentations and comparison reports, a unique 3-character code and a unique symbol was assigned to each participant (Modelling Team). Moreover, a 3-character code and a unique symbol is also assigned to the co-ordinator. The symbol and code of the co-ordinator will be used to identify the experimental data in comparison plots. When possible, a colour (shared by 2 participants) will be used to enhance contrast among curves plotted together. Both the co-ordinator and the participants will use their own code to construct the name of the files to be sent by them. The list with the codes, symbols and colours is given Table 2.1.

Some minor changes in participation took place during the development of the Project. In Part A all the teams included in Table 2.1, except BGR and STUK, participated. In Part B all the working teams, except ANN were active. In Part C, ANN and STUK did not participate.

2.3. Summary of results

2.3.1 Conclusions for Part A

Widely different models for water inflow were used. Some teams (ANN, CNS, and SKB) used uncoupled hydraulic transient models to solve the first part of the exercise, whereas others (ANG, DOE, SKI) used a coupled HM modelling. It does not seem that the mechanical coupling introduces any advantage in this case. In fact, the reason for some of the better predictions (such as SKB calculation) may be associated with previous calibration of the model using other hydraulic data in the same area. Some models describe water circulation in the rock by means of discrete features (tubes, channels such as ANN) equivalent porous medium for different zones (such as DOE,

Table 2.1 Codes, symbols and colours assigned to participants and co-ordinator.

F. O.	**Participant (Modelling Team)**	**Code**	**Symbol**	**Colour**
ANDRA	National Agency for Radioactive Waste Management (G3S-EP), France	ANG	■	red
ANDRA	National Agency for Radioactive Waste Management (LAEGO-EMN), France	ANN	□	red
BGR	Federal Institute for Geosciences and Natural Resources, Germany	BGR	◆	green
CNSC	Canadian Nuclear Safety Commission, Canada	CNS	◇	green
DOE	US Department of Energy, USA	DOE	▲	blue
IPSN	Institute for Protection and Nuclear Safety, France	IPS	△	blue
JNC	Japan Nuclear Cycle Development Institute, Japan	JNC	⊠	brown
SKB	Swedish Nuclear Fuel and Waste Management Co., Sweden	SKB	∷	black
SKI	Swedish Nuclear Power Inspectorate, Sweden	SKI	+	black
STUK	Radiation and Nuclear Safety Authority, Finland	STU	●	orange
	Technical University of Catalonia, Spain (co-ordinator)	UPC	○	orange

SKI) and others combine porous medium and discrete fractures (ANG, CNS, SKB). The overall results do not show a particular advantage of a 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.

Pore water pressure changes in the vicinity of the tunnel excavation are a direct consequence of changes in the volumetric strain of the rock. Later, pore water pressure dissipations are a consequence of the transition flow towards a new equilibrium, which now has a modified boundary condition (the tunnel surface) in the vicinity. Therefore, fully coupled hydro-mechanical analyses are required to try to capture actual measurements. In fact, one-way coupling (hydraulic parameters updated as the rock mass deforms) is not capable of reproducing the observed behaviour.

However, the case has demonstrated that even if a fully HM coupled model is used, the difficulties to capture the actual pore pressure of the granitic mass are very high. It was well established that the volumetric behaviour of the rock in the vicinity of the tunnel depends critically on two aspects: the orientation and the intensity of the initial stress field. “In situ” stresses show often a large variability. Field determinations at Grimsel suggest that the major principal stress at the location of the FEBEX tunnel is horizontal (around 30 MPa), whereas the minor principal stress may be considered vertical and defined by geostatic conditions (around 10 MPa). The intermediate principal stress, also horizontal, may reach intermediate (around 15 MPa) values, but remains substantially higher than the vertical stress. It was shown that this particular distribution of initial stress leads to results which are opposite in trend to the actual measurements (dilation of the rock, instead of compression is computed at the P4 locations). In order to match the actual measurements, changes in the intensity of the vertical stress and on the direction of principal horizontal stresses had to be introduced. Moreover, the same initial stress field does not seem to be valid to reproduce results at P3 and P4. It should be added that local conditions at P3 and P4 do not seem to be the same since a more previous zone (which reduces the trend for a rapid initial increase in pore pressure) is present in P3. The finite length of the measuring intervals allows also an easy connectivity between pervious and impervious zones.

2.3.2 Conclusions for Part B

Only a reduced number of modeling teams participated in the blind prediction of Part B. As shown in the comparisons of RH and stress variables only three teams (CNS, SKB and SKI) were able to provide predictions for the full exercise. Modeling teams who used a 1D coupled model (IPS) provided approximate results for cases, which could be approximated by a radial symmetry. This is the case of sections normal to the test axis at the center of each one of the heaters. Models prepared to solve only the Thermo-hydraulic part of the problem (BGR) could not provide predictions for stress development. In some of the models, (BGR, IPS) phase change and vapor transfer was not considered and this limitation hampered the correct reproduction of measured variables. In fact, vapor transfer plays a dominant role in the early stages of the test.

The three fully coupled models (CNS, SKI, and SKB) behaved in general terms in a quite satisfactory manner. They predicted quite accurately the evolution of relative humidities inside the barrier. Stress prediction, however, has proved to be a more difficult task. There is always some concern about the actual reliability of measuring procedures. It appears that the measured radial stresses, which are essentially induced by the progressive hydration of the bentonite, are higher and develop faster than predictions, especially at the end of the considered period.

2.3.3 Conclusions for Part C

As in Part B, only a reduced number of modelling teams provided blind predictions for the rock behavior, once the expansive bentonite barrier was in place. Coupled THM models are also required for this part of the Benchmark although the temperature increase plays a dominant effect on the rock behavior. As it is frequently the case, temperature changes are well reproduced in general terms. Rock water pressures development integrates two separate phenomena: the modification of the hydrogeological regime in the vicinity of the tunnel due to the presence of the barrier and the temperature effects. Temperature effects, in turn, depend on a number of rock properties: rock dilation coefficient, porosity, stiffnes and permeability. The actual development of excess pore pressures are additionally controlled by the rate of temperature change and by the general drainage conditions in the area. It has been suggested that the limited transient reaction of the pore water pressure in the Grimsel host rock is a natural consequence of the high permeability of the rock and, to a lesser extent, of the averaging effect of the measuring interval (a few meters of borehole). The records of packer water pressures have provided interesting complementary evidence of the transient pore water pressure development. Also, the evolution of total stresses, 3 m away from the tunnel wall, shows a transient initial peak which has also been attributed to excess pore water pressure behavior.

Long-term water pressures increase slowly with time in the tunnel immediate vicinity (a few meters). Measured water pressures after 1000 days of test operation are, however, relatively small (1MPa).

Very small incremental displacements were recorded in the 1000-day period (a tenth of a millimetre in 4 and 8m long intervals).

Rock water pressures were reasonably well predicted by three of the research teams (IPS, DOE, and SKI). More limited success was achieved in the prediction of stresses and displacements, with the exception of SKI.

2.4. Summary of scientific achievements of the task

The FEBEX test is one of the few large-scale tests available to gain an integrated perspective of the behaviour of 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 six years. Part of this data, the data corresponding to the first three years of heating, has been used to conduct Task 1 of Decovalex III. The capabilities of a number of finite element codes developed to handle coupled problems in geological and porous media have been evaluated.

For the purposes of the organization of the exercise into specific tasks the Benchmark was divided into three main parts: A: Rock behaviour during the excavation of the FEBEX tunnel, B: Buffer behaviour and C: Rock behaviour during the heating and (partial) hydration of the buffer. This distribution has been maintained in this Report.

Specific conclusions for each of the mentioned parts have been given before. Only a few concluding remarks will be added here:

- The best predictions of the water inflow into the excavated tunnel are found when the hydrogeological model is properly calibrated on the basis of other known flow measurements in the same area. The particular idealization of the rock mass (equivalent porous media, discrete fractures) plays a secondary role
- The development and dissipation of excess pore water pressures in the vicinity of the advancing tunnel (at the time of the FEBEX tunnel excavation) was a clear example of hydro-mechanical interaction. It was concluded that the development of pore pressures was controlled by the initial stress field state, by the rate of excavation and by the permeability and drainage properties of the granite. However, the available information on the intensity and direction of principal stresses in the area was found inconsistent with the actual measurements. The problem posed by this discrepancy was essentially unsettled since a precise determination of the initial stress state in the vicinity of the FEBEX tunnel was not available.
- Predicting the behaviour of the buffer under the combined heating and wetting actions requires a fully coupled THM formulation, which incorporates all the necessary physical processes controlling the bentonite behaviour. Only a partial set of codes could offer the required features. Particularly relevant to predict the early stages of heating was the inclusion of phase changes of water and the vapour transport. Codes incorporating these features were capable of making good predictions. It should be added that the FEBEX in situ test benefits from a comprehensive experimental information on compacted bentonite properties derived from a large variety of laboratory tests on samples and on small-scale hydration and heating cells.

- It has been shown that the hydration of the bentonite buffer was essentially independent of the heterogeneous nature of the rock hydraulic conductivity features. This is explained by the fact that the rock matrix permeability is higher than the saturated bentonite permeability. Some 3D analyses performed, where the heterogeneous permeability features of the rock have been included, tend to support also this conclusion.
- The heating of the rock resulted in a significant increase in rock stresses in the vicinity of the FEBEX tunnel. Water pressures remained however essentially unchanged. The relatively high rock permeability explains the absence of significant pore water pressure transients. Only one of the participating modelling teams was capable of achieving a consistent prediction of all the measured variables in the rock: temperature, water pressures, rock stresses and radial displacements

2.5. Lessons learned and outstanding issues

The previous section summarizes some of the most relevant findings of the project. They have a specific character. It is possible also to adopt a more general perspective to evaluate the project. As a general introductory statement, the entire project was a learning process experience for all the involved participants. Some of the physical explanations found for specific measurements (i.e. the development of pore water pressures in the granite when the Febex tunnel was excavated) or the progressive improvement of THM codes are aspects of this process.

A second general comment concerns the character of “blind prediction”, which was a pre-requisite for the organization of the work. It turned out that a true prediction (which is, by nature, blind) is difficult to make even if a highly controlled and documented case record (such as Febex) is chosen for benchmark exercises. It is a fact that “predictions” become more and more accurate as the answer to the problem, i.e. the real field measurements, are made available to modellers.

Concerning the modelling philosophy adopted by different groups, it is interesting to realize that a good “a priori” understanding of the relevant physical phenomena at play becomes perhaps the most important item to achieve good results. In particular, decisions concerning the relevant couplings in a particular problem, are a key issue in the modelling exercise. These decisions are not always clear or obvious, and they require the appropriate technical and scientific background. As an illustration of these comments, the following couplings, or main physical phenomena, have been identified as the most relevant ones for the three cases solved under Task 1. Failure to consider them precludes the correct simulation of some features of the observed behaviour.

Part A (Specially the prediction of pore water pressure development)
- Full hydro-mechanical coupling
- Due consideration to a general three-dimensional initial stress field
- Modelling in detail the rate of geometry changes (progress of tunnelling in time)

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

Part C

- Thermal dilation of water and skeleton. (The second provides the main reason for stress development and the difference between water and skeleton dilation is the origin of heat induced pore water pressures).
- Full hydro-mechanical coupling

In a reverse sense, a good understanding of the physical processes may lead to the selection of appropriate simplifications. In parallel to the previous list, the following set of aspects was found of minor relevance in the Febex case:

- The structure of the granite rock played a negligible influence on the hydration of the bentonite buffer. This was explained as a consequence of the difference in saturated permeability of the bentonite and the rock matrix
- The gas pressure may be safely assumed to be constant, due to the high gas permeability
- Plastification of the bentonite does not seem to be an issue because of the high
- confinement provided by the rigid granite. Simple elastic models, provided that suction effects are incorporated may suffice.
- 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.

A number of unresolved, or insufficiently known aspects, remained at the end of the work performed. The following may be mentioned:

- The behaviour of the system at long times. This comment refers to issues such as saturation times, chemical effects and corrosion effects. These problems were not specifically discussed in Decovalex III, although they are part of the general design problem addressed by Febex.
- The effect of the change of scale implied by a real repository where many tunnels carrying waste are closely located in a large disposal area. Same comment as above.
- The difficulty to match with calculations the mechanical response of the buffer (stresses, displacements). The blocky nature of the buffer was not considered by any of the modelling teams.

Concerning the methodological and numerical approaches followed by different groups two additional general comments may be made:

- Numerical analysis performed could be divided into two types: single program fully coupled or a combination, via a staggered approach, of codes solving partial problems. Groups falling in the second category found more difficulties to reproduce adequately the observed phenomena.
- Very few participants took advantage of the small and medium-scale laboratory tests performed on the bentonite in order to derive model parameters. These tests are considered as especially relevant to derive, using backanalysis techniques, accurate material parameters, even if different constitutive models are employed.

3 Executive summary – Task 2

3.1 Introduction

The Drift Scale Test (DST) in Yucca Mountain in Nevada, USA is a large scale, long term field thermal test being conducted for the United States Department of Energy (DOE). The heating phase of the DST, an integral part of DOE’s program of site characterization at Yucca Mountain to assess whether the mountain is suitable site for a repository for the disposal of high level nuclear waste (HLW) and spent nuclear fuel (SNF), was initiated in December 1997. Heating was terminated in January 2002 ushering in the cooling phase of the test that is expected to continue for four years. The overarching objective of the DST is to study coupled thermal, hydrological, mechanical, and chemical processes caused by the decay heat from HLW and SNF emplaced in an underground geologic repository. The layout of the DST est is shown in Fig. 3.1.

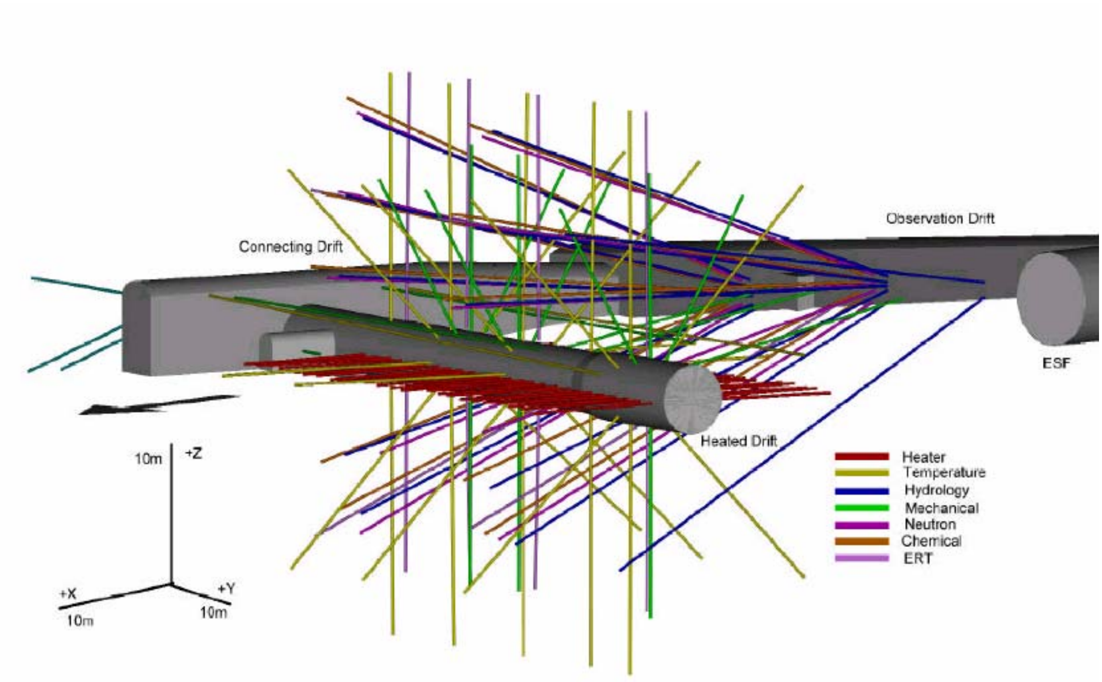


Figure 3.1: Perspective of DST Block Showing Multiple Boreholes to House Heaters and Sensors

The DST consists of a 5 m diameter, 47.5 m long drift heated by nine cylindrical electric heaters placed on the floor. Each heater, 1.7 m diameter and 4.6 m long, is capable of generating a maximum of 15 kW. 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 1). The drift cross-section and the cylindrical heaters are approximately the sizes 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, 10m long, has two distinct segments capable of generating 1145 W and 1719 W. 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 1). As shown in Figure 1, a large number of boreholes drilled from the drifts into the test block house the heaters, instruments, and sensors for the test.

3.2. Problem definition and work organization

In 1998 the DST was included as a test case in the then ensuing DECOVALEX III project, the Task 2. Task 2 of DECOVALEX III organized around the DST had four sub-tasks: 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 the TM response while predicted or calculated temperatures were the input in 2B. Task 2D was to study the thermal-hydrologic-chemical (THC) response.

Table 3.1. Organization and works performed

Funding Organization	**Research team**	**Works performed**
CEA	CEA/DM25/SEMT, France	Task 2C
DOE	LBNL, USA	Co-ordinator
ENRESA	Universidad Politecnica de Catalunya (UPC), Spain	Task 2A, 2B
JNC	JNC, Tokai Works	Task 2D
NRC	Southwest Research Institute, USA	Task 2A, 2C
SKI	LBNL, USA	Task 2C

3.3. Modeling approaches

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 which solves mass conservation equation (air and water), energy conservation equation in non-isothermal state, and momentum balance equation for mechanical equilibrium to predict the TH conditions. Initially, their model used a single equivalent porosity and permeability structure to represent the fractured tuff in the DST block (Datta, 2002). Later the ENRESA/UPC team used double porosity and double permeability structure to represent the co-located fracture medium and the matrix medium (Datta et al, 2003).

The NRC/SWRI researchers used the multiphase simulator MULTIFLO to perform Task 2A TH modeling. Their model involved the dual continuum model (DCM) formulation that is similar to the dual permeability model (DKM) used by the DOE researchers. Both the DOE and NRC researchers invoked the active fracture model for unsaturated flow through fractured rock proposed by Liu et al (1998) to ensure realistic fracture-matrix interaction. The DOE research team used the TOUGH2 code to perform the TH modeling of the DST (Pruess et al., 1999).

For Task 2B, SKI researcher and later DOE researcher performed coupled thermal-hydrological-mechanical (THM) analysis of the DST with the TOUGH-FLAC code which is a simulator based on coupling of two established computer codes: TOUGH2

(Pruess et al. 1999) and FLAC3D (Itasca Consulting Group, 1997). TOUGH-FLAC simulation captures the effect of stress changes on hydraulic properties based on a conceptual model of highly fractured rock mass containing three orthogonal fracture sets. Porosity correction factors and permeability correction factors are calculated from the initial and current apertures assuming equally spaced fractures and adopting the parallel plate fracture flow model. The ENRESA/UPC researchers performed their 2B analysis by CODE_BRIGHT that allows permeability changes to be calculated based on changes in porosity due to stress changes.

For Task 2C, both the CEA and NRC researchers used measured temperature profiles as the thermal input to model the thermal-mechanical process to predict displacements in rock. The NRC team performed a continuum analysis using the FLAC code. The CEA team also performed continuum analysis using the code Castem2000 (Verpeaux et al., 1989).

The works performed for Task 2B and 2C was reported in (Datta et al., 2004a).

For Task 2D, the JNC team performed coupled THC simulation of the DST employing the THM code THAMES (Ito et al., 2003; Ohinishi et al. 1985; Chijimatsu et al. 2000), mass transport code Dtransu (Nishigaki et al. 2001) and the geochemical code PHREEQE (Parkhurst et al. 1980). These three codes are controlled by the coupling system COUPLYS which can exchange common data between the three codes and can synchronize each code in order. The DOE researchers used the TOUGHREACT code (Xu et al., 2003) to model the THC processes in the DST adopting the dual permeability method to capture separate yet interacting processes in fractures and matrix.

Simulations of THC processes included coupling between 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, 2004b).

3.4. Scientific achievements

The DST confirmed that the heat transfer process in the Yucca Mountain fractured tuff is conduction dominated, although pore water plays an important role, especially in the sub-boiling regime. Vaporized water travels away from the heat via fractures and condenses in cooler regions, thereby filling fractures and lowering the permeability.

Various conceptual models were evaluated by comparing simulated and measured temperatures. The dual continuum model (fracture and matrix) and active fracture concept reflecting actual heat load yielded the best agreement.

The effect of dimensionality (i.e., 2D versus 3D) on temperature was evaluated. A maximum reduction of temperature of about 10^0C near the wing heaters was calculated after four years of heating when a 3D model was used compared to a 2D model. The TH calculations indicate that it is 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.

Task 2 researchers presented seven papers based on their DECOVALEX III project work at the GeoProc 2003 conference held at the Royal Institute of Technology in

Stockholm, Sweden in October 2003 (Datta et al., 2003; Rutqvist et al., 2003; Hsiung et al., 2003; Green and Painter, 2003; Olivella et al., 2003; Millard & Rutqvist, 2003). More papers will be submitted for a forthcoming Special Issue of the International Journal of Rock Mechanics and Mining Sciences devoted to achievements in DECOVALEX III/BENCHPAR projects.

3.5. Lessons learned and outstanding issues

The DST is a large and complex field test in which a multitude of measurements were made, and its realistic simulation needs multidiscipline approaches with multiple research teams with different concepts and approaches so as to achieve more in-depth understanding to the coupled THMC processes involved. DECOVALEX III researchers studying the DST for Task 2 performed well in their individual works, but more concentrated efforts with more teams involved is needed for further studies, helped with more active coordinating.

Although the effects of the chemical processes have been investigated in-depth by DOE over the years, the works performed in the Task2 for this effect is not adequate for furthering the scientific understanding due simply the two few numbers of teams involved.

The presence of fractures in the DST site and the long periods of heating-cooling phases of the test may cause residual and long-term variations in physio-chemical properties of the fractured tuff, due to the irreversibility of the coupled THMC processes, for example the residual fracture deformation and its impact on permanent change sin permeability of the near-field. Such residual and permanent changes will be important factors affecting design and performances of post-closure monitoring works and final safety assessment. Study on these effects are not considered in Task 2 of the DECOVALEX III project, but is an important outstanding issue for further research.

4 Executive summary - BMT1, Task 3

4.1. General definition of the problem

In the definition of BMT1, it was proposed that scoping calculations be performed in order to estimate how T-H-M 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 of BMT1 is based on a hypothetical nuclear waste repository in a granitic rock formation at a depth of 1000 m. The typical repository being assessed has rather composite features: it is based on a Japanese conceptual design, the buffer is the same pure bentonite used in the Kamaishi THM experiment in Japan (Fig. 4.1), but the rock mass properties in term of strength and permeability are based on typical Canadian Shield's data. The conceptual design of the repository is illustrated in Figure 4.2a (JNC, 2000). The centreline distance between adjacent tunnels is 10 m and the centreline distance between adjacent depository holes for the wastes is 4.44 m. The depth of each depository hole is 4.13 m and the diameter is 2.22 m. The overpack (canister) for radioactive wastes would be emplaced into the depository hole, and a bentonite buffer material would be compacted around the overpack. The tunnels would also be backfilled with a mixture of gravel and clay. The Performance Assessment analyst in order to assess nuclide transport through the engineered and geological barriers may require feedback on the following key points:

1. What is the temperature evolution in the near-field?
2. How long would it take for the buffer to re-saturate?
3. What are the stresses on the overpack and in the buffer? Will they be structurally stable?
4. How will the permeability and the flow field of the rock mass in the near-field evolve?
5. Is there a potential for rock mass failure in the near-field?
6. What are the uncertainties related to the answers to the above questions, taking into account the variability in the properties of the rock mass?

The BMT1 objective is to answer the above questions through THM simulations of the hypothetical repository. This summary provides an overall presentation of the problem based on three progress reports (Jing and Nguyen, 2001, 2003a and 2003b).

4.2. Implementation steps

In order to address the above points, the research teams will perform T-H-M analyses and adopt the following three-step strategy, which will constitute separate subtasks of BMT1:

Step 1 (subtask BMT1A). Calibration of the computer codes with a reference T-H-M experiment with realistic rock mass conditions and measured outputs of thermal, hydraulic and mechanical variables: The reference experiment chosen for BMT1 is the Kamaishi in-situ experiment at Kamaishi Mine, Japan, performed at the 550 m-Level

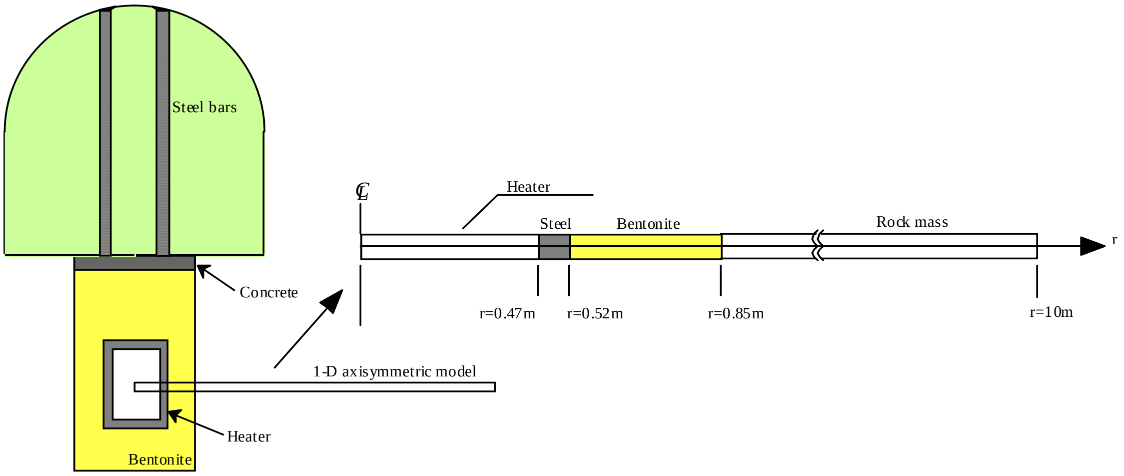


Figure 4.1: Near-field T-H-M experiment with one single heater- the simplified model geometry for BMT1A.

gallery of the experimental site, as illustrated in Fig.4.1. The objective of the BMT1A subtask is to validate the numerical approaches, computer codes and material models, so that the teams simulating tools are at a comparable level of maturity and sophistication.

Step 2 (Subtask BMT1B). Use of the calibrated codes to perform scoping calculations, considering varying degrees of THM coupling, for the generic repository design shown in Fig. 4.2. To simplify the calculation process and focus on the physics of the problems instead of computational efforts, the geometry of the problem, especially regarding the geometry of the fractures, is greatly simplified to regular fracture geometries. In subtaskBMT1B, the rock is considered to be homogeneous without any explicitly represented fractures. However, different permeability values are considered. The aim is to identify the coupling mechanisms of importance for construction, performance and safety of the repository.

Step3 (Subtask BMT1-C). Perform scoping calculations with different coupling combinations for the case where a horizontal fracture intersects the deposition hole and a vertical fracture zone divides two adjacent deposition tunnel/hole system (Fig. 4.2c). A hydrostatic condition is applied along the vertical fracture as a hydraulic boundary condition. In addition to this definition, the SKI/KTH team performed an additional calculation of highly fractured rock mass with two orthogonal sets of fractures with a spacing of 0.5 m)Fig. 4.2d). Figure 4.2e shows a typical FEM model for BMT1C. The aim is the same as that of BMT1B but with the additional influence of explicit fractures.

It was identified from the start that the focus of the analyses in BMT1-B and BMT1-C should be on the following output results, deemed to have a strong influence on the long term safety and performance of the repository:

1. The maximal temperature created by the thermal loading from the emplaced wastes
2. The time for re-saturation of the buffer
3. The maximal swelling stress developed in the buffer
4. The structural integrity of the rock mass
5. The permeability evolution in the rock mass

The combinations of coupling mechanisms and their effects on the above output could be summarized in an interaction matrix shown in Table 4.1. The research teams were asked to perform their calculations considering the coupling combinations shown in the matrix, and compare the output results between the coupling combinations.

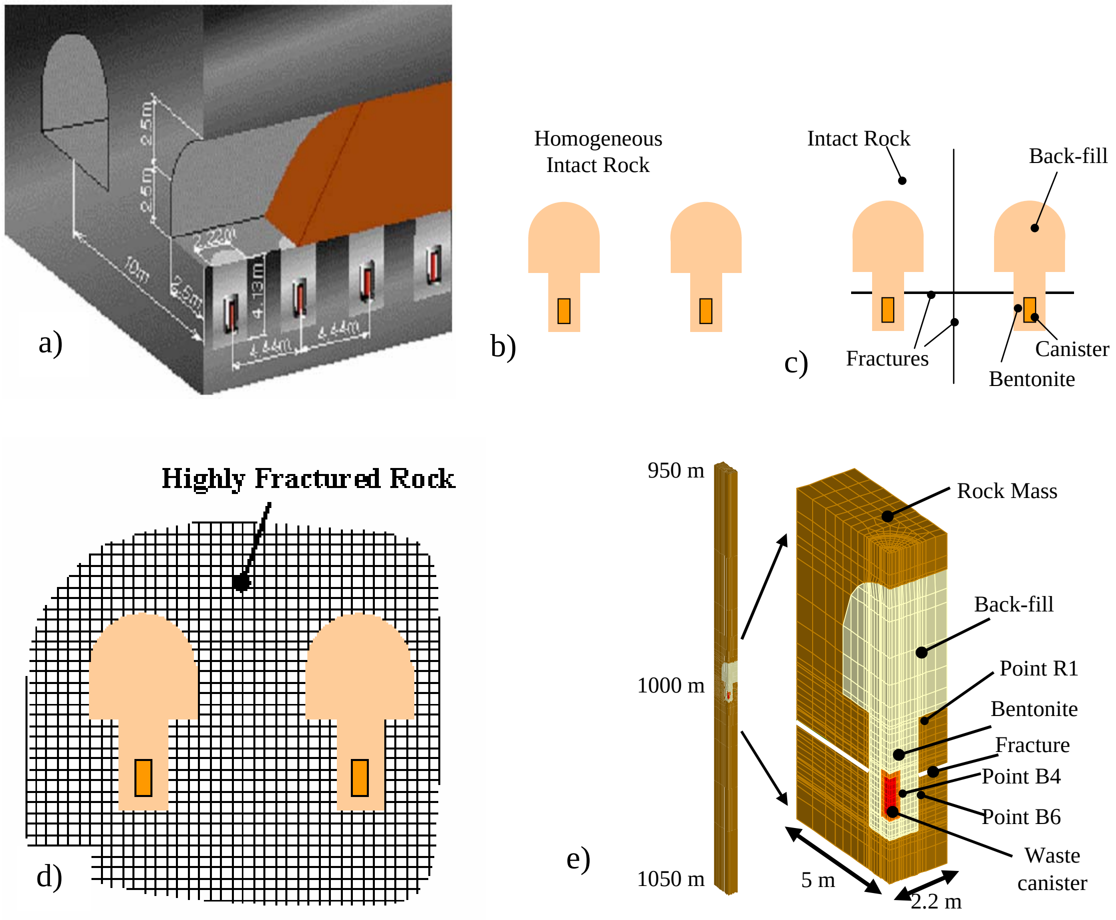


Figure 4.2: Generic design of a hypothetical repository (a), concept of BMt1B (b), concept of BMt1C (c), Additional case studied by the KTH/SKI team (d) and a typical FEM model for BMT1C (e).

Table 4.1. Comparison matrix of for different degree of THM coupling (T-temperature, σ-stress, k-permeability, p-pressure, θ-water content)

Output	T	M	H	H-M	T-H	T-M	T-H-M
T-evolution	Y	N/A	N/A	N/A	Y	Y	Y
σ-evolution	N/A	Y	N/A	Y	N/A	Y	Y
k-evolution	N/A	N/A	N/A	Y	Y	N/A	Y
p-evolution	N/A	N/A	Y	Y	Y	N/A	Y
θ-evolution	N/A	Y	Y	Y	Y	N/A	Y

(Y: Output to be calculated N/A: Not applicable.)

4.3. Work organization and physical processes concerned

Six research teams participated in BMT1, using either finite element (FEM) or finite difference(FDM) methods , as shown in Table 4.2.

The physical processes considered in the BMT1 include mainly:

Table 4.2. The research teams and their approaches for BMT1

Team	FO	Method	Code(s)	Tasks
CEA	IPSN	FEM (3D)	Castem 2000	BMT1A, 1B & 1C
CNSC	CNSC	FEM (3D)	FRACON	BMT1A, 1B & 1C
INERIS	ANDRA	FDM (3D)	FLAC	BMT1A
JNC	JNC	FEM (3D)	THAMES	BMT1A, 1B & 1C
ISEB-ZAG	BGR	FEM (3D)	RF/RM	BMT1B
KTH	SKI	FEM (3D)	ROCMAS	BMT1A, 1B & 1C

- ❑ Water flow in partially and/or fully saturated buffer and rock, in both liquid and gas states, especially the thermally driven water moisture diffusion process;
- ❑ Heat conduction and convection in buffer and rock;
- ❑ Stress, deformation and failure of rock using the Hoek-Brown failure criterion;
- ❑ Variation of swelling pressure, water content and relative permeability fields in buffer due to coupled THM processes as listed above;

4.4. Summary on scientific achievements

4.4.1. Achievement from BMT1A

A number of improvements to the modelling of the Kamaishi Mine heater test were suggested and tested in this study, using a simplified axisymmetric model of the heater test as shown in Fig. 4.1. Although the model geometry is much simplified compared to the field test conditions, improved simulation of the general THM responses were obtained, as compared with the Task 2C results of DECOVALEX II. The measures taken for improvement were:

- ❑ Parameter changes (reduced rock mass permeability and rock mass thermal expansion by the KTH/SKI team, and increased thermal expansion coefficient and reduced swelling pressure constant of the buffer by JNC team)
- ❑ Inclusion of the sealing of rock fractures by penetrating bentonite by the KTH/SKI team, which can explain the uniform (axisymmetric) wetting of the bentonite.
- ❑ An improved swelling/shrinking strain function combined with an increased thermal expansion of the bentonite giving a good match of the mechanical (stress, strain) behavior of the buffer by the KTH/SKI team.
- ❑ Uses of higher Young’s modulus and Poisson’s ratio of the bentonite near the heater, and a “sealed” layer of rock around the bentonite by the CNSC team.

As a results of the above measures, the results from the simplified axisymmetric model used in the re-evaluation of the Kamaishi mine experiment showed general improvement over the original models used in the prediction phase during the DECOVALEX II project, especially in the following aspects:

- ❑ Calculated values of temperature agree very well with the experimental values, for all teams.
- ❑ Generally improved stress and strain behaviour in the bentonite, at least qualitatively though, with the measured results.
- ❑ The water content near the heater (at point 1) is relatively well predicted by all teams, although the saturation front at the bentonite/rock interface are still

predicted to advance much faster than in reality.

In general, the mechanical behaviour of the buffer is complex with forces contributing from shrinking/swelling in all part of the bentonite, external stress from the thermal expansion of the heater and rock, and internal thermal expansion of the bentonite itself. However, a reasonable prediction of the mechanical behaviour can be done if all relevant bentonite properties are known from laboratory tests.

4.4.2. Achievements from BMT1B

The teams successfully performed required scoping calculations and important conclusions were drawn regarding the importance of THM coupling processes for design, construction, performance and safety of the repository. In order to assess the importance of different coupling mechanisms and their combined effects, the research teams have considered different degree of complexity of the coupling mechanisms as shown in Table 4.1. From the modelling results, it was identified that the initial rock mass permeability is a key parameter.

For the typical repository considered in BMT1-B, only the fully 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 on 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 the results of the BMT1B, it appears that from a technical point of view the effect of coupling will be either short lived (several decades to 100 years) and would not impact on long term (thousands to hundred of thousand years) safety issues, or could be rectified by adequate design and operation methodology (e.g. avoid over-cooling the galleries in the Japanese context). The influence of the host rock properties (e.g. permeability) on the long-term safety seems to be much more important than coupling effects, since one has much less control over these properties. However, a fully coupled approach is necessary to help design and construction strategies and to interpret monitoring data that would be 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.

4.4.3. Achievements from BMT1C

This analysis aimed to evaluate the impact of THM couplings on the performance of a repository located in sparsely fractured rocks. The results of this analysis can be summarised as follows:

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

It is clear that the temperature can be predicted accurately without consideration of coupling to hydraulic and mechanical processes since heat convection plays a minor role in temperature evolution and the conversion of the mechanical work (dissipated energy) is not significant at all. On the other hand, it is also clear that the mechanical behaviour (mainly the evolution of stress in the buffer-rock system) cannot be appropriately predicted without consideration of the effects of fluid pressure and temperature. However, it is not clear from the BMT1 analyses whether the hydraulic behaviour (for example re-saturation of the buffer and radioactive nuclide transport) can be significantly impacted by T and M processes. For the parameter set adopted in this analysis, the re-saturation time is slightly impacted by the effect of temperature whereas the mechanically induced changes in permeability (of the rock or the buffer????) do not significantly impact the re-saturation process.

The general 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 re-saturation process.

4.4.4. Generated Publications

Besides the progress reports in the reference list at the end of this summary, additional international publications have been generated by the research teams involved with BMT1 (Chijimatsu et al.,2003; Kohlmeier et al., 2003; de Jonge et al., 2003; Millard et al., 2003; Rutqvist et al., 2003 and Nguyen et al., 2003). They are papers published in the proceedings of the international Conference of GeoProc 2003 (Stephansson et al., 2003).

4.5. Lessons learned and outstanding issues

The BMT1 is a comprehensive numerical Bench-Mark Test problem considering coupled THM processes in the near-field buffer and rocks of a hypothetical repository. The special features of buffer re-saturation and mechanical integrity of the repository are considered for the first time in the DECOVALEX I, II and III project series. Through iterative verification against the results from the in-situ THM experiments at the Kamaishi Mine, significant progress have 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 modelling of complex coupled THM processes in buffer materials and rock masses. Thus, the codes become more reliable tools to aid in the design, construction, performance and safety assessments of nuclear waste repositories.

On the other hand, further improvement in both the models and the hypothetical case definition is always desirable. The main lessons learned and the outstanding issues from the BMT1 problem series may be summarized as follows:

4.5.1. Problem Definition:

The BMT1A definition is a simplification without considering the effects of rock fractures in the near-field of the deposition hole. As demonstrated in the previous DECOVALEX II studies (Task 2), the effects of the rock fractures are important for the mechanical behaviour of the rocks, especially near the intersection area between the tunnel and the deposition hole. The assumption of an axi-symmetric model of BMT1A makes the consideration of fractures impossible to be included, therefore, their effects on the results cannot be considered.

The models for BMT1B and 1C are hybrid models in the sense that the geometry and buffer properties are determined based on the in-situ THM experiment at the Kamaishi mine, Japan, but the rock properties come from the Canadian Shield, due mainly to the incompleteness of data available from any one single source at the time of the project. This hybrid model conceptualisation suffers from the limitation that the simulation results obtained from the BMT1 cannot be compared with observations in Kamaishi or Canada URL for quantitative analyses, especially regarding the failure of the tunnel-hole system.

It is therefore necessary to consider similar simulations with one specific repository site which can provide adequate data support for all aspects of THM simulations against observations so that the impacts of THM processes can be evaluated more realistically and quantitatively to improve confidence building and code/model performance.

4.5.2. Mathematical Models and Numerical Implementation:

It is shown from the BMT1 results 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) and phase change, has to be considered in order 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, thus produced acceptable results for both hydraulic processes in buffer, and thermal processes in the buffer and the rock. The FDM code (FLAC) lacks this important capability to simulate the thermally driven moisture flow and could thus only adequately model the thermal processes.

The finite element codes applied for BMT1 problems have functions in simulating fractures as thin-layer continuum elements with equivalent properties. This strategy suffers from the shortcoming of mesh distortion, displacement locking across the fractures, small deformation, and limited number of fracture elements in order to avoid the problem of numerical singularity in the global stiffness matrix. The codes' performance for BMT1 are acceptable because of the simple fracture size and geometry assumed for the problem. However, this may not be the case when more realistic fracture systems need to be represented in modelling practical problems instead of simplified Bench-Mark Test problems.

4.5.3. Process Representation:

An important issue in repository design, construction and performance/safety assessments is the understanding of the effect of DZ (Disturbed Zone, or Damage Zone) surrounding an excavation. The importance of the DZ is not only on its effects on the mechanical stability of the repository (although it is important to consider this effect in repository design and construction), but also on its effect on the 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 rock failure extent were simulated in BMT1 with the Hoek-Brown criterion based on theory of plasticity, the real mechanism of combined damage, micro-fracturing and plastic deformation and their effects on the behaviour and evolution of the DZ was not considered.

4.5.4. Relevance to Performance and Safety Assessments:

The safety indicators defined in BMT1 are mainly variables such as maximum temperature, re-saturation time, permeability and saturation evolutions, etc. Although they are relevant measures for PA /SA assessments, more direct and interactive linking between the THM modelling and radioactive nuclide transport process was not attempted. It is therefore desirable in the future to consider more integrated approach between THM simulation and PA/SA assessments. In that context, the THM specialists and the PA/SA specialists would work together on the PA/SA of the same repository.

5 Executive summary - BMT2, Task 3

5.1. Background and objectives

The Benchmark Test 2 of DECOVALEX III project (also the Work Package 3 of the BENCHPAR project) concerns the upscaling of the THM processes 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 thermo-hydro-mechanical couplings in a fractured rock mass adjacent to a repository are significant in terms of solute transport typically calculated in large-scale repository performance assessments. Since the presence of even quite small fractures may control the hydraulic, mechanical and coupled hydro-mechanical behaviour of the rock mass, a key of the work has been to explore the extent to which these can be upscaled and represented by 'equivalent' continuum properties appropriate 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 modelling and the analysis of the model 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.

From these general aims the task was set-up as a numerical study of a realistic large-scale reference problem. Analysing this reference problem should:

- help explore how different means of simplifying the geometrical detail of a site, with its implications on model parameters, ("upscaling") impacts model predictions of relevance to repository performance.
- explore to what extent the THM-coupling needs to be considered in relation to PA-measures.
- compare the uncertainties in upscaling (both to uncertainty on how to upscale and uncertainty that arises due to the upscaling processes) and consideration of THM couplings with the inherrent uncertainty and spatial variability of the site specific data.

This summary is based on the final report of BMT2 (Andersson et al., 2003) and teams progress reports and papers on the GeoProc 2003 (Blum et al., 2003; Chan et al., 2003; Gómez-Hernández and Cassiraga, 2003; Guvanasen and Chan, 2003; Kobayashi et al., 2003)

5.2. Task organization

In total eight different teams analysed the BMT2 either as part of DECOVALEX III (five teams) or as parts of BENCHPAR (three teams) (Table 5.1).

Table 5.1. Teams and references to the team reports –BMT2, Task 3

Team/Funding organization	**Acronym**	**Part of**
INERIS/ANDRA, France	INERIS	BENCHPAR
Kyoto University/ JNC, Japan	JNC	DECOVALEX III
KTH/SKI, Sweden	KTH	BENCHPAR
DOE/LBNL, U.S.A.	LBNL	DECOVALEX III
AECL/OPG, Canada	OPG	DECOVALEX III
Uppsala University/STUK, Finland	STUK	DECOVALEX III
Univ. of Birmingham/Nirex UK	UoB	DECOVALEX III
UPV/ENRESA, Spain	UPV	BENCHPAR

5.3. Problem definition

The reference problem (Fig. 5.1) concerns the far-field groundwater flow and solute transport for a situation where 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 at stake are:

- how to assess the far-field hydraulic and transport properties when most data stem from small scale (borehole) tests,
- what is the impact of potential mechanical and hydraulic couplings, and
- if MH or HM couplings are significant how would they affect the upscaling?

It is assumed that the HLW (heat source) is encased within resaturated bentonite within a repository drift shown as a simple horizontal body. (NB no attempt is made to represent repository detail such as deposition holes etc.). The repository sits within a low permeability fractured rock unit which is 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 repository is assumed to comprise of 60 uniformly distributed canisters of HLW embedded in compacted and resaturated bentonite, with a canister density of $6 \cdot 10^{-3}$ canisters/m^2 (or 60 canisters per 100 m x 100 m).

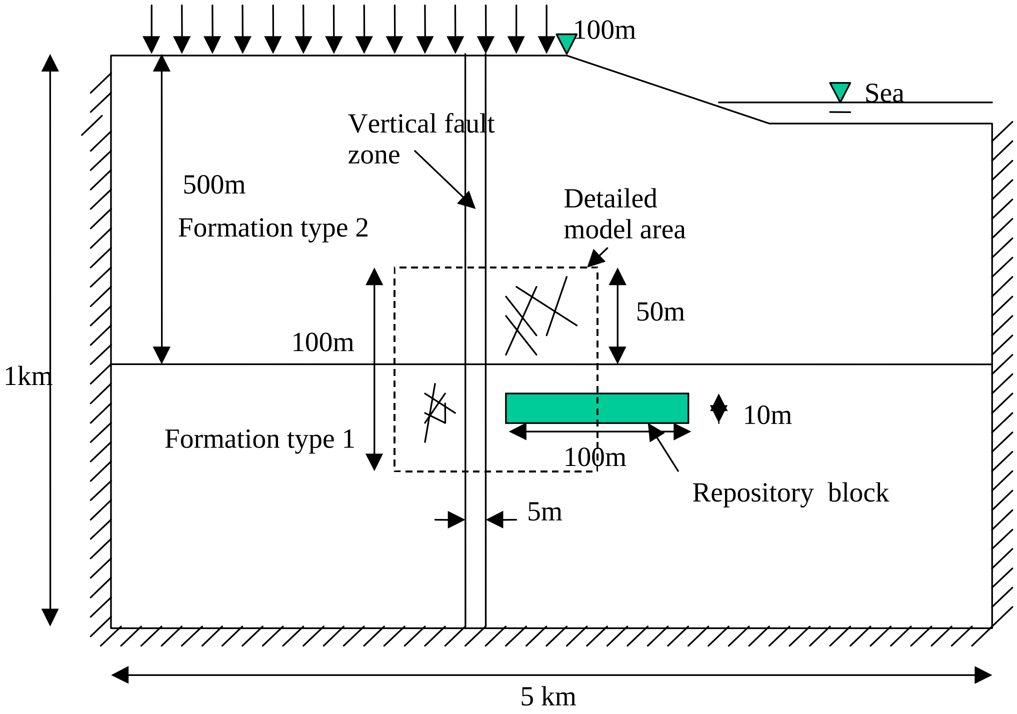
The relevant data for the rock formations and fault are based on Sellafield site characterisation data acquired by Nirex. The data are in the form of statistical distributions of properties. Typically, most of the data concern measurements on a small scale, whereas the problem to be studied mainly concerns the large scale. The types of data include fracture statistics (orientation, length, density, frequency, etc.) and other required thermal, hydraulic and mechanical properties of all materials involved.

The required works for the teams are:

- Analysing the rock mass fracture, hydraulic, thermal and mechanical, data provided by Nirex and abstract appropriate parameters. Derive appropriate conceptual and mathematical models.
- Deriving a description at the small scale using discrete fracture network approaches (2D or 3D) or by continuum analyses.
- Deriving upscaled equivalent hydraulic, mechanical and coupled hydro-mechanical properties from the small scale description. This involves analysis at

a range of scales to ensure that appropriate representative upscaled equivalent continuum parameters are derived (the REV).

- ❑ Parameterise a 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.



Not to Scale

Figure 5.1: Reference problem geometry

The overall performance measures defined for BMT2 are the “transit time (τ) distributions” and "transport resistance (β) distributions" at two output surfaces: a) a perimeter surface at 50m outwards from the boundary (wall/floor/roof) of the repository and b) 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. The works demonstrated that using such intermediate parameters is more practical, and quicker tool, than the ultimate comparison of the overall performance measures.

5.4. Modelling approaches

5.4.1 Approaches for Upscaling at the Small Scale

Table 5.2 summarizes the modelling approaches used by the teams for the upscaling works at small scales.

Table 5.2 Approaches for the upscaling task at small scales

Team	**Main features**
INERIS	3D DEM with flow in fractures only. Independent block generation, code 3DEC and RESOBLOK
JNC	2D fracture system generation and fracture density and permeability estimations based on pixels
KTH	2D DEM with flow in fractures only. Independent fracture system generation using stochastic realizations. Code UDEC
LBNL	Fractal Levy-motion approach for upscaling heterogeneous porous media, based on a series of short-interval hydraulic test results
OPG	2D FEM, extension of crack tensor theory to include THM parameters and BB-model of joints, code MOTIF and FRACTUP
STUK	3D DFN for flow analysis and 2D DEM for thermo-mechanical analysis, code FracMan.Mafic and UDEC
UoB	2D DEM for HM analysis linked with independent DFN flow analysis, code UDEC-BB and FRAC2D
UPV	Laplacian upscaling for HM, with effective hydraulic conductivity tensors evaluated at a REV scale of10 m × 10 m.

5.4.2. Approaches for Large Scale Analysis

The general approaches for the large-scale analysis are similar between the teams, although different software has been used. The approaches used by the teams are summarized in Table 5.3.

5.5. Scientific achievements

5.5.1. The Upscaling at Small Scales

In BMT2, the problem definition did not provide, on purpose, a definitive fracture system geometry model, so as to encourage different approaches to be applied for characterizing the equivalent hydraulic and mechanical properties of the rock masses. This naturally leads to quite different interpretations to the data provided, problem dimensions, and how to use the existing experimental data. This kind of benchmark tests is used first time in the project and played a significant role in deepening understandings on the issues of property upscaling in fractured rocks. Table 5.4 summarizes the resultant permeability and deformation modulus of the rock masses of Formation 1, obtained by using different approaches by the teams. The ranges of the values obtained by one team can be over either the different REV sizes (e.g. INERIS), different permeability components (e.g. KTH), or different techniques used (e.g. LBNL, OPG and STUK) by the same team. The reference data is estimation in the problem definition. For other relevant properties see Andersson et al. (2003).

It is suggested 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 further stress increase due to thermal stresses would not significantly reduce the permeability. However, one must bear in mind that thermal stress does not always increase compressive stress. In some areas there can be reduction of compressive stress. Also, in the near field where temperatures are relatively high, THM coupling through the storage term may not be negligible. Also the TH effects, due to buoyancy, are relatively limited and would add an uncertainty in the order of a factor of 2 or so.

Table 5.3 Approaches for the large scale analysis of THM and transport

Team	**Main features**
INERIS	T, TH, TM and THM computations using code FLAC3D. The equivalent properties derived from the upscaling.
JNC	Solution of the large scale problem using a FEM code THAMES with scaling rules obtained from Crack Tensor theory, but used the mean values provided in the Task. Particle tracking for transport analysis with 300 particles at different starting time (t=0, t=1000 years and t=10000 years).
KTH	Equivalent parameters from small scale analysis for coupled THM analysis of the large scale problem with a FEM code ROCMAS).
LBNL	Multiple realizations of subsurface heterogeneity to determine the mean flow and transport properties and the associated uncertainties. Code T2R3D was used to simulated coupled TH and tracer transport processes - with and without heat. Sensitivity study on the influence of fracture porosity
OPG	Using 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 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 active fractures. Six particles were released from points evenly distributed over the mid-level of the repository block and they were tracked to the 50m boundary and to their discharge points at the right final boundary of the model and in the sea.
STUK	Using code TOUGH2 to solve the head and flux fields, with upscaled parameters of effective conductivity and correlation structures from upscaling. Transport was modelled by particle tracking with multiple realisations concerning H and transport processes. TM effects were studied as sensitivity analysis based on input permeability distributions. A particle was released at a nodal point of a random element within the repository area and was moved 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 sampled from the probability distributions obtained from the small scale analysis.
UoB	The continuum flow and transport code FAT3D was used for the far-field studies, with calculations of particle travel times (t_{50}) for the two considered base cases (H and HM base cases).
UPV	Using a detailed description of the hydraulic conductivity field and by using an upscaled description. The results were then compared.

Table 54 Upscaled properties by different approaches for BMT2.

Team	Permeability (m^2)	Deformation Modulus (GPa)	REV scale (m)
INERIS	5.5×10^{-14} -1.6×10^{-13}	38 – 73	2 – 4
JNC	6.25×10^{-18}	10 – 250	
KTH	3.5×10^{-16} - 3.4×10^{-15}	34-44	5
LBNL	No upscaling		1.56; 12.5 – 50
OPG	7.4×10^{-18} - 7.2×10^{-17}	13 – 17 (32 – 39)	10 – 100
STUK	8.61×10^{-19}		7.5; 50
UoB	5.0×10^{-17}- 5.5×10^{-16}		10
UPV	No upscaling		5
Ref.	**5.7×10^{-18}**	**65**	**50**

These observations support the conclusion that it is the uspcaling of hydraulic properties that are the main sources of uncertainty in a problem of this nature. The added disturbance, in relation to in-situ stress, is small in the far-field of a deep repository. Yet, understanding the stress/permeability relation is important for understanding the nature of the permeability field.

5.5.2. The Large Scale Analysis

In the large-scale analyses all teams used their upscaled properties in various equivalent porous continuum codes to explore the resulting effects on the large scale flow and transport processes, and the impact of the heat source by waste decay.

a) Impact of the heat source

Similar values of the maximum temperature were predicted by different teams, as 55 °C by INERIS and 50 °C by LBN and OPG, respectively.

b) Impact of coupling processes on nuclide transport

The following conclusions were reached for impacts of different coupling mechanism combinations on PA/SA considerations:

- Negligible effect of hydraulic process on stress or displacement variations, with less than 20% difference between TH and THM results. However, significant effects of mechanical processes on the discharge vectors and the pore pressure variations (reached by INERIS).
- TM processes induce relatively small changes in permeability. Thermal loading has a noticeable but insignificant effect on radionuclide transport (reached by LBNL).
- Significant thermal effect on flow process, with 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 50m scale than at the km scale. The fracture density assumed in the modelling, and whether upscaling is performed or not, appear to affect the transit time to final discharge more than THM coupling (reached by OPG).
- Long-term heating affects hydraulic aperture and a decay of about 10-15% of apparent aperture during the first 00 years of heating, implying decay of fracture transmissivity. TM effects on flow and transport processes are small

in comparison to the intrinsic uncertainties in modelling hydraulic flow in fractured rock (Reached by STUK)..

- The results for the HM base case show a very sensitive to the chosen mechanical properties (reached by UoB).
- It can also be noted that most conclusions to be drawn from the large scale analyses could already be drawn from studying the intermediate performance measures such as permeability, deformation modulus and k versus stress relations.

Table 5.4 compares the breakthrough time predicted by different teams.

Table 5.4. Resulting overall performance measures as calculated by the different teams

Team	**τ_{50} at 50 m (in years)**	**τ_{50} final in years/m**	**β_{50} final in years/m**	Comment
JNC	$9.8 \cdot 10^5$ (3.110^{13} s)	$8.8 \cdot 10^6$ (2.810^{14})	$4.1 \cdot 10^{15}$	
LBNL	$(3.9-6.8) \cdot 10^4$	$(1.48-2.09) \cdot 10^4$	$(7.09-9.5) \cdot 10^8$	Only H (years)
	$6.61 \cdot 10^6$			TH
OPG	$4.85 \cdot 10^4$	$7.85 \cdot 10^5$	$2.60 \cdot 10^7$	H only, no upscaling,
	$5.95 \cdot 10^4$	$7.77 \cdot 10^5$	$2.61 \cdot 10^7$	HM, no upscaling
	$3.64 \cdot 10^4$	$5.85 \cdot 10^5$	$1.94 \cdot 10^7$	TH, no upscaling
	$4.34 \cdot 10^4$	$5.79 \cdot 10^5$	$1.94 \cdot 10^7$	THM, no upscaling,
	$8.36 \cdot 10^2$	$2.53 \cdot 10^4$	$6.75 \cdot 10^5$	HM, upscaled property
	$7.70 \cdot 10^2$	$2.00 \cdot 10^4$	$4.70 \cdot 10^5$	THM, upscaled property
	$4.81 \cdot 10^3$	$1.77 \cdot 10^5$	$4.69 \cdot 10^6$	HM, upscaled property (1/3 active fractures)
	$5.37 \cdot 10^3$	$1.40 \cdot 10^5$	$3.82 \cdot 10^6$	THM, upscaled property (1/3 active fractures)
STUK	500 ($1.5 \cdot 10^{10}$ s)	$1.1 \cdot 10^3$ ($3.3 \cdot 10^{11}$s)	$2.7 \cdot 10^{10}$ $7.54 \cdot 10^{17}$s	Without TM
	566 ($1.7 \cdot 10^{10}$s)	$1.2 \cdot 10^3$ ($3.58 \cdot 10^{11}$s)	$2.8 \cdot 10^{10}$ $8.12 \cdot 10^{17}$s	With TM
UoB	-	120 yrs ($3.8 \cdot 10^9$ s)	-	H base case (constant hydraulic aperture = 10 µm).
		$3.72 \cdot 10^5$		HM with (UCS = 39.6 MPa)
UPV		$1.5 \cdot 10^8$		Only H, σ=1detailed
		$1.7 \cdot 10^8$		Only H, σ=1upscaled

(β_{50} is taken as the travel time with Darcy velocity)

5.6. 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 works can only be regarded as a start for understanding both the nature of the problem and the demanding computational skills and resources for further research. Some of the lessons learned and outstanding issues needs to be further investigated are summarized below.

- ❑ If modelling uses relaxed initial apertures as input the HM coupling is essential for capturing realistic permeability at depth. It appears that the 2 order of magnitude decrease as e.g. noted by the KTH team would account for most of the discrepancy between their modelled (assuming relaxed apertures). This raises the issue as to 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 process with uncertainty is the relation between hydraulic residual aperture and maximum mechanical aperture. Evidently this has a strong influence on the impact of the HM coupling. Related to this is the indication found on the significance of the increase of differential stress results in increasing the permeability and in channelling of flow path (potentially caused by fracture dilation).
- ❑ Some results (UoB) suggest that the impact of the variations of the mechanical properties is higher than the HM coupling. However, most of the research teams applied the mean mechanical properties for their HM analysis. However, the variability of mechanical properties and the impact on the performance measurements and the uncertainties were not thoroughly addressed, due at least partly to the extra computational resources demanded for such analysis which was not available for the present project.
- ❑ At the outset it was considered 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 were poorly constrained and that markedly different fracture densities could be generated that were consistent with the data.
- ❑ The fact that only a subset of fractures conducts fluid flow under in-situ conditions was not considered by all the team (except OPG to a certain extent), due partly to the additional time required, but not available for the present project, for more comprehensive characterization of the fracture system and flow testing results. All teams treated all fractures as formed by the same genetic failure mechanism and did not distinguish joints from veins from faults. None considered different scaling laws for each type of fracture. While it cannot be certain that such considerations would improve the predictive capability of flow and migration in fractured media, this nevertheless illustrates needs for more comprehensive system characterization needs for more reliable computer simulations. Besides the development of approaches for upscaling the coupled HM processes in fractured rocks, for which good progresses were made during BMT2, more in-depth considerations and more proper computational representations of actual physics of the problem and existing data ought to be considered in future.
- ❑ There has been relatively little difficulty in interpreting the orientation distribution as given in the test case definition. However, there is room for interpretation on how to use these distributions, which are given in 3D, for the 2D applications.
- ❑ There is considerably more uncertainty in the interpretation of fracture size. Of particular interest are assumptions made on correlation between size and hydraulic properties. Such assumptions may have a large impact on the upscaling rules.

- There was also various approaches to selecting the fracture density. Provided consistency checks are made on various measured properties, this may in fact turn out to be useful for bounding the fracture intensity used in subsequent simulations, but attention to the problem is needed since fracture intensity has a key impact resulting upscaled hydraulic and mechanical properties.
- The spatial model chosen for the generation of fractures might have a significant influence on the calculation and simulation of effective hydraulic conductivity. Again, there are differences between teams, which originate from assumptions (necessary) rather than from hard information data.
- It is judged that differences in results of equivalent permeability between teams depend essentially on whether the team used given apertures as input - and then calculated fracture transmissivity using the cubic law – or if the hydraulic test data were used to calibrate the fracture transmissivity distribution. Still, for teams using the hydraulic information, the deviation between teams is at least an order of magnitude different fromthat given in the test case definition.
- The issue of effects of fracture size versus aperture (or permeability) was not considered in the study. Different assumptions on this would, although not really tested in BMT2, lead to large differences in upscaled properties. While calibrating against single hole hydraulic tests would take away most uncertainty as regards the stress/aperture impact, this is not the case as regards the size/aperture relation.
- From the BMT2 study it cannot be concluded regarding to the question whether upscaling needs to be done using a DFN approach (which most teams applied) or if stochastic continuum approaches would suffice. It can be expected, that more extreme assumptions of the fracture size versus aperture relation would show a more dramatic difference between these approaches.
- It is basically no surprising that the TM processes has very limited impacts on the far-filed nuclide transport processes, since their significant effects is basically at the near-field of the repositories with impacts of excavation and EBS performance, which were not considered in BMT2. For more complete PA/SA studies the THM impacts on the mechanical integrity and operational safety of the repository, and its effect on the change of transport properties, such as EDZ or permanent property change, should primarily be investigated at near-field scale..

6. Executive summary of BMT3, Task 3

6.1. Background and objectives

Geological evidence has indicated that mid- to high-latitude locations in the Northern Hemisphere have experienced glaciation/deglaciation cycles in recent geological history. These cycles are likely to recur in the future within a time frame of several hundred thousand years and have to be considered in performance assessments of deep geological repositories of long lived nuclear wastes.

Bench Mark Test 3 (BMT3) of DECOVALEX III (also Work Package 4 of BENCHPAR) has been designed as a generic numerical study to investigate the coupled Thermo-hydro-mechanical (THM) impacts of a glacial cycle on the long-term (up to 100 000 years), post-closure performance of the geosphere in which a hypothetical repository is located**.**

The objectives of BMT3 are:

1. To study, by analytical and/or numerical modelling, the long-term evolution of a fractured rock mass in which a generic repository is located, as it undergoes a glaciation/deglaciation cycle in a time frame of 100 000 years;
2. To assess the impact of the coupled mechanical and hydraulic responses of the repository system to a glaciation/deglaciation cycle on its long-term performance in waste isolation; and,
3. To improve the geoscientific basis to support the safety case for a deep geological repository.

This summary is based on the final report of BMT3 (Chan et al., 2004), team progress and/or final reports (Chan and Stanchell, 2003; Chan and Stanchell, 2004; Vidstrand et al., 2003; Wallroth et al., 2002; Wallroth et al., 2003; Aalto and Hartikainen, 2004) and papers in the proceedings of GeoProc 2003 (Boulton et al., 2003; Chan et al., 2003a; Boulton and Hartikainen, 2003).

6.2. Work organization

Within BMT3 there were three types of numerical modelling studies:

- Type 1: Continental scale coupled THM ice-sheet/drainage modelling;
- Type 2: Site-scale coupled THM permafrost modelling; and
- Type 3: Site-scale coupled HM rock mass modelling.

The primary purpose of Type 1 modelling 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 modelling focused on simulating the time evolution of subsurface temperature and permafrost although hydraulic heads and stresses were also calculated. Type 3 modelling focused on the first two objectives above. Subsurface heads, Darcy velocities, displacements and stresses were calculated. Naturally, Objective 3 above was a common goal for all three types of modelling.

Four research teams participated in BMT3, as shown in Table 6.1.

Table 6.1. Research teams and their participation in BMT3

FO	**Team (acronym)**	**Code**	**Numerical Method**	**Model Type**
EU[a]	University of Edinburgh (UEDIN)	RC[b]	FDM[c]	Type 1
OPG	Atomic Energy of Canada Ltd. (AECL)	MOTIF	FEM[d]	Type 3
SKB/EU[a]	Chalmers University of Technology (CTH)	ABAQUS	FEM	Type 3
STUK	Helsinki University of Technology (HUT)	RC[b]	FEM	Type 2

[a] Through the BENCHPAR Project; [b] RC = research code; [c] FDM = finite difference method; [d] FEM= finite element method.

6.3. Problem definition

Although BMT3 is a generic modelling exercise, 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.

The model domain encompasses a volume approximately 25 km x 37 km x 4 km (depth) and consists of sparsely fractured rock, moderately fracture 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. Figure 6.1 shows a simplified topographic map of the WRA, as well as the plan view of the conceptual model boundaries and the approximately 2 km x 2 km x 10 m (thick) repository. The model boundary follows the Winnipeg River system except in the Northeast where it coincides with a major fault. 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, that is lake Lac du Bonnet, is 255 masl. For modelling purpose 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 ground surface. Within the WRA the general topographic gradient slopes from SE to NW.

The network of major fracture zones has been idealized so that there are 17 fracture zones (Figure 6.2), 12 at the vertical boundaries and 5 in the interior of the conceptual model. Of the five interior fracture zones two are vertical, one is horizontal and two are dipping at 45°. In particular, the long horizontal fracture zone was included to study the possibility of glacially induced hydraulic jacking. Hydraulically, the background rock mass was represented by 13 layers with horizontal permeability, k_H, decreasing with depth from 10^{-15} m^2 near surface to 3.35 x10^{-20} m^2 at the assumed repository level just below 500-m depth and to approximately 10^{-21} m^2 at 750-m depth. Below this depth k_H remains constant at approximately 10^{-21} m^2. Vertical permeability was assumed to be 10 k_H for the top 300 m. Below this depth the rock was assumed to be isotropic hydraulically. Porosity was assumed to be 0.003 for the background rock mass. For the vertical fracture zones k was assumed to be 10^{-13} m^2 from surface to 400-m depth, below which it decreases rapidly downward. The horizontal and dipping fracture zones were assumed to have k value of 10^{-13} m^2 at all depths.

The following mechanical properties were assumed for the rock mass: density = 2650 kg.m^{-3}, Young's modulus = 35 GPa, Poisson's ratio = 0.22, cohesion = 5 MPa and internal friction angle = 30°. For the fracture zones Young's modulus = 3.5 GPa, cohesion = 3 MPa and friction angle = 25°. Biot's hydroelastic coefficient, α, was assumed to be 1.0 everywhere. The in-situ stresses were the mean of typical Canadian Shield values and Beberg (Sweden) values..

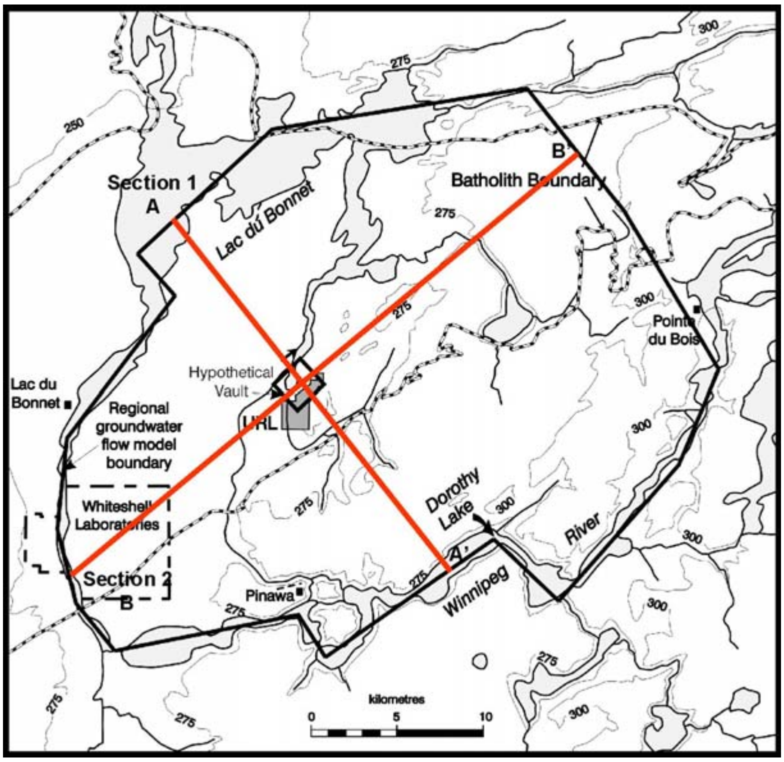


Figure 6.1: Simplified map of the WRA.

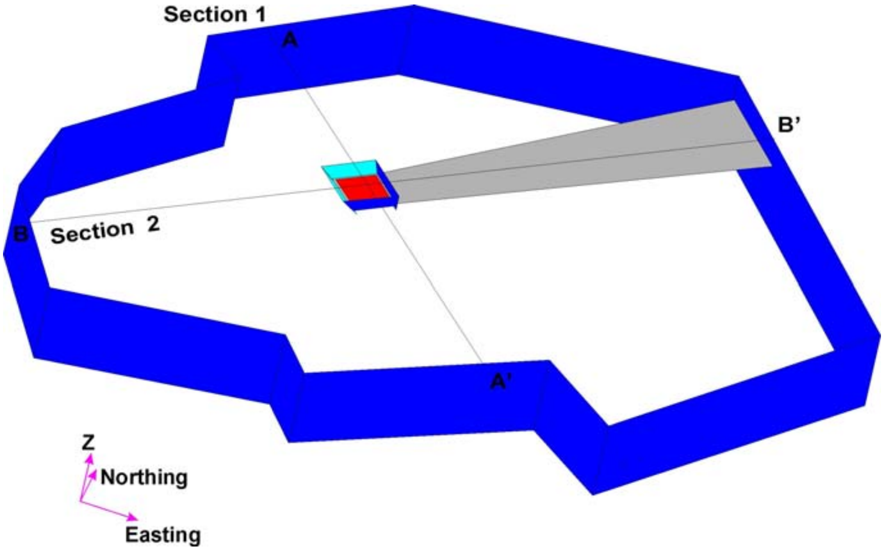


Figure 6.2: A 3D view of the simplified WRA fracture zone structure for BMT3. The dark blue panels are vertical fracture zones, the light blue panels are low dipping fracture zones, the grey panels are horizontal fracture zones and the red panel is the hypothetical repository location.

The modelling exercise was divided into three phases. In Phase I the UEDIN team enhanced its numerical tools for simulations of the climate drive, ice-sheet loading and basal thermal and hydrological regime; the HUT team conducted some preliminary studies on coupled 1D and 2D processes pertaining to permafrost development, while the AECL and CTH teams performed 2D site-scale coupled HM subsurface modelling using several sets of generic steady-state boundary conditions.

In Phase II the UEDIN team performed 3D ice-sheet/drainage modelling and averaged over 2D swats to generate transient thermal boundary conditions for 2D permafrost modelling by HUT and transient hydraulic and mechanical boundary conditions for the 2D transient site-scale coupled HM subsurface modelling by AECL and CTH. Permafrost modelling in Phase II involves coupled analytical THM-salinity modelling and 2D coupled THM numerical modelling with effects of salinity on the water/ice phase change.

In Phase III UEDIN 3D ice-sheet/drainage simulations to generate time-dependent 2D mechanical and hydraulic boundary conditions to be used directly by AECL in its 3D coupled HM site-scale rock mass modelling while CTH extended its 2D model to 3D.. 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 (Boulton and Hartikainen, 2003) and to the WRA (Aalto and Hartikainen, 2004).

6.4. Modelling approaches

6.4.1 Ice-sheet/drainage modelling

Several steps are taken in ice-sheet/drainage modeling. A highly simplified description follows:

Step 1 – Simulation of the climate drive

The simulations covered the whole of the last glacial period from 120,000 years ago (120 ka) to the present. The pattern of climate change was derived from the record from the Greenland ice sheet (Johnsen et al., 1992), adapted to the region using palaeo-climatic data from southern Canada and the northern USA and synoptic extrapolations.

Step 2 – Ice sheet loading and basal thermal and hydrological regime

A transient thermo-mechanical ice sheet model (Boulton and Payne, 1994) coupled with the Earth model of Lambeck et al. (1998) was driven by the climate function over a prescribed topography of North America with a 15 km resolution. The model computes the temperature at the base of the ice sheet and the rate of basal melting in time and space. This was used to compute the spacing between channels that are required to exist at the ice/bed interface to discharge meltwater that cannot be discharged by groundwater flow (Boulton et al., 2001), and thereby the head distribution at the ice/bed interface.

6.4.2 Permafrost modeling

A transient model of permafrost development based on macroscopic thermodynamics of mixtures and implemented in a finite-element code (Mikkola and Hartikainen, 2001) is driven directly by the climate function when there is no ice sheet present. When the ice overrides the site, one of the following approaches is used:

i. The temperature at the base of the ice sheet is used as a boundary condition for permafrost development (Phase II).
ii. Excess heat flux from ice shearing and, in case of ice sheet sliding, frictional heating is transferred to the subsurface permafrost model through the ice/bed interface (Phase III).

6.4.3 Coupled hydro-mechanical rock mass modeling

The AECL team used an in-house MOTIF finite-element code (Guvanasen and Chan 2000), which is based on the classical poroelastic theory of Biot (1941). In this code the solutions of the fluid flow equation and the mechanical equilibrium equation are iteratively coupled. The CTH team employed the commercially available, general-purpose finite-element code ABAQUS/Standard 6.3 (ABAQUS manuals). The porous medium is considered as a multiphase material (comprising solid grains, free wetting water and trapped water) and an effective stress principle is used to describe its behaviour. Biot’s (1941) analytical solution for 1D consolidation in the form presented in (Chan et al., 2003b) was utilized to guide the selection of an appropriate value for the bulk modulus of the “mineral grains” for the low-permeability, low-porosity rock in BMT3. Time-dependent mechanical and hydraulic boundary conditions were transferred from the ice-sheet/drainage model to the subsurface rock mass model at the ice/bed interface. Details of other boundary conditions can be found in the references given in Section 6.1.

6.5 Summary of results

Ice-Sheet/Drainage Modeling

Glaciological modelling of the Laurentide ice sheet through the last glacial cycle suggests that the WRA was glaciated at about 60ka and during the glacial maximum, between about 22.5ka and 11ka B.P. (before present), which is compatible with geological evidence from the region. The ice front advanced across the model domain in about 100 years. During the 11 000-year glaciation period at this site maximum ice sheet thickness reached approximately 2500m while maximum water pressure head at the ice-bed interface exceeded 2000m. Three subglaical channels, with significantly reduced (by up to 500-m head) water pressures, developed at the top of the site-scale model domain.

Permafrost modelling

Under extreme periglacial conditions permafrost is able to develop into depths comparable to or below the assumed 500-m repository horizon. As the glacier overrode the model domain, the warming effect of the ice sheet progressively increased subglacial temperatures and caused permafrost to decay to almost zero thickness 6000 years after the glacier arrived at the site. During the last glacial maximum large hydraulic heads and gradients developed in the in the thawing zone of permafrost wedge under the glacier. Salinity seems to have only a slight effect on temperature distribution but affects development of perennially frozen subsurface somewhat more by depressing the freezing point of water.

Rock mass hydro-mechanical modelling

Simulation results indicate the following subsurface consequences of glaciation:

- High sub-glacial hydraulic heads are rapidly transmitted down fracture zones to 500-m depth in less than 10 years. Heads at 500-m (assumed repository depth) increases rapidly, reaching values >2 000 m as ice-sheet thickness increases to 2 400 m in about 2 000 years. During ice sheet advance head values in fracture zones can be 400-500 m higher than in the surrounding low-permeability rock or the repository zone. Very high downward hydraulic gradients, up to 10m/m, develop at nominal repository depth as the ice sheet advances across the model domain. Upon deglaciation these hydraulic gradients reverse their direction.
- The glacially induced hydraulic response completely dominates over the gravity gradient due to local topographic variations.
- Maximum average linear groundwater velocities are of the order of 10 m/year in the fracture zones and 10 cm/year in the repository zone, 2-3 orders of magnitude higher than under non-glacial conditions.
- A particle-tracking analysis by AECL indicates that surface water recharges to greater depths than that under non-glacial conditions but does not reach the repository depth.
- Disconnecting two fracture zones reduces the linear ground water velocity there by about two orders of magnitude.
- Coupled HM simulations using transient boundary conditions obtained from UEDIN's ice-sheet/drainage simulations to represent a glacial event have yielded markedly different evolution of the flow field than in 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 throughout the model domain increase dramatically, up to 800-m head, equivalent to about 1/3 of the pressure due to the weight of the ice sheet by HM coupling. With uncoupled simulations hydraulic head distribution below a certain depth remains unchanged from the initial non-glacial conditions.
- High residual excess pore pressure (approximately 250 m higher than hydrostatic at 800-m depth) remains 10 000 year after the ice sheet has retreated off the model domain at nominal repository depth or below due to the very low hydraulic diffusivity of the rock, suggesting the flow system is currently in a transient state of slow recovery towards equilibrium.
- Due to the counter-balancing 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 fraction zone shown in Figure 6.2) of the values predicted by uncoupled mechanical modelling. The minimum effective stress in this fracture zone is compressive with a magnitude of few MPa so that no hydraulic jacking is predicted. Neither is shear failure predicted. Principal effective stress ratio and orientation vary during glaciation. Uncoupled stress analysis leads to

significantly higher (i.e., optimistic) factor of safety than the coupled HM model.
- In a 3D model the fracture zones are better connected than in 2D models. Consequently, the influence of sub-glacial channels - the remnants of which are eskers - is stronger and maximum groundwater velocities are twice as high as those found in 2D simulations.

6.6. Scientific achievements

The transient coupled hydro-mechanical modelling in this study represents a major step forward in advancing the state of the science for modelling and understanding geosphere response to glaciation. Although models of glacier-groundwater, glacier-permafrost-groundwater and glacier-groundwater-shallow failure systems have been presented previously, this BMT is one of the first attempts to assess impacts 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 to interface with site-scale subsurface modelling. The results provide valuable insights into the magnitude and rate of change of site-specific hydro-geological and geo-mechanical responses to external, transient climate forcing. They clearly demonstrate the importance of glaciation scenarios in performance assessments and the reality of 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 the two computer codes, ABAQUS and MOTIF, in modelling site-scale subsurface response to a glacial event. Although no enhancement to these two codes were undertaken within the BMT3 study, 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 reasonably site-specific, though somewhat simplified, hydraulic and mechanical attributes. Results indicate the possibility of high hydraulic gradients, high flow velocities and flow reversal during deglaciation, high residual pore pressure long afterwards, and faster and deeper surface water recharge. Large hydraulic gradients can appear at the glacier terminus or near the sub-glacial channels. The extensive and thick ice-sheet diminishes the influence of topographic gradients, so that the groundwater flow regime beneath a continental ice-sheet is controlled primarily by the glacially induced hydraulic and mechanical boundary conditions, the geometric structure of the fracture-zone network and the spatial distribution of hydraulic properties. Additional groundwater pressure on waste containers during glaciation approaches that equivalent to the ice thickness. Mechanical responses, though complicated, are relatively mild. No hydraulic jacking or hydraulic shearing is indicated at nominal repository horizons although changes in orientation and ratio of principal effective stresses have been predicted. Coupled HM modelling with Mohr-Coulomb failure criterion suggests significantly lower factor-of-safety values than uncoupled modelling. Further work may be necessary to investigate whether the latter changes need to be taken into consideration in repository design for some waste management organization.

Other achievements include thermodynamic coupling between the ice-sheet and permafrost modeling, enhancement of the permafrost model with regard to salinity effects and demonstration of applicability to 2D (simplified) site-specific coupled THM simulations of permafrost development and effects.

6.7. Lessons learned and outstanding issues

Although our approach has provided a systematic and structured framework for assessing the relative importance of coupled H-T-M impacts on geosphere performance, a number of improvements on problem definition, work organization and numerical modeling have been identified in the course of this BMT3 study. Some of the lessons learned and outstanding issues are summarized below.

Problem definition

It was found in Phase I that using in situ stresses that represent averaged values in the shield areas in conjunction with pessimistic fracture zone mechanical strength, can lead to inconsistent model predictions of some fracture zones failing under ambient in situ stress and hydraulic pressure conditions even without glaciation. It is the opinion of some participants that in similar future numerical studies, it would be preferable to use site-specific data from one site, or at least one type of geological environment, in defining the problem right from the beginning. An added advantage of using site-specific data is that subsurface modeling results can be compared with hydrogeological monitoring, paleohydrogelogical and hydrogeochemical data to check for consistency.

Work organization

In BMT3 initiation of ice-sheet/drainage modeling, which was funded by EU through BENCHPAR, lagged behind initiation of rock mass HM modeling, which was funded by DECOVALEX III FOs, by one year. Since the former type of modeling generates boundary conditions for the latter type of modeling, this has made it difficult for the latter work to be completed on schedule. Similar future work should be organized in such a way as to avoid this type of situation.

Mechanisms and processes

For simplicity, the effects of variable salinity and effective stress-dependent permeability have been excluded from the coupled HM rock mass modeling in BMT3. These should be included in future studies. Secondly, additional sensitivity analysis should be performed to investigate the effects of uncertainty in input parameters and boundary conditions on coupled HM rock mass modeling results. For example, the possibility of re-activation of faults can be studied using mechanical boundary conditions different from the zero-normal displacement or fixed bottom boundary condition in BMT3/WP4. Thirdly, the influence of permafrost was only investigated in Phase I by AECL and CTH using no-flow boundary conditions. Improved representation of permafrost, e.g., as a zone of reduced permeability may be attempted in the future. Finally, the ice-sheet/drainage model and the site-scale models were performed sequentially and interfaced through boundary conditions in BMT3, but should really be coupled to allow feedback to occur.

Code improvements

The participating codes may be enhanced to incorporate the capability to model the above-mentioned mechanisms and processes as well as improved numerical efficiency and accuracy, especially in computing derivative quantities such as Darcy velocity and effective stress. Some of the codes already have special types of finite elements that can be used to simulate discrete fractures or fault zones. Other codes would need to be further developed to incorporate such capability. Once these improvements have been made the codes should be used with simple structural models to explore the importance of the various processes before being applied to site-specific problems.

Implications for performance assessment

Performance measures in BMT3 have included changes in hydraulic heads, Darcy velocities, mechanical displacements and stresses, together with failure evaluation using the Mohr-Coulomb criterion and particle tracking. It is recommended by some participants that radionuclide transport simulations be also undertaken in future studies to better assess the impact of glaciation on the performance of the geosphere in which a deep geological repository is located.

7 Executive summary-Task 4

7.1. Background

The Task 4 is a part of the International DECOVALEX III project on coupled thermo-hydro-mechanical (T-H-M) processes focuses on T-H-M modelling applications in safety and performance assessment of deep geological nuclear waste repositories. A previous phase, DECOVALEX II, saw a need to improve such modelling (Stephansson et al., 1999). As a result of an elicitation and compilation of the state-of-knowledge statements, and subsequent extensive internal and external reviews, four of the most important issues are identified as follows:

- Clarifying the Role of THM Processes for PA.
- Demonstration Analysis of Disposal System Stability.
- Study of the Scale-Dependent Properties Relevant to Repository Design and Performance.
- Technical Auditing Demonstration of the Overall Modelling and a Specific Numerical Code.

These issues were considered for further evaluation and study in the Task 4 of DECOVALEX III. This summary presents the findings and strives for reaching recommendations in addressing coupled T-H-M issues in safety assessments, based on the final report of Task 4 (Andersson, 2003).

7.2. Objectives and scope

The task sets out to derive conclusions and recommendations on practices in addressing THM issues in Performance and Safety Assessment Applications, based on the findings of DECOVALEX III. More specifically the task intends:

- to provide concrete examples on when T-H-M couplings may need to be considered in a quantitative fashion in post-closure performance assessment of nuclear waste repositories in hard rock formations and when T-H-M couplings not need to be considered in such assessments,
- to provide a practical approach for the general problem of simplifications of T-H-M analyses such that they can be properly incorporated in Performance Assessment analysis, and to evaluate uncertainties introduced through such simplifications.

7.3 Works performed

In order to address the issues as addressed above, Task 4 has:

- Analysed two major T-H-M experiments (Task 1 and Task2) and three different Bench Mark Tests (Task 3) set-up to explore the significance of T-H-M in some potentially important safety assessment applications.
- Compiled and evaluated the use of T-H-M modelling in safety assessments at the time of the year 2000, using a questionnaire and answers by the concerned

funding organizations in the DECOVALEX III project (see Appendix A in Andersson, 2003).
- Organised a forum of interchange between PA-analysts and THM-modellers at each DECOVALEX III workshop.

7.4. Major findings through the questionnaire-answers forum

The answers received during 2000 were compiled with the following conclusions:

Most organisations already apply standardised procedures for identifying processes and couplings to be considered in assessments. However, it seems that these procedures are more as a means of stating the confidence in that all relevant (T-H-M) processes are indeed considered in the safety assessment rather than as tools for identifying previously non-considered processes or couplings. Providing a motivated statement of confidence is indeed a crucial part of a safety assessment report, and here the formal approaches are valuable. Judging from the answers the impression is that most T-H-M issues are already identified. One should not expect dramatic surprises if applying such procedures. (It is rather the means of analysing the couplings that needs to be discussed.)

Several examples of identified problems where T-H-M couplings are shown to be important or are judged to be potentially important to be considered directly in a safety assessment context are given such as:

- The migration of vapour, water and heat in partially saturated systems.
- The mechanical stability of the underground excavations before and during construction.
- The potential for and the effect of rock creep.
- Mechanical effects such as rock fall or fracture shear displacements resulting from earthquakes.
- The understanding and modelling the formation and resulting hydraulic properties of a disturbed zone (EDZ) around tunnels.
- Stress and stress change impact on fracture hydraulics.
- The consequences of a glacial ice cover.
- Full thermo-hydro-mechanical couplings when analysing the resaturation of the buffer.
- Heat pulse driven rock fracturing and permeability changes due to theromechanical deformation of fractures, where a full thermo-hydro-mechanical analysis is potentially needed.

In conclusion, T-H-M issues need to be considered in repository R&D, both as regard modelling, field experiments and repository design and Safety Assessment.
Although PA/SA is built around simplifying abstractions/assumptions, T-H-M modelling coupled with appropriate testing is still needed to understand how the hydrological system works, in order to rationalize the abstractions.

7.5. Presentation cases at the Task 4 themes of the DECOVALEX III workshops

A number of PA/SA experts were invited to give presentations on PA7SA practices of different organizations, related coupled processes and their treatments in PA/SA practice. They include:

- P. Zuidema, NAGRA, Switzerland: Safety case and THM coupling;
- J. Alonso, ENRESA, Spain: THM issues in the ENRESA 2000 project;
- M. Yui, JNC, Japan: Safety Assessment, THM(C) and Monitoring – Japanese experiences;
- T. Vieno, VTT, Finland: THM Aspects in the POSIVA Safety Case.

7.6. Issues discussed at DECOVALEX III workshops

A set of issues evolved during the course of Task 4 discussions that can be summarized as follows:

Are most THM-related FEPs both identified and sufficiently understood?
Can we formulate workable performance measures for judging relevance of THM coupling?
Can the identified FEPs be managed through the appropriate combination of design, process modelling and scenario analysis?
Do we need to consider coupled HM outside the near-field?
Is there a need to couple THM with transport of RN (apart from the indirect coupling though hydrogeology)?
What do we need to now as regards short term EBS evolution and monitoring and its relation to System Safety?
Is the interaction with the "PA-people" actually taking place within your organisation and is it used to inform, set priorities and define needed level of accuracy?
Where should (further) THM-related R&D focus?

7.7. Findings and implication of the different DECOVALEX III tasks

7.7.1. Task 1

a) Relevance to safety case

The work is aimed at gaining confidence on predicting models for barrier performance. Clearly, the bentonite buffer and its interaction with the near-field rock is an essential component of most deep geological repository concepts. This warrants both experimental and theoretical studies as better understanding in general will support statements on the evolution of this repository component. However, for repository performance the outstanding issue is to assess the barrier performance over long times. Details in the re-saturation phase are not necessarily important unless they would imply long term remaining effects. The test case was focused on short term effects – and its relevance for long term effects remain to be addressed.

b)Performance measures

Given that the Test Case is only indirectly connected to the safety case, i.e. through its potential for enhancing understanding, also the useful performance measures could only be indirectly connected to the ultimate needs. This means that for the Test Case a typical performance measure is to compare model predictions with actual behaviour of the benchmark experiments. Furthermore, it must be understood that gaining confidence requires not only benchmark exercises but good experimental research at a basic level (material behavior should be understood).

c) Importance of couplings

These findings are summarized in Table 7.1.

Table 7.1 Task 1: Assessed Importance of Couplings

Coupling	Rating	Comments
HM and HM	High for pore water pressure	The development and dissipation of excess pore water pressures in the vicinity of the advancing tunnel is a clear example of hydro-mechanical interaction. However, the coupling did not seem important for modelling water inflow.
MT and TM	Low/Med	Stresses and deformations do not modify in a significant way thermal parameters. A limited second order effect comes through the change in porosity due to deformation Thermally induced strains significantly controls stresses in rigid/confined materials. Mechanical constitutive properties are not much affected in the range 20º-80º. Limited information beyond 100º.
THM	High in the buffer	Predicting the behaviour of the buffer under the combined heating and wetting actions requires a fully coupled THM formulation.

7.7.2. Task 2

a) Relevance to safety case

Task 2 involves developing a good understanding of heat-driven coupled processes such as TH, THM, THC and THMC surrounding a high-level nuclear waste repository. With respect to the safety case for the potential repository at Yucca Mountain, THM processes are considered to have little direct impact on the performance of the potential repository. Studying the heat-driven coupled processes enhances the thoroughness and credibility of the safety assessment by expanding and reinforcing the knowledge base supporting it.

At the highest level the overall performance measure is, of course, the calculated radiological risk (dose) to the public in the accessible environment within the performance period. At a much lower level the performance measure to assess the relevance of THM processes on the safety case is the nature and quantity of seepage into the drifts and their effects on the performance of the waste package.

b) Importance of couplings

According to the assessment team, see Table 7.2, there are no highly important THM-couplings going on at the experiment. The evolution could approximately be explained with uncoupled T, H, and M analyses.

c) Uncertainties

The major source of uncertainties in Task 2 is characterising the rock with large spatial variability of properties, especially hydrological properties. The other source of uncertainty is in effectively modelling the consequences of THM coupling capturing all the phenomena of significance.

Table 7.2 *Task 2: Assessed Importance of Couplings*

Coupling	Rating	Comments
TH	Medium	Changes in fracture water content cause changes in fracture permeability that may be recovered as the thermal pulse dies, and liquid water drains down emptying the fractures.
TM	Low	
HT	Low	
HM	Low	
MT	Low	
MH	Low	

7.7.3. BMT1-Task 3

a) Relevance to safety case?

From a safety point of view, engineering measures could be easily carried out to minimize the coupled effects. From the results of the present work, it appears that from a technical point of view the effect of coupling will be either short lived (several decades to 100 years) and would not impact on long term (thousands to hundred of thousand years) safety issues, or could be rectified by adequate design and operation methodology (e.g. avoid over-cooling the galleries).

b) Importance of couplings

Table 7.3 (Table 7.6 in Nguyen and Jing, 2003) summarizes the effect of different degree of coupling on the key performance and safety indicators in the near field of a repository. The rating of low, medium and high is rather qualitative and arbitrary, as explained in the preceding discussion. The definitions of low, medium and high are qualitative and given in the text. This table is also dependent on the case and scenario being analyzed and no generalization should be done.

From the results of the present work, it appears that from a technical point of view the effect of coupling will be either short lived (several decades to 100 years) and would not impact on long term (thousands to hundred of thousand years) safety issues, or could be rectified by adequate design and operation methodology (e.g. avoid over-cooling the galleries). The influence of the host rock properties (e.g. permeability) on the long term safety seems to be much more important than coupling, since one has much less control over these properties. However, the short term period where coupled processes are important corresponds to the repository construction and post closure

Table 7.3. BMT1: The effect of different degree of coupling on the key performance and safety indicators in the near field as assessed in BMT1.

	Temperature	Resaturation	Swelling stress	Rock stability	Rock permeability
THM	Low	Medium/High	High	High	Medium/high
TH	Low	Medium	-	-	Medium
TM	Low	-	Low	Low	Medium
HM		Low	High	Low	Low

monitoring periods for most disposal systems. These periods are crucial for confidence building, demonstration purposes, and public acceptance. In order to interpret and assess the monitoring data collected during the construction and post closure periods, we believe a fully coupled approach is necessary.

c) Uncertainties

The influence of the host rock properties (e.g. permeability) on the long-term safety seems to be much more important than coupling, since one has much less control over these properties. However, for confidence building and demonstration purposes, a fully coupled approach is necessary to interpret monitoring data that would be collected the first few decades after repository closure, since coupled processes would prevail during that period of time.

7.7.4. BMT2-Task 3

a) Relevance to safety case?

The scale of PA-models, or at least the far-field radionuclide transport models, is usually large compared to the scale where there is some understanding and data on HM couplings. This raises several issues:

- How should coupled processes and associated parameters be upscaled?
- Are the HM couplings significant in relation to the geometrical factors controlling the upscaling of permeability and rock mass mechanical properties (such as deformation modulus)?
- Are couplings at all significant compared to other uncertainties (network geometry, hydraulic properties, fracture constitutive laws)?
- What are the Site Characterisation Implications?

BMT2 is designed to address these issues. Ultimately, the performance measure for a repository PA would be doses or risk, however, in order not to introduce too many assumptions about the waste, release mechanisms or the retention properties of different species the general performance measures being studied here are restricted to the groundwater specific contribution to retention. The research teams were thus asked to predict:

- Flow related migration parameter in the form of “transit time distributions” and "transport resistance distributions" at two output surfaces.

- Intermediate results of upscaling (effective parameters) like effective permeability and rock mass deformation modulus for different block sizes.

b) Importance of couplings

Table 7.4 displays the assessed importance of the different couplings in BMT2. In short it is not evident that there are any highly significant THM couplings to be considered for this problem. Upscaling permeability from small scale measurements is indeed a difficult task, but there is little evidence from the test case suggesting the upscaling also needs to consider the added complexity of the THM-coupled effects.

Table 7.4. BMT 2: Assessed Importance of Couplings

Coupling	Rating	Comments
TH	Low	Not significant in large scale
TM	Low	
HAT	Low	
HM	Potentially important	Considered potentially significant. Important starting point in DFN upscaling. Not necessary to consider given other uncertainties, and given that hydraulic data is sampled at appropriate depths.
MT	Low	
MH	Potentially important	See HM

c) Uncertainties

It appears that the main uncertainties encountered in BMT 2 concern upscaling the parameters of individual processes. The currently listed major uncertainties include:

- Conceptualisation if fracture network data (the resulting upscaling is also very sensitive to this).
- Results sensitive to interpretation of fracture data.
- Software limitations especially with hydromechanical codes.
- THM uncertainty in relation to other uncertainties: the findings certainly suggest
- THM uncertainties in this case are small in relation to the upscaling and
- Geometrical uncertainties explored.

7.7.5. BMT3-Task 3

a) Relevance to safety case?

Boulton et al. (2003) conclude that safety assessments of the disposal of long lived radioactive wastes in the middle to high latitudes of the northern hemisphere must recognise that these areas have been repeatedly glaciated in the recent geological past, and that were it not for the prospect of human induced global warming, would expect an imminent descent into glaciation.

Glaciation has the potential to influence strongly the geosphere to the preferred depths for deep disposal sites of between 500 and 1000m. The strongest potential impacts in periods of glaciation are associated with the extension of ice sheets in and perennial ground freezing to create “permafrost” to depths of several hundred metres. The involved processes are the product of a system driven by the Earth’s climate and characterised by strong thermo-hydro-mechanical coupling, in which both chemical processes and transient phenomena are important.

Boulton et al. (2003) also conclude that although models of glacier-groundwater, glacier-permafrost-groundwater, glacier-groundwater-shallow failure systems have been presented (e.g. Boulton et al, 1995), BMT3 is the first attempt to assess impacts at repository depths using site specific data. The results provide valuable insights into the magnitude and rate of change of site-specific hydrogeologic and geomechanical properties in response to external, transient climate forcing.

The most important general conclusions of BMT2 are that:

- Glaciation occur on a depth scale that is relevant to the safety of repositories buried several 100m beneath the surface;
- Glaciation occur on timescales that are relevant to safety assessments for long lived waste;
- Assessed impacts implies transient but several orders of magnitude effects on groundwater flow.

Boulton et al. (2003) thus conclude that the coupled processes connected to glaciation must be considered in safety assessments.

b) Importance of couplings

While the analysis points out several potentially important effects of future glaciations, still only some THM couplings need to be considered. For the analyses of the Whiteshell site Boulton et al. (2003) conclude that:

- The Hydro-Mechanical coupling effects on pore pressure is significant as there are high residual pore pressure for 1000s of years after glacier has retreated from the site,
- The thermal impact on hydrology and mechanics may be significant in terms of permafrost since permafrost may develop at repository depths,
- The Hydro-Mechanical impact in terms of potential hydraulic jacking at depth is unlikely to be important,
- The impact on stress and mechanical stability at depth is minor.

Table 7.5 displays the assessed importance of the different couplings in BMT3. In addition Boulton et al. (2003) remarks that the BMT used used four separate components, a climate model, an ice sheet-earth model, a permafrost model and an earth hydro-mechanical earth model. The ice sheet-permafrost models are weakly coupled but the climate and hydro-mechanical earth models are uncoupled from other components. The development of a model in which the system is fully coupled and driven only by global climate, with feedbacks between the ice sheet and local climate is necessary if the full consequences of coupling are to be understood.

c) Uncertainties

- The modelling teams note the following main uncertainties related to BMT 3.
- External climate driving ice sheet model.
- Site specific properties (rock type, fracture network geometry & connectivity, hydraulic properties, fracture zone strength) and scaling.

- Boundary Conditions, especially the hydraulic and mechanical state in the ice and in the bedrock at the ice/bedrock boundary, but also the hydraulic boundary conditions at the vertical boundaries.
- Model approximations, influence of salinity on flow omitted, representation of permafrost in HM models, Mesh fineness, model size.
- THM uncertainty in relation to other uncertainties: the modelling teams suggest the importance of e.g. spatial variability of rock mass permeability in relation to the process uncertainty is difficult to assess. The uncertainties due to THM coupling are not a subset of uncertainties due to spatial variability. It is judged that the two types of uncertainties are comparable in magnitude for the BMT3 case.

Table 7.5. BMT 3: Assessed Importance of Couplings

Coupling	Rating	Comments
TH, HT	Low (High in terms of permafrost)	The thermal impact on hydrology and mechanics may be significant in terms of permafrost since permafrost may develop at repository depths;
TM, MT	Low (High in terms of permafrost)	See above
HM, MH pore pressure	High	High residual pore pressure for 1000s of years after glacier has retreated from the site
HM, MH hydraulic jacking and stress	Low	The Hydro-Mechanical impact in terms of potential hydraulic jacking at depth is unlikely to be important; the impact on stress and mechanical stability at depth is minor;

7.8. Lessons learned and outstanding issues

7.8.1.Judging Relevance – Performance Measures

Although the geosphere is a system of fully coupled processes, this does not directly imply that all existing coupled mechanisms must be represented numerically for all the problems. Modelling is conducted for specific purposes and the required confidence level should be considered. The modelling style and content depends on the objectives — which are to be judged, inter alia, against performance measures and the confidence required, given the available capabilities in terms of codes and data. Performance measures should be identified, making it possible to explore how assumptions, uncertainties and confidence affect the issues of concern.

Useful performance measures should be sought in the context of model predictions that may affect decisions. The decisions may concern a wide range of issues e.g. licensing a nuclear waste repository, selecting a proper grouting scheme or deciding whether a scientific investigation is good enough for the overall objectives. A common performance measure for a nuclear waste repository is the yearly risk of death to an individual due to the repository evolution and potential radionuclide releases. Such overall performance measures are usually to be found in regulations. However, useful performance measures can also be related to intermediate conditions potentially affecting these ultimate measures.

The key impact of T-H-M processes as regards repository performance is of course disposal concept and site dependent. Nevertheless, the following T-H-M-related conditions often are linked to overall repository performance:

- The water pressure or water content in buffer and rock
- Temperature in buffer and rock,
- Formation and properties of an EDZ,
- T-H-M effects on parameter estimation from site or laboratory experiments,
- Mechanical stability of emplacement drifts
- Significant changes of permeability (temporal and permanent)

In conclusion, when assessing importance of T-H-M for repository performance, care is needed to formulate relevant yet revealing performance measures against which to assess the outcome of the analysis.

7.8.2. Identification of T-H-M Processes

During the course of DECOVALEX III there has been little reason to alter the conclusion made already at the beginning of the work that *Most processes/issues (i.e. FEPs) where there potentially is need to consider T-H-M-couplings for the currently considered waste disposal concepts are identified.* However, there is still a need to evaluate to what extent potentially important processes or couplings actually need to be included in an assessment.

The uncertainty stemming for potential improper incorporation of coupled processes has to be weighed against the importance of other uncertainties. In particular spatial variability of properties is often a very important source of uncertainty in geologic media. Another aspect of model uncertainty in geologic media concerns the basic principles for describing the host rock mass, or as often called the conceptual model of the rock mass, such as ‘fractured crystalline rock’, ‘complex deformation zones’, ‘sedimentary rock’, volcanic regions’, ‘high stress rock’ etc. Clearly, the conceptual model affects how data are interpreted and the overall confidence in the system description.

7.8.3. Examples where T-H-M Couplings Need to Be Considered in Safety Assessments

a) Near-field effects

Resaturation of the buffer: Task 1 concludes that predicting the behaviour of the buffer under the combined heating and wetting actions requires a fully coupled THM formulation, which incorporates all the necessary physical processes controlling the bentonite behaviour. However, the only safety implications would occur if the resaturation process implied any long term effects. In many assessments, where container failures happen long after the saturation, the details of the resaturation phase are inconsequential.

Interactions between rock and EBS: The analysis of Task 1, Task 2 and BMT1 demonstrates the saturation of the buffer between the heat producing waste container and the near field rock involves the interaction between heat, vapour, flowing water transport and stress. From the results of the present work, it appears that the effect of coupling will be either short lived (several decades to 100 years) and would not impact on long term (thousands to hundred of thousand years) safety issues, or could be rectified by adequate design and operation methodology (e.g. avoid over-cooling the galleries). In general, it seems that the influence of the host rock properties (e.g. permeability) on the long-term safety seems to be much more important than coupling, since one has much less control over these properties. However, for confidence building and demonstration purposes, the coupled effect should be considered.

Long term mechanical stability of disposal vaults: This issue has not really been studied within the DECOVALEX III framework.

b) Far-field effects

Groundwater flow in the far-field: The analyses of BMT2 in particular, suggest that modelling groundwater flow in the far-field would generally not need to consider mechanical or thermal impacts, even thought they exist. The effects are small in relation to performance measures and the uncertainties due to spatial variability. However, in understanding the permeability field and its anisotropy, coupled effects may be crucial, as processes like fracture dilatation caused by past stress changes may have a large impact.

Future large scale events (glaciation and permafrost.): BMT3 demonstrates that future large scale events, like glaciations and permafrost, will mobilise several processes and couplings. Still, it is not evident that all these processes actually need to be modelled, since the details of the glaciation may have little impact on actual performance. Nevertheless, further assessment of the processes affecting hard rock formations during glaciations and other extreme climate effects, like deep permafrost, are warranted.

Need to consider THM directly when modelling radionuclide transport: BMTs of the DECOVALEX III project demonstrated impact of THM couplings on the groundwater flow. However, in none of these cases were the T or M impacts on H anything but secondary (see previous paragraphs). TM impacts on the rock matrix aspects of radionuclide migration have not been explored within DECOVALEX III project, but the effects, if any, are judged to be small.

c) Implications on site characterisation.

There are also coupling implications as regards site characterisation. This concerns the formulation of an appropriate conceptual model and how to interpret what is actually measured in a field test.

As demonstrated both in BMT1 and BMT2 a key process, where there still is uncertainty is the relation between hydraulic residual aperture and maximum mechanical aperture. Evidently this has a strong influence on the impact of the HM coupling. Related to this is the indication found in BMT2 on the significance of the increase of differential stress results in increasing the permeability. Still, this does not necessarily imply that the actual data analysis needs to be conducted with coupled codes.

d) T-H-M related to monitoring, retrievability and closure

Coupled processes need also be considered in relation to short term monitoring. Arguably, it will be necessary to explain and predict monitored changes at a repository site, even if these changes may not have implications for repository safety. Confidence in the safety predictions may be in jeopardy in case observed changes in the short term are not reasonably understood. Here, more coupled phenomena, including chemical couplings, may potentially be significant. Still long term monitoring needs to be connected to issues of relevance to performance. Also decisions not to seal a repository or to retrieve waste from it have long term implications, and such decisions should only be made in case they really can be justified.

e) Reporting Safety Assessments - the Safety Case

In making the Safety Case of geological disposal considering THM processes is important for demonstrating understanding. It is necessary for scientific credibility in general but also for the demonstration of the confidence in the understanding of the system. Performance and safety assessments are built around simplifying abstractions (rather than assumptions). It is necessary to acquire a knowledge base supporting an understanding of how the hydrological system works, in order to construct the abstractions. Regardless of the approach selected to PA/SA, evidence should be provided to substantiate simplifying assumptions that consider both time and space. The knowledge base needs to be presented, and reasonable conclusions should be drawn, directly in the PA/SA report.

7.9. Conclusions

The full development of T-H-M modelling is still at an early stage and it is not evident whether current codes provide the information that is required for PA/SA. However, although the geosphere is a system of fully coupled processes, this does not directly imply that all existing coupled mechanisms must be represented numerically. Modelling is conducted for specific purposes and the required confidence level should be considered. It is necessary to match the confidence level with the modelling objective.

Coupled THM modelling has to incorporate uncertainties, in the conceptual model and in data. Assessing data uncertainty is important when judging the need to model coupled processes, but also the confidence in the prediction need to be assessed. Even if comparing THM models with real data is a fundamentally difficult problem, it is not impossible, as demonstrated by Task 1 and Task 2 of DECOVALEX III.

- The emphasis on the need for THM modelling differs among disciplines. For geological radioactive waste disposal in crystalline and other similar hard rock formations DECOVALEX III shows it is essential to:
- Understand the stress-permeability couplings when interpreting stress and permeability field data,
- Understand the coupled processes involved in the re-saturation of the near-field,
- Understand the coupled processes involved in the development of an Excavated Disturbed Zone and
- Understand the coupled processes involved in the impact of large-scale and significant climatic events, like glaciations and permafrost.

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