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Research

DECOVALEX-THMC Project

Task D
Long-Term Permeability/Porosity Changes in the EDZ and Near Field due to THM and THC Processes in Volcanic and Crystalline-Bentonite Systems

Phase 1 Report

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Foreword

The DECOVALEX-THMC project is an ongoing international co-operative project that was stared in 2004 to support the development of mathematical models of coupled Thermal (T), Hydrological (H), Mechanical (M) and Chemical (C) processes in geological media for siting potential nuclear fuel waste repositories. The general objective is to characterise and evaluate the coupled THMC processes in the near field and far field of a geological repository and to assess their impact on performance assessment:

- during the three phases of repository development: excavation phase, operation phase and post-closure phase;
- for three different rocks types: crystalline, argillaceous and tuff;
- with specific focus on the issues of: Excavation Damaged Zone (EDZ), permanent property changes of rock masses, and glaciation and permafrost phenomena.

The project involves a large number of research teams supported by radioactive waste management agencies or governmental regulatory bodies in Canada, China, Finland, France, Germany, Japan, Sweden and USA, who conducted advanced studies and numerical modelling of coupled THMC processes under five tasks:

- **Task A**: Influence of near field coupled THM phenomena on performance assessment, initiated by CNSC, Canada.
- **Task B**: The Excavation Disturbed Zone (EDZ). MHC studies of the EDZ, initiated by SKB, Sweden.
- **Task C**: Excavation Damaged Zone (EDZ) in the argillaceous Tournemire site, France, initiated by IRSN, France.
- **Task D**: Permanent permeability/porosity changes due to THC and THM processes, initiated Department of Energy, USA.
- **Task E**: THM Processes Associated with Long-term Climate Change: Glaciations case study, initiated by OPG, Canada.

Work defined in these five tasks are divided into different phases or steps so that the progress can be monitored and achievements documented in project reports.

The present report presents the definition, achievements and outstanding issues of the Phase 1 of Task D, concerning the research activities, achievements and outstanding issues within Task D. with additional information provided in an attached CD, which includes various appendices.

Lanru Jing, Fritz Kautsky, Ove Stephansson and Chin-Fu Tsang

Summary

The DECOVALEX project is an international cooperative project initiated by SKI, the Swedish Nuclear Power Inspectorate, with participation of about 10 international organizations. The name DECOVALEX stands for **DE**velopment of **CO**upled models and their **VAL**idation against **Ex**periments. The general goal of this project is to encourage multidisciplinary interactive and cooperative research on modeling coupled processes in geologic formations in support of the performance assessment for underground storage of radioactive waste.

Three multi-year project stages of DECOVALEX have been completed in the past decade, mainly focusing on coupled thermal-hydrological-mechanical processes. Currently, a fourth three-year project stage of DECOVALEX is under way, referred to as DECOVALEX-THMC. THMC stands for **T**hermal, **H**ydrological, **M**echanical, and **C**hemical processes. The new project stage *aims at expanding the traditional geomechanical scope of the previous DECOVALEX project stages by incorporating geochemical processes important for repository performance. The U.S. Department of Energy (DOE) leads Task D of the new DECOVALEX phase, entitled "Long-term Permeability/Porosity Changes in the EDZ and Near Field due to THC and THM Processes for Volcanic and Crystalline-Bentonite Systems." In its leadership role for Task D, DOE coordinates and sets the direction for the cooperative research activities of the international research teams engaged in Task D.

The research program developed for Task D of DECOVALEX-THMC involves geomechanical and geochemical research areas. THM and THC processes may lead to changes in hydrological properties that are important for performance because the flow processes in the vicinity of emplacement tunnels will be altered from their initial state. Some of these changes can be permanent (irreversible), in which case they persist after the thermal conditions have returned to ambient; i.e., they will affect the entire regulatory compliance period. Geochemical processes also affect the water and gas chemistry close to the waste packages, which are relevant for waste package corrosion, buffer stability, and radionuclide transport.

Research teams participating in Task D evaluate long-term THM and THC processes in two generic geologic repositories for radioactive waste, with the ultimate goal of determining the impact of geomechanical and geochemical processes on hydrologic properties and flow patterns. The two repositories are simplified representations of possible repository sites and emplacement conditions considered by the participating countries. One repository is a simplified model of the Yucca Mountain site, featuring a deep unsaturated volcanic rock formation with emplacement in open gas-filled tunnels. The second repository is located in saturated crystalline rock; emplacement tunnels are backfilled with a bentonite buffer material.

During the past year, four international research teams from China, Germany, Japan, and USA have started research activities for the geomechanical and geochemical scenarios of Task D. As shown in the table, these teams are using different simulators with different model capabilities. Thus, good agreement of model results between the different teams (that use different simulators) would provide valuable supporting evidence for the validity of the various predictive models simulating THM and THC processes. Since all research teams model the same task configuration, research results from the participating teams can be compared.

Numerical simulator	Coupling	Research Team	Mechanical/ chemical model	Hydraulic and transport model
TOUGH-FLAC	THM	DOE/LBNL	Elastic Elastoplastic Viscoplastic	Single or dual continuum; multiphase liquid and gas flow
ROCMAS	THM	DOE/LBNL	Elastic Elastoplastic Viscoplastic	Single continuum; unsaturated liquid flow; thermal vapor diffusion
GeoSys/ Rockflow	THM	BGR Center for Applied Geosciences	Elastic Elastoplastic Viscoplastic	Single continuum; unsaturated liquid flow; thermal vapor diffusion
FRT-THM	THM	CAS Chinese Academy of Sciences	Elastic Elastoplastic Viscoplastic	Single continuum; unsaturated liquid flow; thermal vapor diffusion
THAMES	THM	JAEA Japan Atomic Energy Agency*	Elastic Elastoplastic Viscoplastic	Single continuum; unsaturated liquid flow; thermal vapor diffusion
TOUGHREAC T	THC	DOE/LBNL	Equilibrium and kinetic reactions, using HKF activity model	Single or dual continuum; multiphase liquid and gas flow; advection/ diffusion of total concentrations (sequential)
GeoSys/ Rockflow with PHREEQC	THC	BGR Center for Applied Geosciences	PHREEQC	Single continuum; unsaturated liquid flow; thermal vapor diffusion; advection/ diffusion of total concentrations (sequential)
COUPLYS with THAMES, Dtransu-3D-EL and PHREEQC	THMC	JAEA Japan Atomic Energy Agency*	PHREEQC	Single continuum; unsaturated liquid flow; thermal vapor diffusion; advection/ diffusion of total concentrations (sequential)

* The Japanese organization was recently renamed from JNC to JAEA. We have not been able to update the report parts accordingly; thus the text and figure references in this report still use the old name JNC.

The research work is performed in a collaborative manner with close interaction between the international research teams during meetings, visits, via email, and per telephone. This close collaboration among international top scientists and engineers is one of the major benefits from participation in DECOVALEX-THMC. First, interaction with top international scientists helps to further the understanding of geomechanical and geochemical processes related to geologic storage of radioactive waste. Second, the cooperative research work conducted in the field of THMC modeling provides valuable peer-review of the modeling analyses in this field.

The international research teams involved in Task D have made significant progress during the past year. At the current project stage, the geomechanical and geochemical modeling studies are conducted separately. (In later stages, the separate THM and THC model analyses may be integrated to a fully coupled geomechanical and geochemical analysis.) The teams working on THM processes finalized the model development work, and all four teams presented results of the first modeling phase (assuming simplified geomechanical processes). Comparison of these results indicates a good overall agreement between the research teams (see example for comparative evaluation in below figure). The research teams participating in the geochemical tasks have mostly been working on code and model development during the last year. Preliminary simulation results showed good agreement for a simplified geochemical system. Results from both geomechanical and geochemical simulations provide a good basis for adding another layer of complexity in the next project phases, e.g., evaluating the changes in hydrological processes due to geomechanical and geochemical changes, developing alternative model approaches, and estimating conceptual as well as data uncertainties.

This status report summarizes the research activities conducted within Task D of the international DECOVALEX project (status October 2005). Additional information is provided in the attached CD, which includes various appendices. The appendices comprise a detailed description of the DECOVALEX THMC Task D definition, three meeting summaries from workshops in Kunming, Berkeley, and Ottawa, as well as separate status reports on research results provided by the participating research teams. To bring out similarities and discrepancies, the LBNL research team has conducted a comparative evaluation of all status reports with regards to the conceptual models used and the simulation results. This comparative evaluation is provided in Sections 4 and 5 of this report.

Content

1. Introduction

This status report summarizes the research activities of several international research teams with respect to Task D of the international DECOVALEX project. The DECOVALEX project is an international cooperative project initiated by SKI, the Swedish Nuclear Power Inspectorate, with participation of several international organizations. The name DECOVALEX stands for **DE**velopment of **CO**upled models and their **VAL**idation against **Ex**periments. The general goal of this project is to encourage multidisciplinary interactive and cooperative research on modeling coupled processes in fractured rocks and buffer materials, in support of the performance assessment for radioactive waste storage in geologic formations.

Three multi-year project stages of DECOVALEX have been completed in the past decade, mainly focusing on coupled thermal-hydrological-mechanical (THM) processes. The most recent project stage, DECOVALEX-III, included THM modeling work on two large-scale *in situ* heater experiments, the FEBEX experiment at Grimsel in Switzerland and the Drift Scale Test (DST) at Yucca Mountain in the USA. This modeling work has greatly enhanced our understanding of the coupled near-field processes in two different rock formations (crystalline rock versus volcanic tuff), hydrological settings (saturated versus unsaturated), and emplacement designs (backfilled drift versus open drift), and has added confidence in the predictions by comparison of measured data with the model results (e.g., Rutqvist et al., 2005a, 2005b).

Currently, a fourth multi-year project stage of DECOVALEX is under way, referred to as DECOVALEX-THMC. THMC stands for **T**hermal, **H**ydrological, **M**echanical, and **C**hemical processes. The project was initiated in January 2004 and will run through June 2007. Participating organizations are from USA, France, Japan, Sweden, Germany, China, and Canada. Five individual research tasks are defined within DECOVALEX-THMC, each of which is headed by a different participating organization. DOE leads Task D of the new DECOVALEX phase, entitled “Long-term Permeability/Porosity Changes in the EDZ and Near Field due to THC and THM Processes for Volcanic and Crystalline-Bentonite Systems.” In its leadership role for Task D, DOE coordinates and organizes the cooperative research activities of the international research teams engaged in Task D (China, Germany, Japan, USA), and conducts its own modeling work for Task D. Scientists at Lawrence Berkeley National Laboratory (LBNL) support DOE in organizational matters and conduct the respective modeling studies.

The research program developed for Task D of DECOVALEX-THMC involves both geomechanical and geochemical research areas. The geomechanical project, referred to as D_THM, builds on the knowledge gained from modeling the short-term *in situ* heater experiments in DECOVALEX-III, and applies that knowledge to the evaluation of long-term THM processes in two generic geologic repositories for radioactive waste, where the regulatory compliance periods span over thousands to tens of-thousands of years. THM processes lead to changes in hydrological properties that can be very important for performance, because the flow processes in the vicinity of emplacement tunnels will be altered from their initial state. Some of these changes can be permanent (irreversible), in which case they persist after the thermal conditions have returned to ambient; i.e., they will affect the entire regulatory compliance period. In general, THM changes are strongest close to the tunnels; i.e., they will be particularly relevant for the long-term flow behavior in the Excavation Disturbed Zone (EDZ) and the near-field environment. Research teams participating in Task D_THM model the THM processes in the fractured rock close to representative emplacement tunnels as a function of time, predict the mechanically induced changes in hydrological properties, and evaluate the impact on near-field flow processes. Currently, research teams from China, Germany, Japan, and the U.S. conduct modeling work on Task D_THM, each using different conceptual approaches and computer codes.

The new DECOVALEX-THMC project aims at expanding the traditional geomechanical scope of the previous DECOVALEX project stages by incorporating geochemical processes important for repository performance. As discussed in Section 2.2, chemical processes can permanently alter hydrological properties and flow paths in the near field by mineral precipitation and dissolution. They also affect the water and gas chemistry close to the waste packages, which are relevant for waste package corrosion, buffer stability, and radionuclide transport. Recognizing their increasing importance, Task D includes a geochemical research area, referred to as D_THC, that addresses long-term THC effects and their relevance in two generic repositories for radioactive waste. Research teams participating in Task D_THC model the THC processes in the fractured rock close to representative emplacement tunnels as a function of time, and predict the changes in water and gas chemistry, mineralogy, and hydrological properties. Currently, research teams from Germany, Japan, and the U.S. conduct modeling work on Task D_THC, each using different conceptual approaches and computer codes.

The generic waste repositories evaluated in Task D represent simplified versions of two possible repository sites and emplacement conditions considered by the participating organizations. The first repository is located in saturated crystalline rock; emplacement tunnels are backfilled with a bentonite buffer material. This repository is referred to as a *FEBEX* type, since many of its features are similar to the *FEBEX* field test setting. The second repository is a simplified model of the Yucca Mountain site, featuring a deep unsaturated volcanic rock formation with emplacement in open gas-filled tunnels (Yucca Mountain type). At first, each generic repository will be analyzed separately within the geomechanical and the geochemical research areas, respectively. (At later stages, the separate THM and THC model analyses may be integrated to a fully coupled geomechanical and geochemical analysis.) However, as D_THM and D_THC modeling studies are conducted assuming identical site and emplacement conditions, the results from the geomechanical and geochemical models can be easily compared.

The following activities were conducted during the first year of Task D research work: First, DOE and LBNL finalized the Task D description and produced a detailed report containing all necessary specifications for geomechanical and geochemical modeling analyses of the two generic repositories (see Appendix A). Then, four international research teams from China, Germany, Japan, and USA started their research work on D_THM and D_THC (see approaches and results in Sections 4 and 5 of this report). Three full DECOVALEX workshops were held to share research ideas and compare modeling results (Utrecht, Netherlands, June 15-16, 2004; Kunming, China, February 21-24, 2005; Ottawa, Canada, October 4-7, 2005). In addition, DOE organized three meetings just for Task D research participants to discuss organizational and modeling issues specific to this task (Kunming, China, February 20, 2005; Berkeley, USA, July 21-22, 2005; Ottawa, Canada, October 4, 2005; see meeting summaries in Appendix B).

In between workshops and meetings, the international research teams collaborated closely via email and telephone.

The close collaboration among international top scientists and engineers is one of the major benefits from participation in DECOVALEX-THMC. First, interaction with top international scientists helps to further the understanding of geomechanical and geochemical processes related to geologic storage of radioactive waste. Second, the cooperative research work conducted in the field of THMC modeling provides valuable peer-review of the modeling analyses in this field. Since all research teams work on identical tasks (but use different conceptual approaches and computer codes), research results from the participating teams can be easily compared. Good agreement between the different teams provides an additional proof of confidence into predictive models for THM and THC processes, which are important feeds for assessing the performance of the geologic repositories studied in different countries.

The value of analyzing two different repository sites and emplacement conditions is twofold: One repository setting resembles the geologic repository at Yucca Mountain, the designated site in the DOE program. Another repository setting (*FEBEX* type) is representative of the possible emplacement conditions considered in many European countries and Japan. Since the geomechanical and geochemical processes expected in such settings are different from each other, the demands and requirements on THM and THC simulation models are different. It is important to show that all models, proven to be capable of simulating one repository type, are equally valuable for the simulation of an alternative repository setting with different THM and THC processes.

2. Task D Summary Description

The following section gives a brief summary of the problem definition for the simulation analyses to be conducted in Task D. A document containing a more comprehensive task description with all necessary specifications for modeling work was distributed to the individual research teams in May 2004 (Barr et al., 2004a). A first revision was issued in December 2004 (Barr et al., 2004b). The latest revision of this document is attached in Appendix A (Barr et al., 2005).

The nomenclature used for the different simulation problems defined in Task D is as follows. Simulation tasks with focus on geomechanical processes are referred to as D_THM, while simulation tasks with focus on geochemical processes are referred to as D_THC. Since two different generic repository settings are considered (*FEBEX* type and *Yucca Mountain* type), there are two subtasks each for D_THM and D_THC:

- Task D_THM1: Geomechanical simulations for a generic repository located in saturated crystalline rock, where emplacement tunnels are backfilled with buffer material (*FEBEX* type).
- Task D_THM2: Geomechanical simulations for a generic repository located in unsaturated volcanic rock, with emplacement in open gas-filled tunnels (*Yucca Mountain* type).
- Task D_THC1: Thermal-hydrological-chemical simulations for a generic repository located in saturated crystalline rock, where emplacement tunnels are backfilled with buffer material (*FEBEX* type).
- Task D_THC2: Thermal-hydrological-chemical simulations for a generic repository located in unsaturated volcanic rock, with emplacement in open gas-filled tunnels (*Yucca Mountain* type).

2.1 Basic Concepts of Generic Repositories

Figure 2.1 presents the basic functions of the two repository types analyzed in Task D of DECOVALEX-THMC (*FEBEX* type and *Yucca Mountain* type). Both repository types depend on a multibarrier system relying on an engineered system (e.g., waste, canister, buffer, and excavation) and a natural system (rock mass). In the *FEBEX* case, the tunnels hosting waste canisters are backfilled with a low-permeability buffer material such as bentonite. Since the crystalline rock formation surrounding the repository is saturated with water, the tight (low-permeability) bentonite is necessary to prevent water flow and solutes from coming into contact with the waste canister. On the other hand, for an open-drift repository in an unsaturated tuff formation similar to *Yucca Mountain*, there is no protective bentonite buffer, but the open drift itself provides a natural capillary barrier that can limit liquid water from entering the drift. There is also a difference in the amount of heat and temperature rise. In a bentonite-backfilled repository, considered in most European countries and Japan, the temperature is generally kept below 100°C to prevent chemical alterations of the bentonite material. For the open-drift alternative (considered for the *Yucca Mountain* repository), the current design results in above-boiling temperatures within the tunnels and in the near field rock.

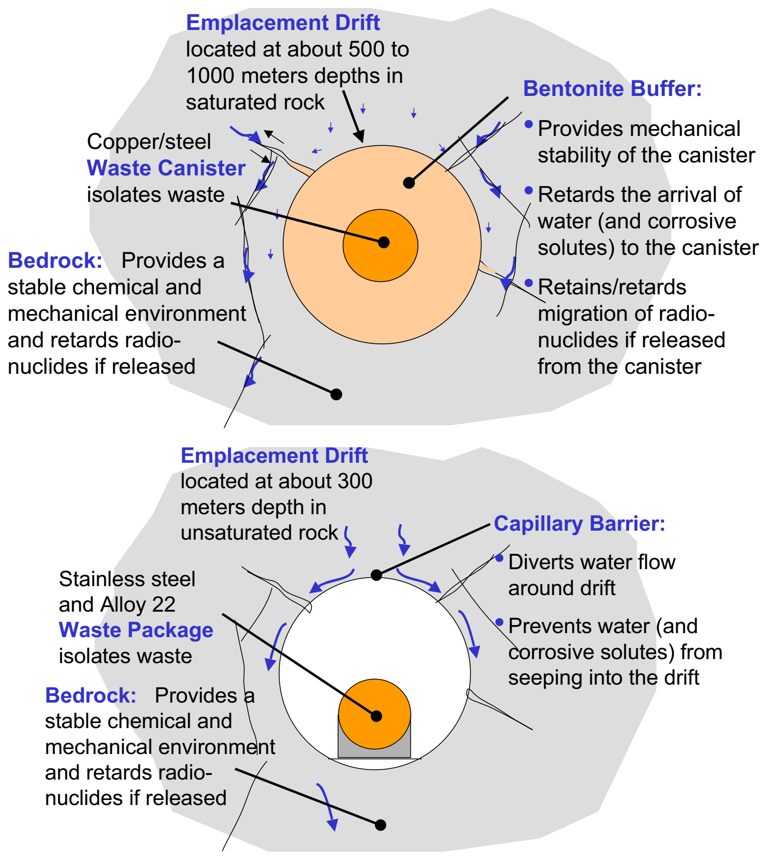

*Figure 2.1: Schematic showing the two repository types evaluated in tasks D_THM and D_THC: (a) bentonite-back-filled repository in saturated rock (*FEBEX type*), and (b) open-drift repository in unsaturated rock (*Yucca Mountain type*)*

2.2. Geomechanical and Geochemical Processes Affecting Hydrological Properties

The ultimate research topic in Task D is to evaluate and predict long-term changes in near-field hydrological properties as a result of heat-driven geomechanical and geochemical alterations. Such changes in hydrological properties (mostly with respect to fracture porosity and permeability) affect the flow and transport processes in the vicinity of emplacement tunnels and can thus be very important for performance assessment. The following section gives a brief description of the coupled processes expected to occur in the two repository types.

Geomechanical Processes and Related Research Work

Significant geomechanical alterations are expected to occur in response to the heat output of the decaying radioactive waste. The strongest effects typically coincide with the period of the highest temperatures; i.e., depending on the repository type, during the first decades or centuries after emplacement (Figure 2.2). For example, in the case of a bentonite-backfilled repository, the drying and wetting of the bentonite induces shrinkage and swelling in various part of the buffer, with resaturation expected to occur within tens of years. In the case of an open-drift repository, the boiling of water creates a dryout zone in the near-field rock that will prevent liquid water from entering the drift for several hundred to more than one-thousand years.

At the same time, thermally induced stresses will act upon pre-existing fractures, which will open or close depending on the local stress. One of the important effects, i.e., thermal expansion of the rocks (with impact on fracture aperture), is generally recoverable as the temperature drops. However, increased thermal stress may also lead to irreversible or permanent impacts, which are most relevant for performance assessment (Figure 2.3). For example, if changes in the stress field during the heating period are sufficiently large, inelastic mechanical responses may be induced in the form of fracture shear slip or crushing of fracture asperities. These processes may change the fracture porosity and permeability permanently, since the rock loses its integrity. Furthermore, the elevated temperatures and stresses will be maintained for long time spans, which could give rise to increased microcracking and subcritical crack growth through stress corrosion or other related phenomena. Such inelastic mechanical responses in the fracture system would induce irreversible (permanent) changes in the hydrological properties of the rock mass.

Figures 2.1 and 2.2 suggest that for long-term THM processes, there are differences but also many similarities between the two repository cases, indicating that modelers face similar challenges and issues. Working together on both cases will help in evaluating similarities and differences, in comparing approaches and results, and in gaining a better overall understanding.

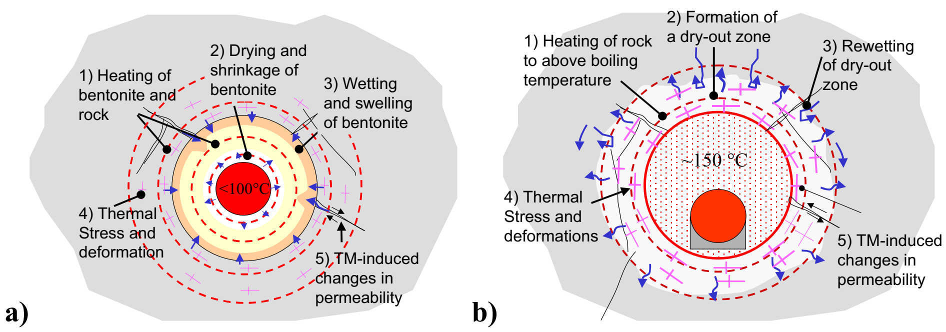

Figure 2.2: Short-term coupled THM processes at (a) a bentonite-backfilled repository in saturated rock and (b) an open-drift repository in unsaturated rock

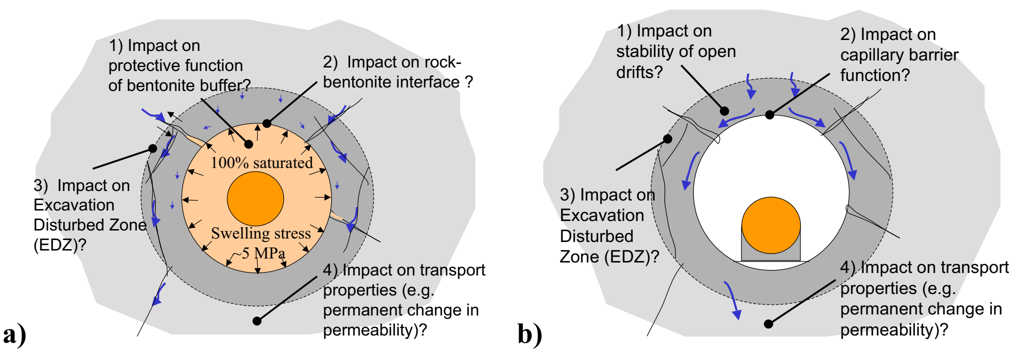

Figure 2.3: Potential long-term impact of coupled THM processes at (a) a bentonite-back-filled repository in saturated rocks and (b) an open-drift repository in unsaturated rock

Geochemical Processes and Related Research Work

The heat output of the decaying radioactive waste will induce important geochemical reactions in the host-rock formations, owing to the changes in stabilities of minerals with increasing temperature and changing water chemistry and also to greatly increased reaction rates. Geochemical alteration include changes in water and gas chemistry in the near field and within the tunnels, which affects the waste package environment and may also jeopardize the integrity of buffer materials. In turn, buffer materials will interact with formation water and minerals in the adjacent host rock, thus altering the buffer mineral assemblage, pore water chemistry, physical, and hydrological properties.

In both formation rocks and buffer materials, mineral precipitation and dissolution will give rise to long-term, possibly permanent changes in hydrological properties. Increased temperature results in mineral-water disequilibrium and increases the reaction rates of minerals with water, leading to enhanced mineral dissolution and precipitation. Effects of mineral precipitation on fracture porosity and permeability are particularly strong when temperatures are above boiling. In this case, vapor is driven away by the heat in all directions and cools as it moves farther from the heat source, eventually condensing into the liquid phase. Above the heat source, condensate flows back down by gravity and capillary suction, only to boil again as it gets closer to the heat source. This cycle of vaporization, condensation, and reflux can result in strong mineral alteration processes where dissolution is dominant in the condensation zone and precipitation takes place at the boiling front.

Figures 2.4 and 2.5 give a schematic illustration of the main long-term THC processes expected in the two repository types.

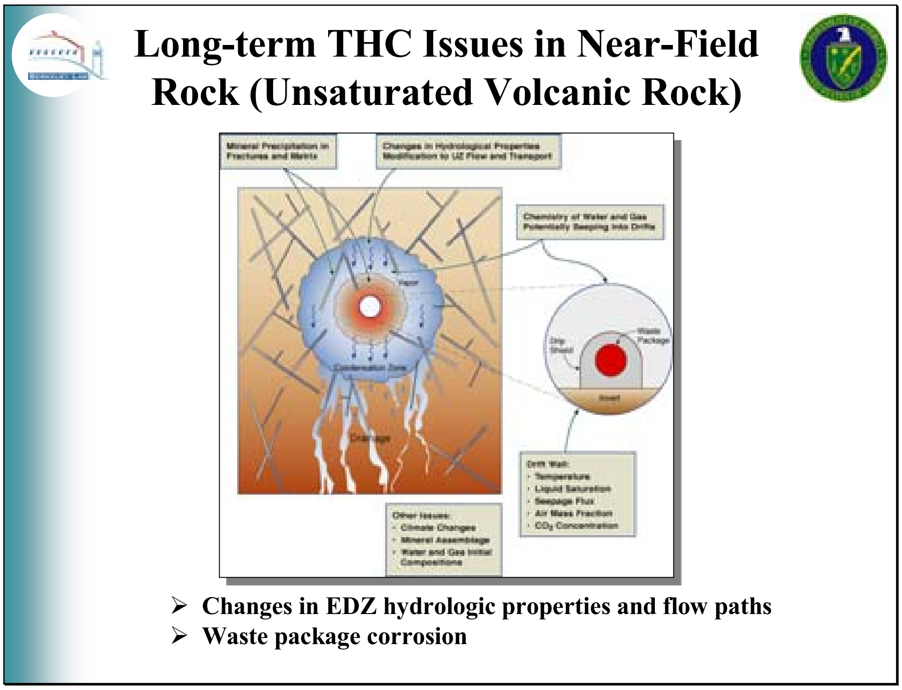

Figure 2.4: Possible THC processes with impact on hydrological properties near emplacement tunnels in unsaturated volcanic rock

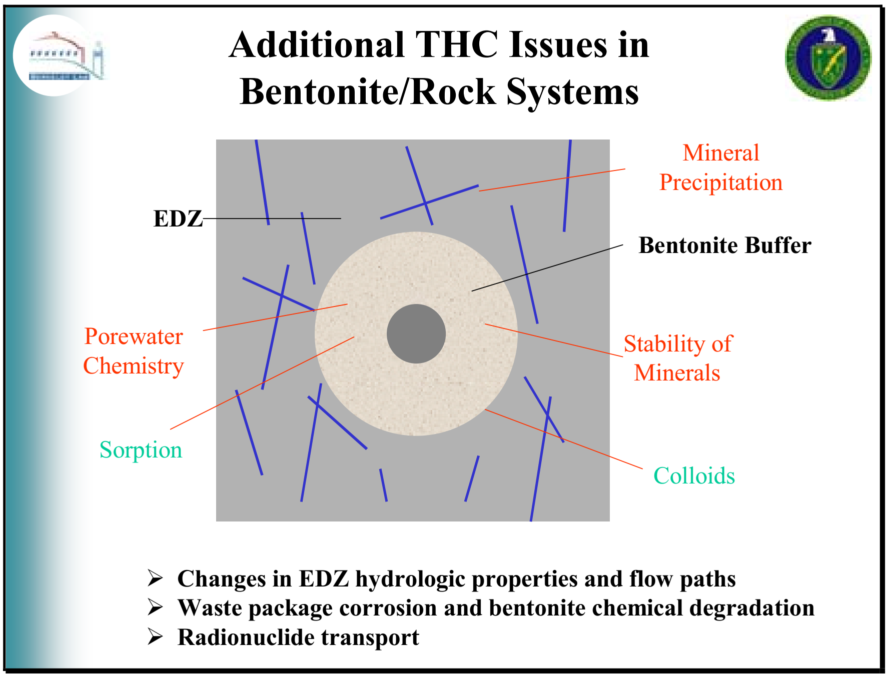

Figure 2.5: Additional THC processes and their impact on hydrological properties in and near emplacement tunnels with bentonite backfill

2.3. Brief Description of Simulation Tasks D_THM and D_THC

The task description for D_THM and D_THC is designed such that the expected physical processes in future repositories are incorporated in a realistic manner, yet allow for somewhat simplified modeling as the geometries and boundary conditions have been simplified. Definitions are given such that model concepts as well as relevant property and parameter choices will have to be developed by the individual research teams (based on reports, data, and other sources), rather than being imposed in the task description. The idea is to encourage model comparison, not just code comparison.

Each task includes two different repository scenarios with similar geometry (depicted in Figure 2.6). Both analyze 2-D vertical cross sections perpendicular to the tunnel axis. The emplacement tunnels are assumed to be parallel, with a given distance between them. Symmetry considerations allow limiting the model to one representative emplacement tunnel, with the lateral boundaries at the centerlines of neighboring tunnels. Upper and lower boundaries are such that they remain unaffected by the heat. Waste packages are placed into the center of the tunnels. Heat emitted from the waste packages is provided as a time-dependent line load. Undisturbed flow is from top to bottom, either driven by hydraulic head gradients (saturated flow) or by gravity (unsaturated flow).

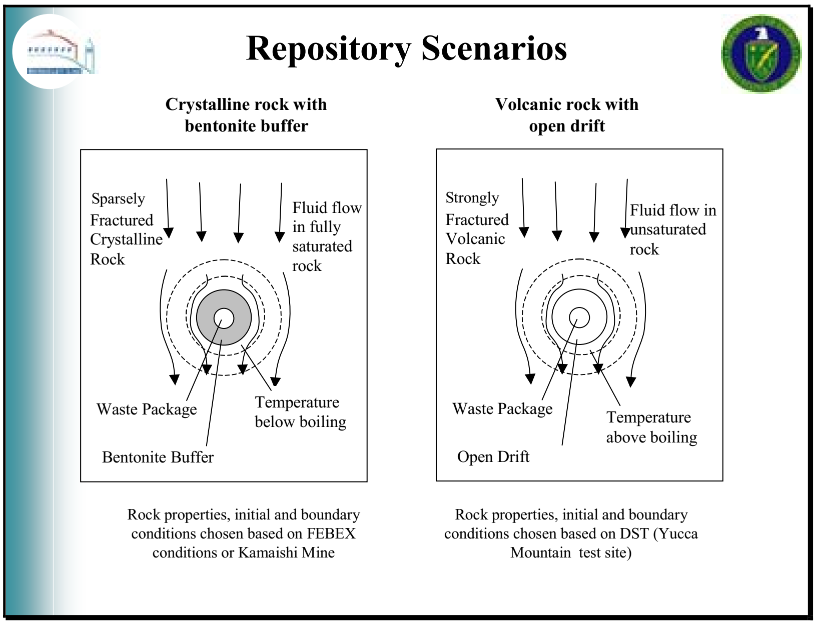

Figure 2.6: Schematic showing the two repository scenarios chosen for D_THM and D_THC (vertical cross sections perpendicular to drift axis)

Tasks D_THM and D_THC are conducted simultaneously, since the researchers working on THM processes are mostly different from those working on THC processes. In each task, participating teams are encouraged to work on both repository scenarios, either simultaneously or sequentially, to enhance process understanding, and to ensure close cooperation. Both tasks may include an analysis and/or simulation component, using measured data to identify relevant processes and to allow for model comparison with experimental results. At later stages of Task D, i.e., after finalizing D_THM and D_THC, results from THM and THC analyses will be compared, and the need for a fully coupled thermal-hydrological-mechanical-chemical (THMC) simulation study will be evaluated. This latter subtask will require close interaction between THM and THC research teams.

2.3.1 Task D_THM: Workscope, Research Topics, and Modeling Phases

In this task, research teams conduct geomechanical modeling analysis of the long-term coupled processes in two generic repositories with simplified conditions and dimensions. Participating research teams model the THM processes in the fractured rock close to a representative emplacement tunnel as a function of time, predict the mechanically induced changes in hydrological properties, and evaluate the impact on near-field flow processes. Geochemical processes are neglected in Task D_THM. Two subtasks analyze the coupled THM processes in two generic repositories as follows:

- Task D_THM1: Generic repository located in saturated crystalline rock, where emplacement tunnels are backfilled with buffer material (*FEBEX* type).
- Task D_THM2: Generic repository located in unsaturated volcanic rock, with emplacement in open gas-filled tunnels (*Yucca Mountain* type).

Figure 2.7 gives a summary of the problem setup and the main challenges for D_THM.

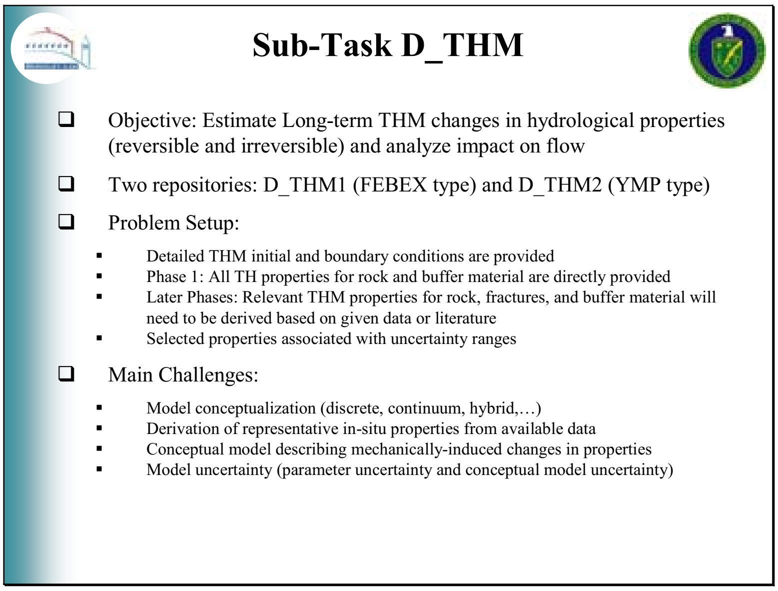

Figure 2.7: Problem setup and main challenges for D_THM

The main processes considered in Task D_THM are heat transfer, fluid flow, stress and deformation, and geomechanical alterations in hydrologic properties (e.g., porosity and permeability). Specific THM research interests addressed in Task D_THM include, but are not limited to:

- Relative importance of thermal-mechanical changes to near-field hydrological properties and flow fields
- Relative importance of irreversible mechanical changes versus reversible mechanical changes
- Comparative analysis of THM effects in different host rock types and repository designs
- Evaluation of stress-permeability and stress-porosity relationships
- Importance of THM processes for performance assessment
- Assessment of fully coupled THMC processes (necessity, approaches)
- Assessment of uncertainties in the predictions resulting from uncertain parameters, alternative conceptual models, heterogeneities, and other factors

The predictive THM simulations may be conducted using various modeling techniques, for example discrete fracture models or continuum models. Model predictions should include the most likely results on THM-induced property changes as well as an evaluation of the uncertainties related to these predictions. This could involve stochastic modeling, resulting in a probability distribution of possible results or, at a minimum, estimation of upper and lower limits of results. In addition to the data and background information provided by the task leads, the research teams should utilize any available literature data to build their case, to ensure providing the best possible prediction of potential permanent changes based on the current state of knowledge.

The description of Task D_THM1 is based on data from the Grimsel Test Site (GTS) and the FEBEX *in situ* experiment, which were used in DECOVALEX III, Task 1. The design and material properties of the engineered system (canister, bentonite, and drift) are taken from the FEBEX *in situ* experiment. The rock properties and *in situ* conditions are also taken from the GTS/FEBEX site. However, in a few instances, data from the

Kamaishi Mine in Japan (from DECOVALEX II) and the Laxemar site in Sweden are utilized to complement the GTS/FEBEX data set. The crystalline host rock in D_THM1 is sparsely fractured, which would suggest that the fractures might be modeled using discrete approaches, if necessary. The data set for Task D_THM2 is entirely derived from the Yucca Mountain site in Nevada and the lithographic rock units surrounding the Yucca Mountain Drift Scale Test. Here, the porous tuff rock is densely fractured, which would suggest that the fractures could be treated as a continuum. For both repository settings, a complete set of rock properties and *in situ* conditions with uncertainty ranges is given to the research teams, upon which to build their models for Task D_THM2 (see specifics on task definition in Appendix A).

The simulation work in Task D_THM is being conducted in three modeling phases that tackle increasing degrees of difficulty. After each phase, the results of the different research teams are compared to ensure that there are no systematic differences before moving into the next, more complex model phase. The three phases for D_THM are defined as follows (Figure 2.8):

Phase 1. Model Inception
Phase 2. Preliminary Prediction and Sensitivity Study
Phase 3. Final Prediction and Uncertainty Analysis.

The purpose of the Model Inception Phase (Phase 1) is for the research teams to familiarize themselves with the problem by performing simulations in which all the properties are provided with explicit values while permanent changes are neglected. The results of the research teams are compared at the end of this phase to assure that all teams are starting the problem from a common basis. The comparison shall focus on the evolution of temperature and stress, because these are the driving forces behind mechanical and hydrological changes in the fractured rock mass. When research teams are satisfied with their analysis and their results agree with other research teams, they should go on to the next phase.

In Phase 2, the research teams start to develop their model with the goal of predicting mechanically induced permanent changes. This phase may include development of continuum models for representing the hydromechanical couplings at the two sites. It may also include generation of fracture networks based on available statistical data if a discrete model approach is used. Using the available site data and developed data (e.g., stress-permeability relationships), the research teams should conduct an initial parameter study. The purpose of this study is twofold, as follows:

- To demonstrate how the model is able to predict permanent changes in mechanical and hydrological properties
- To find conditions (e.g. strength properties, initial stress state) at which permanent changes are likely

The research teams should then predict coupled THM responses and potential permanent changes (if any). This should be conducted with whatever modeling approach the respective research team has developed. It may be a continuum model using homogenous properties or a heterogeneous stochastic continuum model. It may also be a discrete fracture model using fracture sets with regular fracture spacing or even stochastically generated fracture networks. At the end of this phase, the output results from the different research teams are compared. In particular, the evolution of permeability changes and their impact on the flow field needs to be studied. When research teams are satisfied with their preliminary model prediction, they should go on to the next phase to obtain the final prediction results.

In Phase 3, the research teams are asked to make their final prediction, including estimation of the resulting uncertainties. Examples of uncertainties includes:

- Uncertainties associated with parameters
- Uncertainties associated with model concepts (i.e., representation of discrete structures such as fractures and faults, constitutive relationships)

Parameter uncertainties could be related, for example, to uncertainties in input properties, such as permeability, *in situ* stress, or thermal expansion. Model uncertainties could be related to representation of the *in situ* fracturing. They may also be related to the constitutive models of the mechanical behavior of fractures or the constitutive models developed for continuum approaches. In part, estimation of these uncertainties will be based on scientific judgment. The end result of the uncertainty analysis can be a statistical distribution of the simulation outputs or, at a minimum, upper and lower bounds of possible results.

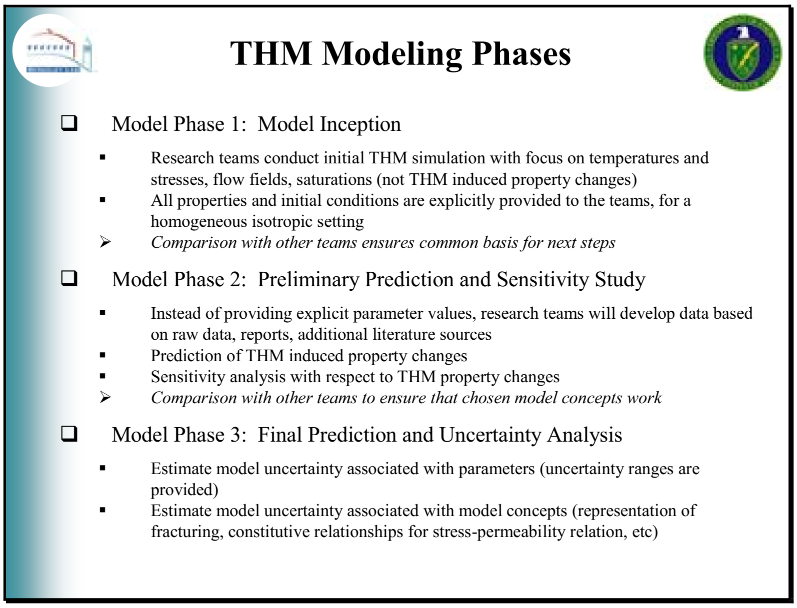

Figure 2.8: Definition of Three Modeling Phases of Task D_THM

2.3.2 Task D_THC Workscope, Research Topics, and Modeling Phases

In this task, research teams conduct geochemical modeling analyses of the long-term coupled THC processes in two generic repositories, similar to those described for Task D_THM. Participating research teams model the THC processes in the fractured rock close to a representative emplacement tunnel as a function of time, and predict the changes in water and gas chemistry, mineralogy, and hydrological properties. The impact of geomechanical processes is neglected in this task. Two subtasks analyze the coupled THC processes in two generic repositories as follows:

- Task D_THC1: Generic repository is located in saturated crystalline rock, where emplacement tunnels are backfilled with buffer material (*FEBEX* type).
- Task D_THC2: Generic repository located in unsaturated volcanic rock, with emplacement in open gas-filled tunnels (*Yucca Mountain* type).

Figure 2.8 gives a summary of the problem setup and the main challenges for D_THC.

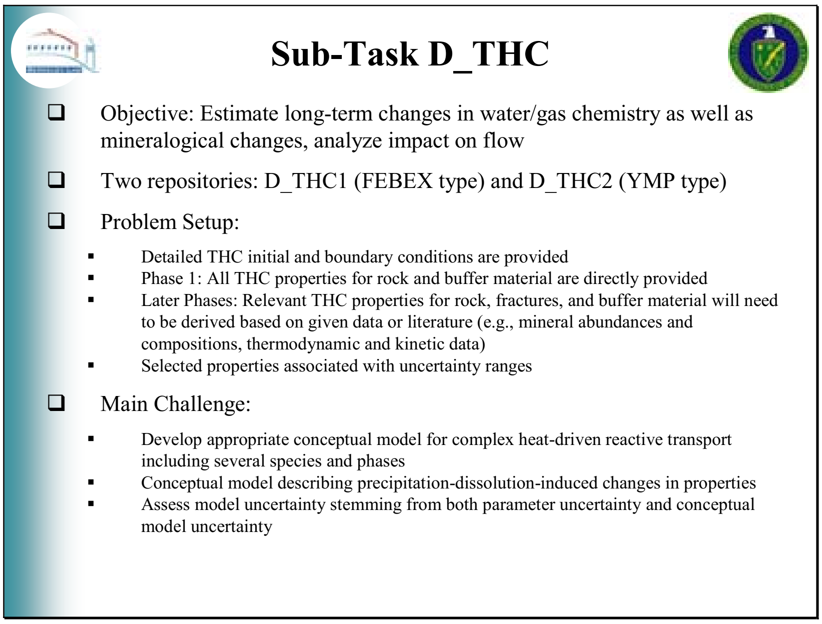

Figure 2.9: Problem setup and main challenges for D_THC

The main processes considered in Task D_THC are heat transfer, fluid flow, reactive transport, and alterations in hydrologic properties. Specific THC research interests addressed in Task D_THC include, but are not limited to:

- Relative importance of thermal-chemical changes on the near-field hydrological properties and flow field
- Evolution of water and gas chemistry close to waste package
- Mineral precipitation/dissolution in the near-field and in bentonite
- Comparative analysis of THC effects in different repository designs/rock types
- Evaluation of the relation between mineral alteration, and hydrological properties
- Importance of THC processes for performance assessment
- Assessment of fully coupled THMC processes (necessity, approaches)
- Assessment of uncertainties in the predictions resulting from uncertain parameters, alternative conceptual models, heterogeneities, and other factors

The predictive THC simulations can be conducted using various modeling techniques—for example, discrete fracture models or continuum models. Model predictions should include the results of THC-induced changes to water and gas chemistry, mineralogy, hydrological properties, flow fields, and an evaluation of the uncertainties related to these predictions. This could involve systematic sensitivity studies, resulting in a distribution of possible results or, at a minimum, estimation of upper and lower limits of results.

The description of Task D_THC1 is based on various sources. The thermal-hydrological properties and their origin are identical to those defined in D_THM1, featuring a bentonite-backfilled emplacement tunnels hosted by a sparsely fractured crystalline formation. Properties of the bentonite buffer material are based on a sample investigated by the Japanese program. The chemical properties of the bentonite buffer and the host rock are taken from the Aspö site in Sweden and from the Japanese program. The input data for Task D_THC2 are entirely derived from the Yucca Mountain site in Nevada and the rock units surrounding the Yucca Mountain Drift Scale Test (densely fractured porous tuff formation). A complete set of geochemical data, rock properties, and *in situ* conditions with uncertainty ranges is provided to the research teams, upon which to build their models for Task D_THC (see Appendix A).

The simulation work in Task D_THC is conducted in three modeling phases that tackle increasing degrees of difficulty. After each phase, the results of the research teams are compared to ensure that there are no systematic differences before moving into the next, more complex model phase. The three phases are defined as follows (see Figure 2.10):

Phase 1. Model Inception
Phase 2. Preliminary Prediction and Sensitivity Study
Phase 3. Final Prediction and Uncertainty Analysis

The purpose of the Model Inception Phase (Phase 1) is for the research teams to familiarize themselves with the conceptual model and problem setup by performing one simulation in which all the properties are provided for a limited set of mineral, aqueous, and gaseous species. The results of the research teams are compared at the end of this phase to assure that all teams are starting the problem from a common basis. The comparison focuses on the evolution of temperature, gas and water composition, and mineral precipitation/dissolution (in fractures, matrix, and the bentonite) for a simplified geochemical system. When research teams are satisfied with their analysis and their results agree with other research teams, they should go on to the next phase.

In Phase 2, a more complete geochemical system is considered. Also, the research teams focus on predicting permanent changes caused by mineral dissolution/precipitation concomitant with the evolution of water and gas chemistry. Using the available site data and various developed data (e.g., mineral dissolution/precipitation-porosity-permeability relationships), the research teams should conduct an initial parameter study. The purpose of this study is twofold, as follows:

- To demonstrate how the model is able to predict permanent changes in chemical (gas, water, and mineral) and hydrological properties
- To find conditions (e.g., initial mineralogy, fracture aperture, water chemistry, flow rates) at which permanent changes are possible

The research teams should then predict coupled THC responses and potential permanent changes (if any) for one realistic realization. This should be conducted with whatever modeling approach the respective research team has developed. It may be a continuum model using homogenous properties or a heterogeneous stochastic continuum model. It may also be a discrete fracture model using fracture sets with regular fracture spacing or even stochastically generated fracture networks. At the end of this phase, the output results from the different research teams needs to be compared. In particular, the evolution of chemistry and permeability changes and their impact on the flow field will be studied. When research teams are satisfied with their preliminary model prediction, they should go on to the next phase to obtain the final prediction results.

In Phase 3, the research teams are asked to make their final prediction, including estimation of the resulting uncertainties. Examples of uncertainties include:

- Uncertainties associated with parameters (e.g., thermodynamic and kinetic data, reactive surface areas)
- Uncertainties associated with model concepts (mineral representations—ideal endmembers vs. solid solutions, mineral textures, equilibrium vs. kinetic reactions, distributions of mineral precipitates, etc.)

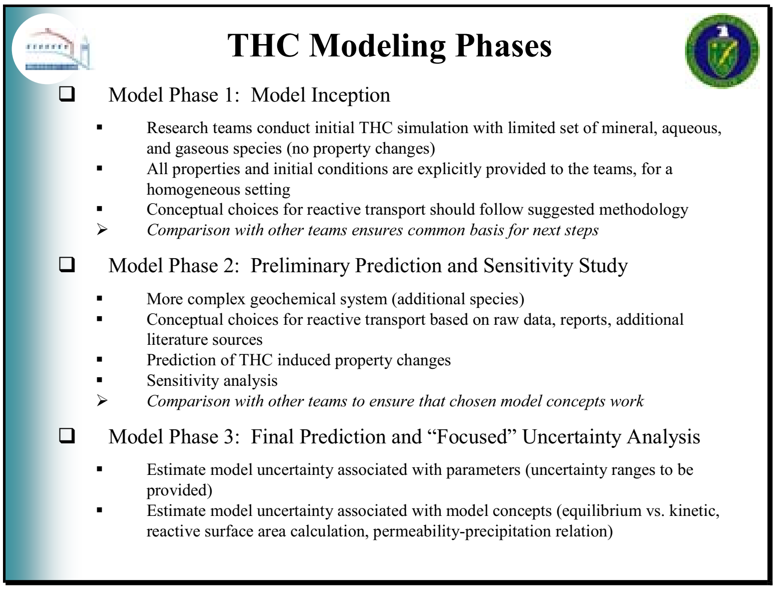

Figure 2.10: Definition of three modeling phases of Task D_THC

2.3.3 Details of Task Description

Much more detail on all task specifications is given in the task description report (Barr et al., 2005) in Appendix A, including specifics on model geometry, boundary and initial conditions, modeling sequence (simulating initial state, excavation state, emplacement state), input data, supporting data, references, suggestions for potential model simplifications (in case certain model features are not available for research teams), proposed schedule, and output specifications.

3. Participating Countries And Team Members

Japan, Germany, and the U.S. participate in both D_THM and D_THM. China participates in D_THM only. The following list gives names and addresses of all team members from the participating countries. Team members may either be representatives of the funding organizations or may be working for research institutes that support these funding organizations in conducting the scientific analyses.

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4. Task D_THM: Geomechanical Analysis

The research teams involved in modeling Task D_THM (from China, Germany, Japan, and the U.S.) have made significant progress during the first year of task D work. Section 4.1 gives a brief summary on the current status of the geomechanical modeling work. Each team has provided a status report, which describes the conceptual model approaches and discusses modeling results. With some minor editing for format consistency, these status reports have been added as Appendices C through F of this letter report (see attached CD). To bring out similarities and discrepancies between different research approaches, the LBNL research team has conducted a comparative evaluation of all status reports with regards to the conceptual models used and the simulation results. This comparative evaluation is summarized in Section 4.2 for D_THM1 and Section 4.3 for D_THM2.

4.1. Summary Status of D_THM Research Work

All teams involved in modeling of D_THM have finalized model development work and have conducted simulation runs for at least one of the two repository scenarios (Table 4.1). Altogether, five different numerical codes were applied to simulate the test cases. DOE uses two alternative codes, TOUGH-FLAC (which is widely used within the Yucca Mountain Project) and ROCMAS. JNC uses a code named THAMES, BGR uses the GeoSys/Rockflow family of codes, and CAS works with a FEMLAB application referred to in the text as FRT-THM (FRT = Fluid-Rock Simulator). All these codes have been developed by the respective organizations or their supporting research institutions; i.e., no off-the-shelf software is used.

Table 4.1: Research teams and numerical models applied within the Task D_THM of DECOVALEX-THMC

Team	Affiliation	Computer Code	Test Case Simulated
DOE-Team	Lawrence Berkeley National Laboratory (LBNL) for DOE	TOUGH-FLAC and ROCMAS	D_THM1 and D_THM2
JNC-Team	Japan Nuclear Cycle Development Institute (JNC)	THAMES	D_THM1 and D_THM2
BGR-Team	Center for Applied Geosciences Tuebingen, for BGR	GeoSys/Rockflow	D_THM1 and D_THM2
CAS-Team	Chinese Academy of Sciences	FRT-THM (FEMLAB application, combined with Mathlab)	D_THM1 and D_THM2

All teams started with the Model Inception Phase, where the problem is well defined, with most of the material properties and conditions specified in the task description report (Barr et al., 2005). The Task D meetings in Kunming, China, and in Berkeley, USA, and various email/telephone exchanges were utilized to conduct in-depth comparison of approaches and results between the different research teams. Various discrepancies were evaluated in a team effort by going through some of the key plots of THM results. It was found that often these discrepancies were caused by differences in rock properties and boundary conditions, because some teams had misinterpreted the task description. These teams made adjustments in their model setup to be consistent with the other teams and conducted revised simulation runs. Eventually, all teams submitted Phase 1 simulation results together with a status report.

Our comparison of the individual status report results indicates that the overall agreement between the research teams is fairly good (see Sections 4.2.2 and 4.3.2 below). In a few cases, model revisions (mostly properties) are still necessary to improve the THM predictions of individual teams. These necessary revisions have been identified and will be conducted in the near future. Otherwise, the discrepancies between teams are rather small and can be explained by subtle differences in conceptual approaches (model simplifications). The good agreement provides a valuable basis for moving into Phase 2 of D_THM. Phase 2 modeling includes prediction of THM property changes with conceptual models chosen by the different research teams, sensitivity analysis with respect to THM property changes, application of alternative conceptual models for fractured rock (i.e., discrete, vs. continuum), and development of model data based on various reports and site data instead of using pre-defined values.

4.2. Repository Case D_THM1 (FEBEX TYPE)

4.2.1 Comparison of Model Approaches

The basic modeling approaches employed by the four international teams (DOE, BGR, CAS, JNC) modeling D_THM1 are summarized in Table 4.2. All codes are capable of modeling thermal-hydrological-mechanical (THM) coupling. However, since TOUGH-FLAC currently does not account for the swelling pressure changes in a bentonite buffer material, it was run in a TH-only mode. In all other cases, simple elastic models are used for simulation of the rock-mechanical behavior, consistent with the simplified task definition for Phase 1 work. However, all models are generally capable of simulating elasto-plastic behavior, which can become necessary when stress-induced changes in hydrologic properties are to be considered in the next phases of D_THM1.

While the mechanical models for the rock-mechanical behavior are identical, the treatment of the evolution of swelling pressure in the bentonite is not consistent between the teams. All teams consider some sort of a saturation-dependent swelling impact, but use different functional relationships. For the scope of D_THM1, one is mostly concerned about the correct magnitude of the fully developed swelling stress, because this value defines the impact of bentonite swelling on the near-field rock during most of the postclosure time period (swelling is roughly expected fore the first 10 years after bentonite emplacement).

At this point, all teams use a single-continuum representation of the crystalline rock mass. This may change in later project phases, when the effect of sparsely distributed fractures may be considered in a more rigorous manner.

TOUGH-FLAC simulates complex multi-phase flow behavior, solving flow equations for both liquid and gas phases. In contrast, all other codes solve for variably saturated flow according to Richard's equation (assuming constant gas pressure), but do not explicitly account for gas flow along a gas pressure gradient. However, recognizing the impact of vapor movement in a thermally perturbed setting with evaporation processes, these codes account for transport of water vapor in a simplified manner, by solving a diffusion problem with diffusivity dependent on pressure and temperature gradients (e.g., see Appendix C, Equations 3.9 through 3.13).

Table 4.2: Comparison of basic modeling approaches used for D_THM1

Team	Numerical simulator	Couplings considered	Mechanical model	Treatment of Buffer Swelling	Hydraulic model
DOE	TOUGH-FLAC	TH	NA	NA	Single continuum; multiphase liquid and gas flow
DOE	ROCMAS	THM	Elastic	Linear swelling strain model as a function of water saturation (targeted to give 5 Mpa at full saturation*)	Single continuum; unsaturated liquid flow, no gas flow; thermal vapor diffusion
BGR	GeoSys/ Rockflow	THM	Elastic	Alternative swelling model as a function of water saturation (possibly not targeted for 5 Mpa)	Single continuum, unsaturated liquid flow, no gas flow; thermal vapor diffusion
CAS	FRT-THM	THM	Elastic	Linear swelling strain model as a function of water saturation (targeted to give 5 Mpa at full saturation)	Single continuum, unsaturated liquid flow, no gas flow; thermal vapor diffusion
JNC	THAMES	THM	Elastic	Alternative swelling model as a function of water saturation (possibly not targeted for 5 Mpa)	Single continuum, unsaturated liquid flow, no gas flow; thermal vapor diffusion

* The target pressure of 5 MPa was specified in the task description (Barr et al., 2005).

4.2.2 Comparison of Model Results

In this section the calculated THM responses for Case D_THM1 (FEBEX type) are compared following output specification given in Barr et al. (2005, Section 6.5). The results of five different model analyses are compared. Those results were developed by DOE, using TOUGH-FLAC and ROCMAS, by CAS using FRT-THM, by BGR using GeoSys/Rockflow, and by JNC using THAMES.

Temperature Evolution

Figures 4.1 and 4.2 show that the general trends and magnitudes of temperature are in agreement for the five different model analyses. Some of the differences that can be observed in Figures 4.1 and 4.2 are related to differences in the interpolation of the tabulated inputs of the heat decay function. The heat power function for D_THM1 was given in a graphical form, and each team extracted tabular values from this graph as input to the model. In addition, each numerical analysis evaluates the heat power at the current time step by interpolating between the tabulated input values. It is apparent from the comparison of the temperature evolution that a small difference in the heat input over a longer period of time can have a quite significant effect on the calculated temperature evolution. Figure 4.2 shows that the difference in temperature near the drift also results in a corresponding difference in the vertical temperature profiles at 1,000 and 10,000 years.

Four out of the five models predict a peak temperature of about 90°C to occur at about 20 years after emplacement, given at Point V1, located at the canister-buffer interface (see definition of points in Appendix A, Figure 6.1). The temperature evolution for the JNC model shows a much higher temperature in V1. These differences in the early temperature evolution are likely related to differences in the evolution of the liquid saturation in the bentonite buffer. The evolution of saturation in the buffer affects its thermal conductivity, which in turn impacts the temperature evolution at the canister-buffer interface (Point V1). However, with the exception of early JNC results in V1, Figure 4.1 shows that the overall agreement between the different models is quite good, especially in Point V6, located about 10 m from the drift.

Evolution of Water Saturation and Fluid Pressure

Figure 4.3 shows a general agreement in the evolution of liquid water saturation in the buffer for a point located in the buffer near the canister surface. In the first few years the initially 65% water-saturated bentonite dries to about 45 to 50%, followed by gradual resaturation. Three out of five models predict a time to full resaturation of about 25 years, whereas the BGR and JNC analyses indicate 70 and 250 years of resaturation time, respectively. Two main processes determine the resaturation time. First, there is a continuous capillary-driven liquid water flux from the fully saturated rock mass into the unsaturated bentonite. Initially, the capillary pressure in the buffer is about –70 MPa (at 65% saturation), leading to a steep capillary pressure gradient. The capillary-driven liquid flux is initially more than offset by thermally driven vapor diffusion, which tends to transport evaporated moisture from the inner hot regions of the buffer, along the thermal gradient, toward outer cooler regions. In the first few years, when the thermal gradient is steep, evaporation and thermal diffusion are sufficiently strong to cause a certain degree of drying near the canister surface. After a few years, as the thermal gradient becomes smaller, the vapor diffusion rate decreases, the inward capillary-driven liquid flux becomes dominant, and finally the entire buffer becomes fully saturated. Differences in the modeling approach and properties for unsaturated fluid flow and thermal diffusion in the bentonite could cause the observed differences in resaturation time.

Figures 4.4 and 4.5 present comparisons of the evolution of fluid pressure in the model domain. During the steady state analysis of the excavation sequence, the open drift tends to drain water from the surrounding rock mass, thereby reducing the pressure. The drainage is shown in Figure 4.5a as the pressure at t = 0 (after excavation) is reduced to be close to zero near and above the drift. After emplacement of the canister and buffer, the water inflow from the formation into the backfilled tunnel decreases and the fluid pressure in the surrounding rock mass increases slowly toward ambient hydrostatic conditions. The results in Figure 4.4 indicate that the ambient hydrostatic fluid pressure is fully restored after about 100 to 1,000 years. The time to restore the ambient fluid pressure depends mainly on the hydraulic properties of the rock mass, and may also be affected by the resaturation of the buffer. The time evolution of the fluid pressure is important for calculation of THM responses, since it affects the time evolution of effective stresses in the rock mass.

Evolution of Stress

Figure 4.6 compares the evolution of stress in the bentonite buffer. The results show that the calculated stress evolution is very different for different teams. The stress evolution is quite consistent between DOE and CAS results, though the final stress magnitude is different. The evolution of total stress in the buffer is mainly affected by the two sources:

1) Moisture swelling of bentonite as the buffer becomes fully saturated
2) Restoration of fluid pressure from an initially drained condition to fully restored hydrostatic pressure.

In addition, thermal expansion of the bentonite has some effect on the total stress evolution in the buffer. The differences in the stress evolution in Figure 4.6 are most likely related to differences in the model approaches and input parameters for moisture swelling. Because the evolution of swelling stress is important for the stability of the drift walls, a more consistent result of the evolution of stress in the buffer is desirable: The final magnitude of the swelling stress after resaturation and the approximate time at which it is achieved should at least be consistent between the different models. Further work is needed to resolve this inconsistency.

Figures 4.7 and 4.8 compare the evolution of horizontal stress in the rock mass. The first figure shows an apparent input error in the initial stresses in the JNC simulation results. Moreover, the initial stress is slightly lower in the DOE (ROCMAS) and CAS simulation results compared to those of BGR. The lower initial stress in the DOE and CAS simulation is an effect of the drainage of formation water into the excavated opening, leading to fluid pressure decrease (See further explanation in Appendix C, Section 4.3.2.) In the BGR results, water drainage is considered, but does apparently not affect the stress field. This needs to be checked in the BGR model.

Figure 4.8 shows that the profiles of horizontal stresses look similar to those of the vertical temperature profiles. The horizontal stresses increase strongest near the drift, where the temperature changes are most prominent. Also, the differences in stress profiles in Figure 4.8 are consistent with differences in temperature profiles in Figure 4.2.

Apart from the differences in the initial stress field, it seems that the thermally induced stress changes are quite consistent between the different models. (Note that the thermally induced stress is the difference between the initial stress and the peak stress.) The calculated stress in Point V3, which is located close to the drift wall, may be somewhat affected by the discretization differences between the four models. Because the stress gradient is very large near the drift wall, any interpolation between model grid points will lead to some inaccuracies.

Evolution of Displacement

Figures 4.9 and 4.10 present the evolution of vertical displacement. In the DOE (ROCMAS) and CAS analyses, the entire column settles initially about 0.05 m, caused by the drainage of water into the open excavation (V7 in Figure 4.9). The BGR model results do not indicate any initial settlement. The vertical profiles in Figure 4.10 show that the general shapes of the displacement profiles are consistent between the different models, except for the excavation phase.

All four models agree that the vertical displacement peaks at about 2,000 years after emplacement of waste. The magnitude of the peak displacement is controlled by the temperature change and the thermal expansion coefficient. (There is no impact of fluid pressure on the peak displacement because the fluid pressure has already been restored to the ambient hydrostatic fluid pressure at 2,000 years.) The peak displacement calculated by DOE (ROCMAS), CAS (FRT-THM) and JNC (THAMES) is about 0.25 m, whereas the peak value calculated by BGR is about 70% that of the three other teams. This difference in peak displacement should be resolved; the peak displacement depends exclusively on the correct temperature distribution and the value of the thermal expansion coefficient.

Evolution of Vertical Water Flux

Figure 4.11 presents a horizontal profile of the vertical percolation flux calculated by the DOE (ROCMAS) and CAS (FRT-THM) teams. So far, results for vertical percolation flux have not been provided by other teams. The numerical value of an initial vertical water flux of about 0.3 mm/yr was confirmed by analytical solution in Appendix C, Section. 4.3.5. The vertical flux is a result of the vertical hydraulic head gradient since the fluid pressure at the lower boundary was fixed at a pressure slightly less than hydrostatic. After long time (over 100 years) the water flux stabilizes somewhat with a diversion around the bentonite filled drift. The results of water flux are dependent on the temperature dependent hydraulic properties, in particular the fluid viscosity. The vertical percolation flux is important since it forms the basis for studying the impact of THM couplings on fluid flow.

Summary of Comparison of Model Results for THM1 Case

In summary, the overall trends and the magnitude of THM evolution are quite consistent between the different models. However, there is room for improvement regarding several aspects that have an impact on the evolution of stress. The current differences in calculated THM responses are related to:

(1) Differences in the interpolation of the tabulated heat decay function
(2) Differences in the treatment of fluid pressure effects on the stress and displacement evolution
(3) Differences in the modeling approaches and input data for bentonite swelling.

These differences could be resolved as follows:

(1) The heat decay function could be more accurately defined by providing closely spaced tabular values for each team to use.

(2) The water drainage during the excavation phase and its effect on stress and strain should be considered in all models, choosing a finite excavation time of 30 years.
(3) The properties for the bentonite swelling need to be strictly defined, perhaps using a target swelling pressure.

Nevertheless, a reasonably good agreement has been achieved regarding the temperature and thermal stress in the rock mass. Therefore, research teams could begin the analysis of the next phase of Task D_THM, while continuing to resolve the remaining differences for Phase 1 results.

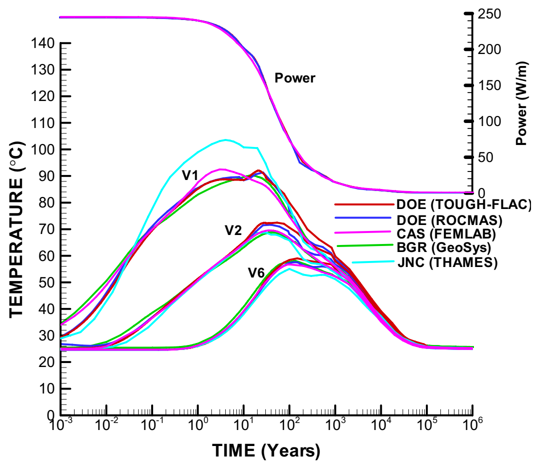
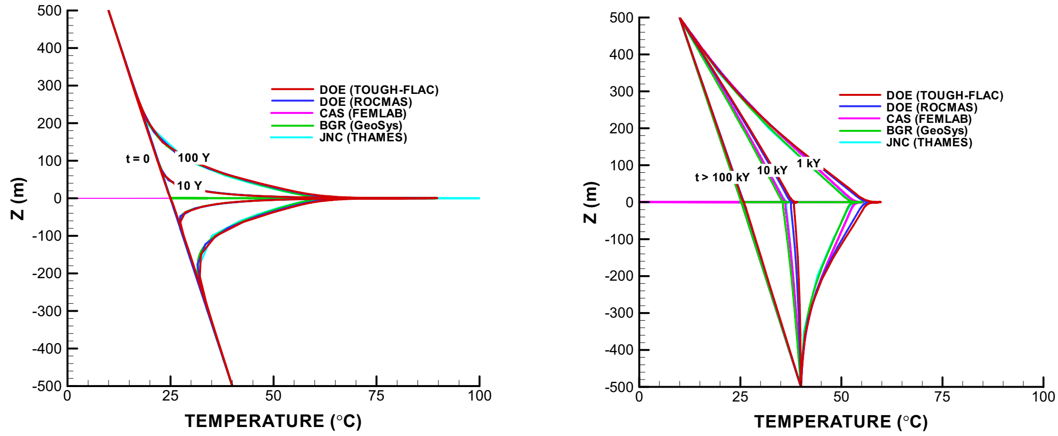


Figure 4.1: Comparison of input power and temperature evolution at selected output points



(a) Profiles for t ≤ 100 years (b) Profiles for t ≥ 1000 years

Figure 4.2: Comparison of vertical temperature profiles

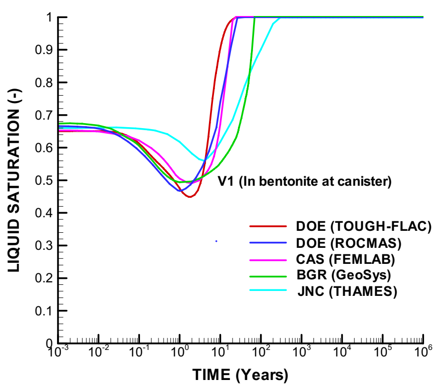


Figure 4.3: Comparison of simulation results for the evolution of degree of saturation in bentonite (Point V1).

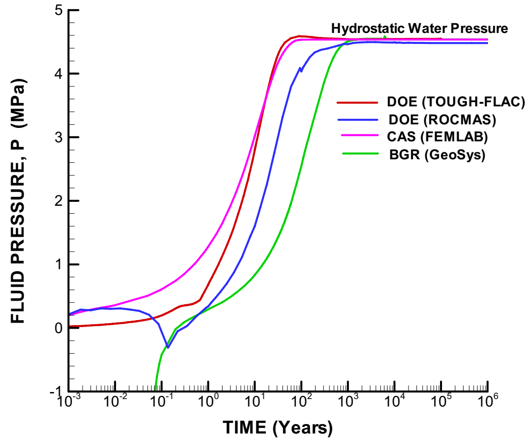


Figure 4.4: Comparison of evolution of water pressure at Point V3 located at the drift wall.

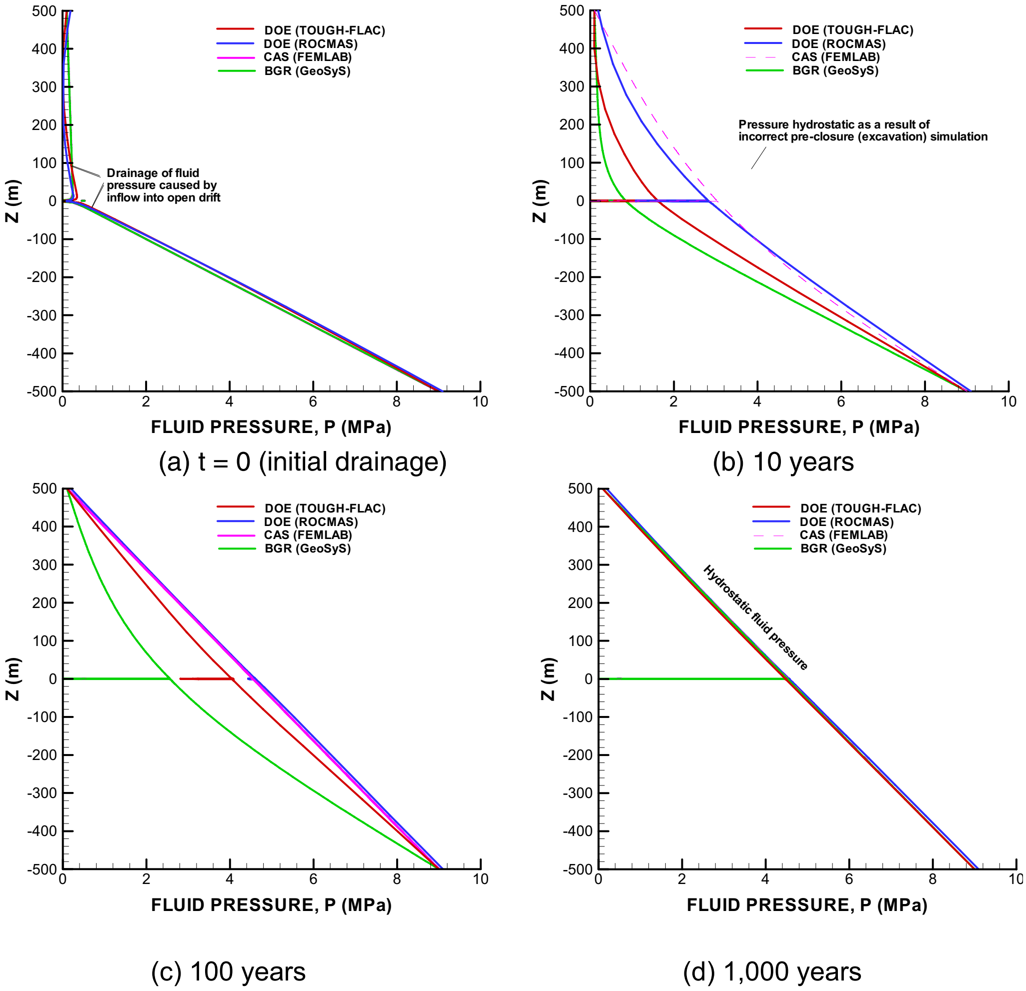


Figure 4.5: Comparison of simulation results of vertical pressure profiles

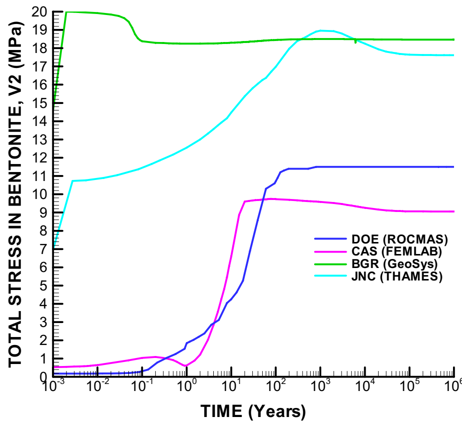


Figure 4.6: Comparison of evolution stress normal to the rock wall at point V1 located at the rock/bentonite interface

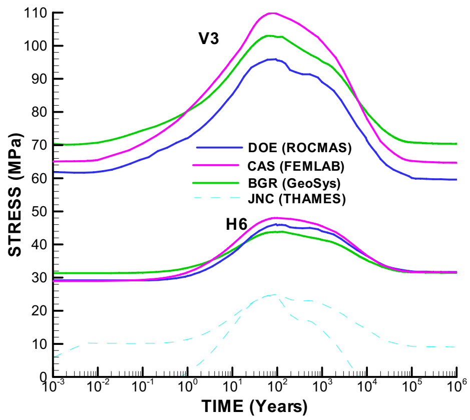


Figure 4.7: Comparison of evolution of horizontal stress in points V3 and H6

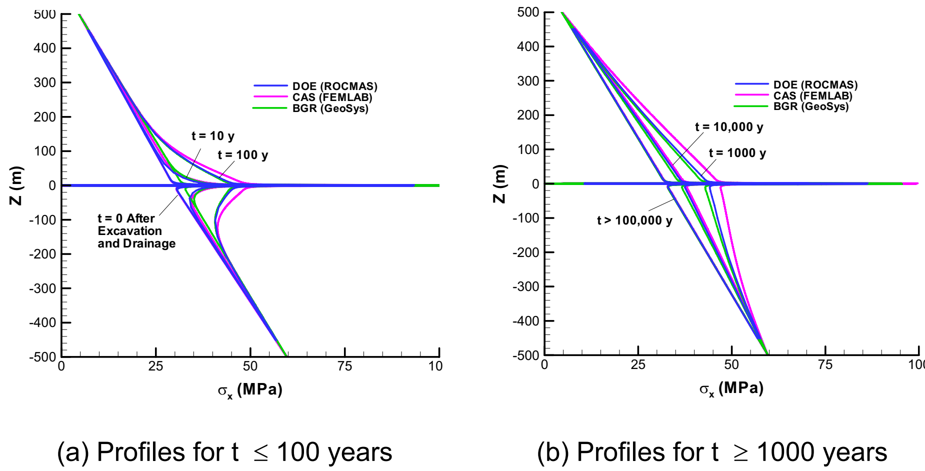


Figure 4.8: Comparison of vertical profiles of horizontal stress

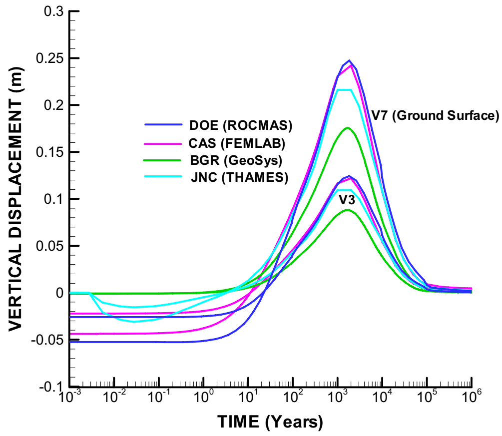
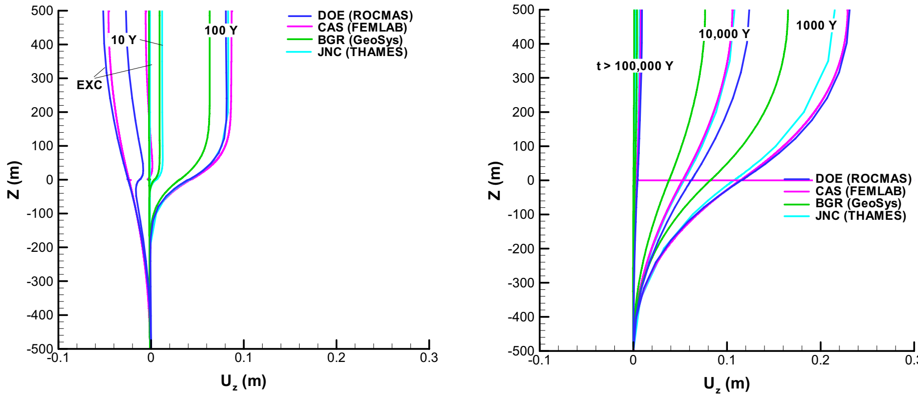


Figure 4.9: Comparison of evolution of vertical displacement at the ground surface (V7) and at the drift (V3)



(a) Profiles for t ≤ 100 years (b) Profiles for t ≥ 1,000 years

Figure 4.10: ROCMAS simulation results of vertical displacement profiles

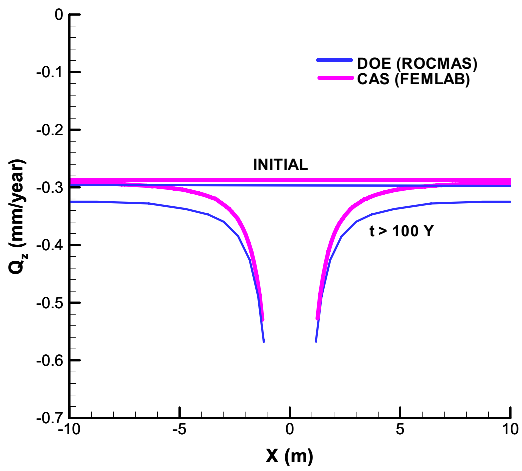


Figure 4.11: Comparison of DOE (ROCMAS) and CAS simulation results of vertical flux through the repository horizon

4.3. Repository Case D_THM2 (Yucca Mountain Type)

4.3.1 Comparison of Model Approaches

The basic modeling approaches employed by the four international teams (DOE, BGR, JNC, CAS) modeling D_THM2 are summarized in Table 4.3. All codes are capable of handling fully coupled thermal-hydrological-mechanical (THM) processes; however, the simulations with ROCMAS have been conducted in a TM-only mode for the sake of comparison with more complex models. Simple elastic approaches are used for simulation of the rock-mechanical behavior, consistent with the simplified task definition for Phase 1 work. However, all models are generally capable of simulating elasto-plastic behavior, which may become necessary when stress-induced changes in hydrologic properties are to be considered in the next phases of D_THM2.

The Yucca Mountain type of repository simulated in case D_THM2 involves complex two-phase flow (gas and liquid phases with components of air and water) interactions between fractures and matrix rock at high (above boiling) temperatures. Because of the higher peak temperatures, the thermal-mechanical effects are likely stronger than in the FEBEX case (D_THM1). Boiling and subsequent condensation of pore water triggers moisture redistribution processes in the rock surrounding the repository drift that last for hundreds of years. The thermally induced liquid and gas flow processes are strongly affected by the vastly different hydrological properties of the fractures and the rock matrix, respectively. The matrix holds significant amounts of water even at ambient conditions, but has a very small permeability, so that overall matrix fluxes are small. The fracture network, on the other hand, is highly permeable, but has a small capillarity, and thus is typically dry under ambient conditions. However, as the near-drift rock is heated up and significant flux perturbation occurs, the fractures become important flow conduits for vapor and liquid. A proper analysis of near-field TH processes in the fractured porous rock would ideally require multi-phase flow and heat transport capabilities employed in a model that can account for the specific hydrologic properties and conditions of fractures and matrix, with their vastly differing permeabilities and moisture retention characteristics.

TOUGH-FLAC, which has been extensively applied in the modeling of coupled THM processes for the unsaturated zone at Yucca Mountain, has all the necessary modeling capabilities listed above. The code accounts for multi-phase flow in liquid and gas phases and deals with phase transition from boiling and condensation in a rigorous manner. Fracture and matrix conditions can be distinguished using the dual continuum model (DKM). A dual continuum model is based on the continuum concept, but uses two separate, overlapping continua for fractures and matrix. At each location, there are two nodes (or volumes) representing the fractures and the matrix, respectively, each having a pressure, saturation, temperature, or stress value. Thus, local disequilibrium between fractures and matrix can be modeled without explicitly accounting for all individual fractures and matrix blocks. This allows considering the hydrologic properties and conditions of fractures and matrix with their vastly different hydrologic properties. Dual continuum models are a good choice for D_THM2 (except for using discrete fracture-matrix continuum models or hybrid models), but require significant code development.

At this point, none of the other codes used for D_THM2 has the full multi-phase capability that is incorporated into TOUGH-FLAC, and certain simplifications become necessary. For example, as mentioned above, ROCMAS solves for thermal-mechanical processes only. Since saturation is unknown, the changes in thermal properties (as the formation dries out at above-boiling temperatures) are accounted for by a simplified temperature-dependent approach described in Barr et al. (2005, Section 6.4.2). The other codes solve Richard's equation for liquid flow, but neglect gas flow. Instead, they account for transport of water vapor in a simplified manner, by solving a diffusion problem with diffusivity dependent on pressure and temperature gradients.

Also, only TOUGH-FLAC is capable of representing the fractured rock mass as a dual continuum; single continuum models are used in all other simulations. It is clear from previous modeling exercises that the flow processes predicted with single continuum models are not adequate when the near-drift rock is heated up and significant flux perturbation occurs (with the fractures becoming important flow conduits for vapor and liquid). For future project phases, when understanding of flow processes becomes more important, teams that strive for a better hydrological response but want to avoid dual continuum modeling may consider the so-called effective continuum model (ECM) (after Pruess et al. [1990]). An effective continuum model captures the different hydraulic characteristics of fractures and matrix, but assumes a local THM equilibrium between fractures and matrix at all times. For systems that are not too dynamic in nature, the ECM model gives quite adequate flow results.

Table 4.3: Comparison of basic modeling approaches used for D_THM2

Team	Numerical simulator	Couplings considered	Mechanical model	Hydraulic model	Thermal Model for Boiling
DOE	TOUGH-FLAC	THM	Elastic	Dual continuum; multiphase liquid and gas flow	Full phase-change model for boiling
DOE	ROCMAS	TM	Elastic	NA	Temperature-dependent thermal properties adopted from (Barr et al., 2005, Section 6.4.2)
BGR	GeoSys/ Rockflow	THM	Elastic	Single continuum, unsaturated liquid flow, no gas flow; thermal vapor diffusion	Temperature-dependent thermal properties adopted from (Barr et al., 2005, Section 6.4.2)
JNC	THAMES	THM	Elastic	Single continuum, unsaturated liquid flow, no gas flow; thermal vapor diffusion	Unknown, probably simple conduction model without boiling
CAS	FRT-THM	THM	Elastic	Single continuum, unsaturated liquid flow, no gas flow; thermal vapor diffusion	Temperature-dependent thermal properties (Barr et al., 2005, Section 6.4.2)

4.3.2 Comparison of Model Results

In this section, the calculated THM responses for Case D_THM2 (Yucca Mountain type) are compared following output specification given in Barr et al. (2005, Section 6.5). The results of four different analyses are compared. These were developed by DOE, using TOUGH-FLAC and ROCMAS, by CAS using FRT-THM, by BGR using GeoSys/Rockflow, and by JNC using THAMES..

Temperature Evolution

Figures 4.12 and 4.13 compare the temperature evolution calculated from the five alternative models. The agreement between the different models is good. Similarly to the THM_1 case (*FEBEX* type), the temperature evolution in the THM_2 case (*Yucca Mountain* type) depends somewhat on the interpolation of the tabulated input heat decay function. However, in the case of THM_2, the heat decay function is better defined through closely spaced tabular values.

In the THM_2 case, the temperature evolution is significantly affected by drying (through boiling of pore water) and rewetting of the near-field rock mass. A peak temperature of 120 to 125°C is calculated by the different models, with the CAS analysis yielding the highest value. It is likely that the slightly higher peak temperature obtained by the CAS is a result of a simplified analysis of the boiling-zone effect on heat transfer (simplified treatment of changes in thermal conductivity as the rock mass dries, simplified treatment of latent heat of vaporization as water boils; see Barr et al., 2005). A similarly high peak temperature was obtained by the DOE team when using the same kind of simplified boiling effect model (see Appendix C). The DOE team found that the simplified boiling model tends to overestimate the effect of boiling on the heat transfer. A pure conduction model yielded a temperature evolution that better matched that of a fully described two-phase fluid flow and heat transport model.

Evolution of Water Saturation

Figure 4.14 compares the initial saturation values in the entire domain for DOE (TOUGH-FLAC) and CAS (FRT-THM). The DOE (TOUGH-FLAC) model, featuring a dual continuum representation of the fractured rock, predicts matrix saturation values between 80 to 92%, whereas fracture saturation varies between 2 to 2.5%, with the highest values occurring at large depth. The CAS (FRT-THM) model uses a single continuum approach with retention properties equal to those of the matrix. Consequently, the CAS single continuum saturation distribution is close to that of the matrix results from the DOE (TOUGH-FLAC) model.

Figure 4.15 compares the evolution of liquid saturation at the drift wall for four models. The figure shows that rock at the top of the drift begins to dry at about 50 years, when boiling occurs at the drift wall. In the DOE (TOUGH-FLAC) analysis, the fractures dry quickly, whereas the matrix has not completely dried until about 100 years. Rewetting of fractures occurs after about 400 years, and the matrix is resaturated to original conditions at about 700 years. In contrast, the CAS and BGR models do not predict a full dryout to zero saturation. This is probably a result of neglecting fracture gas flow in the model. As a result, vapor produced from boiling cannot as easily migrate away from the boiling location as in a dual continuum model, where the fractures offer highly efficient conduits for vapor flow. The total dryout time till rewetting calculated by CAS (FRT-THM), DOE (TOUGH-FLAC) and BGR (GeoSys) models is similar, while the time evolution of saturation is somewhat different. The JNC (THAMES) results indicate limitations in solving the above boiling TH effects using the simplified single continuum approach. Better agreement is expected in future project phases, when more rigorous models (not just single continuum) will be used by the other teams to simulate flow in fractures and matrix rock.

Evolution of Stress

Figures 4.16 and 4.17 present the evolution the horizontal stress. The calculated results for four of the five model calculations are very consistent, both in trends and magnitudes. In contrast, the model results submitted by JNC (shown as a dashed line in Figure 4.16) suffer from some error in the input data. Based on the initial stress results, it appears that the JNC analysis does not properly account for the excavation of the drift. In the analyses by DOE,CAS and BGR, the initial stress is higher at Point V3 as a result of stress concentrations near the drift wall. In the JNC results, on the other hand, the initial horizontal stresses in V3 and H6 are the same, indicating no stress redistribution around the excavated drift. For the DOE, CAS and BGR simulations, the peak stress at V3 varies between 33 to 35 MPa, whereas the peak stress at H6 is almost identical at about 14 MPa. The slight variation in peak stress at V3 is likely caused by interpolation inaccuracies, stemming from different mesh discretizations in a region of steep stress gradients, as well as from differences in the exact location of the point representation in the numerical mesh. However, overall a good agreement in the calculated stress evolution has been achieved. More work is needed by the JNC team to improve the current prediction.

Evolution of Displacement

Figures 4.18 and 4.19 present the evolution of vertical displacements. The peak displacement at the ground surface is about 0.23 m and occurs after about 1,000 years. The agreement between the calculated displacements among three out of four models (DOE models, CAS model and JNC model) is very good. The result by BGR shows similar trend and magnitude but displays an unexplained kink at about 100 to 200 years.

Evolution of Vertical Water Flux

Figure 4.20 presents a horizontal profile of the vertical percolation flux calculated by the DOE (TOUGH-FLAC) and CAS (FRT-THM) models. The vertical flux has not been provided by other modeling teams at this time and the comparison in Figure 4.20 is made only for flux at t = 0 (after excavation). Figure 4.20 shows that the vertical flux away from the drift is 6 mm/year, which is dictated by the water flux supplied as infiltration at the top boundary of the model. The effect of the excavated drift and dryout zone around the drift on vertical flux is evident. At t = 0, the vertical flux is diverted around the drift (due to capillary barrier effects) leading to a water flux of about 15 to 20 mm/year near the drift wall. The DOE (TOUGH-FLAC) results also shows that at 100 years, the water is diverted around the dryout zone, which extends to a few meters from the drift wall (not shown in this figure). Within that dryout zone, water saturation is either zero (fractures) or very small (matrix) and liquid fluxes are practically zero.

Summary of Comparison of Model Results for THM2 Case

Overall, a good agreement in the evolution of temperature and stress was achieved. A small difference in peak temperature is caused by the simulation approach for TH coupling, but this has a minor impact on the mechanical responses. The thermal-mechanical effects can be accurately calculated using a simple thermal-elastic heat conduction model. The analysis of fluid flow, which involves complex interaction between matrix and fractures, has only been fully analyzed with DOE's TOUGH-FLAC model, featuring a dual continuum model. All other teams have used simple single continuum approaches, which are not capable of simulating the complex interaction between fractures and matrix in a thermally perturbed system. Improved single continuum models, such as the effective continuum model approach (ECM), should be used by these teams in case they want to avoid the complexity of a full dual continuum representation. This should provide more consistent and comparable results in vertical flux and liquid saturation. This is important for a proper comparison of the impact of THM processes on the vertical percolation flux. However, the comparison of stress evolution by three models is good and sufficient for moving on to the next phase of Task D_THM2. Some revision is needed for the JNC model, which currently has difficulty predicting the stress conditions.

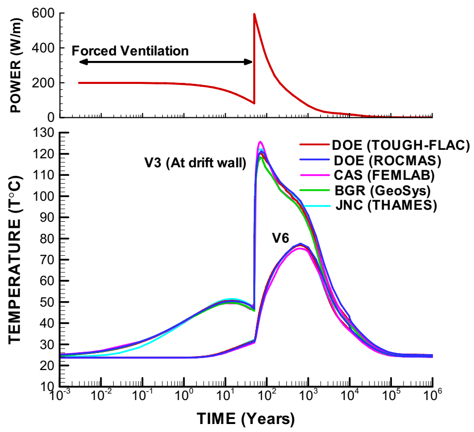
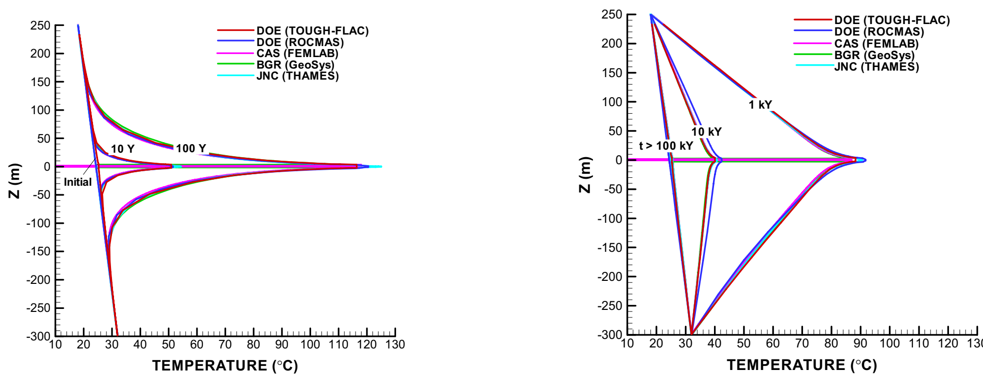


Figure 4.12: Power and comparison of temperature evolution at two selected points



(a) Profiles for t ≤ 100 years (b) Profiles for t ≥ 1000 years

Figure 4.13: Comparison of vertical temperature profiles

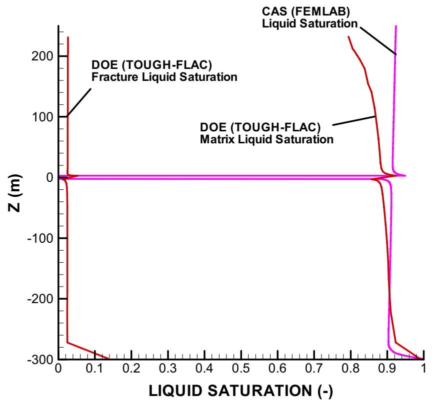


Figure 4.14: Simulation results of vertical profiles of initial saturation for a dual permeability model (DOE, TOUGH-FLAC) and a single continuum model (CAS, FEMLAB)

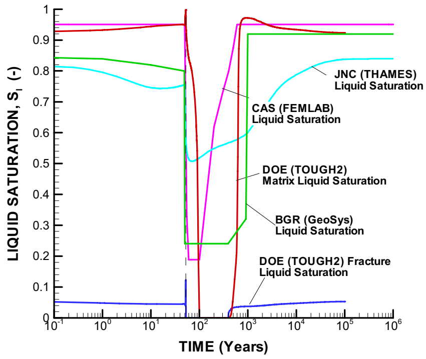


Figure 4.15: Evolution of liquid saturation in fracture and matrix continua at Point V3 located at the drift wall on top of the drift for a dual permeability model (DOE, TOUGH-FLAC) and single continuum models (CAS-FEMLAB, BGR-GeoSys, and JNC-THAMES)

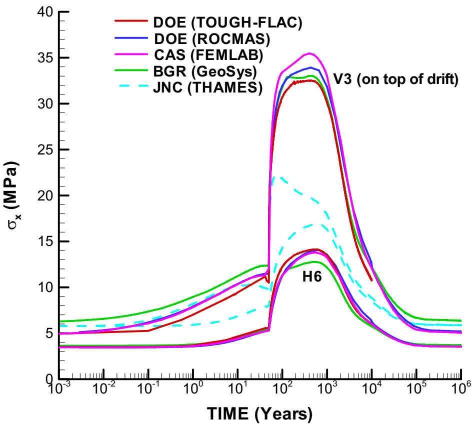
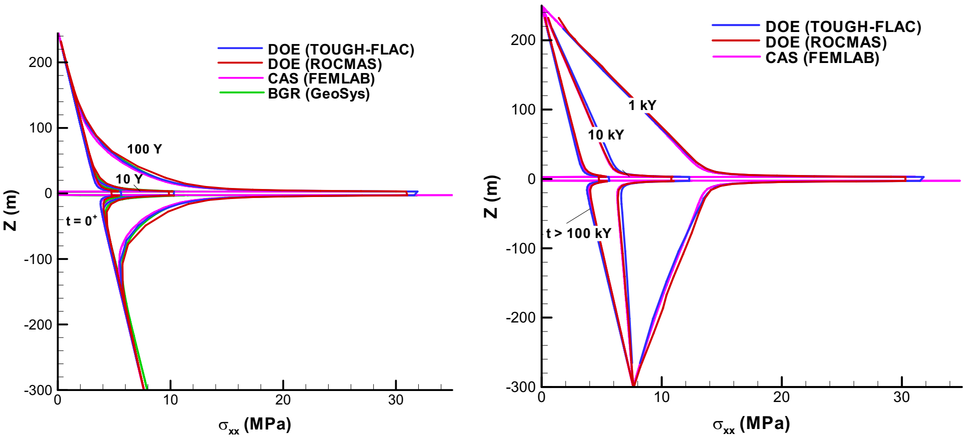


Figure 4.16: Comparison of simulation results of evolution of horizontal stresses in monitoring points V3 (near drift) and H6 (away from drift)



(a) Profiles for t ≤ 100 years (b) Profiles for t ≥ 1000 years

Figure 4.17: Comparison of vertical profiles of horizontal stress

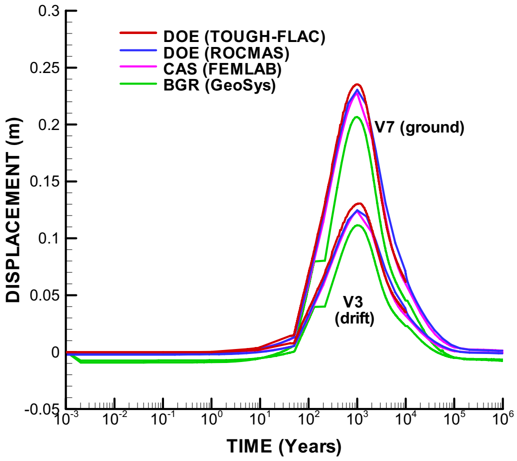
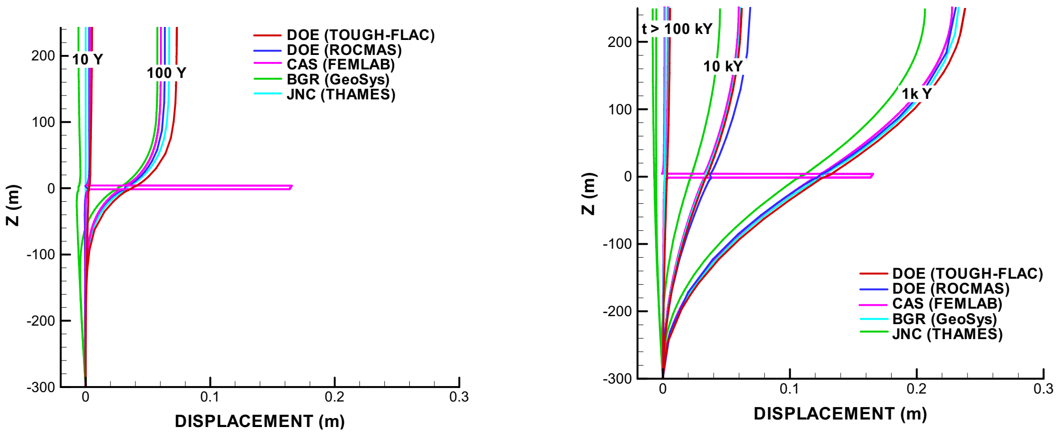


Figure 4.18: Comparison of simulated evolution of vertical displacement



(a) Profiles for t ≤ 100 years (b) Profiles for t ≥ 1000 years

Figure 4.19: Comparison of simulation results of vertical displacement profiles

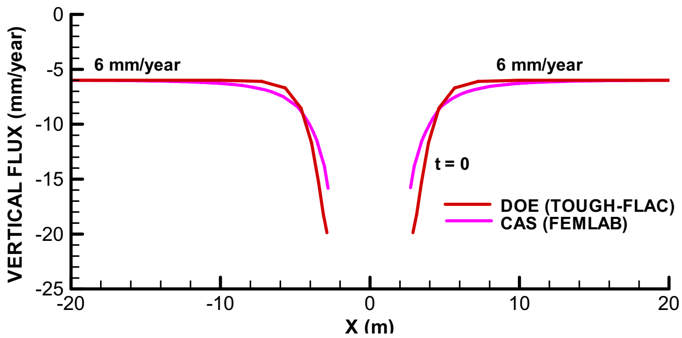


Figure 4.20: Comparison of TOUGH-FLAC and CAS simulation results of vertical flux across a horizontal profile

4.4. Future THM Workscope

As discussed in previous sections, the Phase 1 (Model Inception Phase) activities have largely been finalized, with good agreement among all teams for thermal and mechanical processes. A few remaining model discrepancies have been identified, and a few revised simulations will have to be conducted by individual teams for full completion of Phase 1. Thus, the next step for all team is to move forward into Phase 2 modeling. As summarized in Section 2.4.1, Phase 2 modeling involves more focus on hydrological processes, including prediction of THM property changes with conceptual models chosen by the different research teams, sensitivity analysis with respect to THM property changes plus uncertainty analysis, application of alternative conceptual models for fractured rock (i.e., discrete vs. continuum), and development of model data based on various reports and site data, instead of using pre-defined values (see Appendix A). Reports that may be used for D_THM1 are listed below, together with web sites from where they can be retrieved.

Table 4.4: Supporting information for Phase 2 of D_THM1

Reference	Comment
Keusen H.R., Ganguin J., Shuler P. and Buletti M. (1989). Grimsel Test Site: Geology NAGRA NTB 87-14E, FEb 1989.	Download from LBNL web site: http://esd.lbl.gov/people/kavina/DECOVALEX/THM1_Phase2_Docs/
Amiguet J.-L. (1985). Grimsel Test Site. Felskennwerte von intaktem Granit. Zusammenstellung felsmechanisher Laborresultate diverse granitische Gesteine. NAGRA, NIB 85-05, Sep. 1985.	Download from LBNL web site: http://esd.lbl.gov/people/kavina/DECOVALEX/THM1_Phase2_Docs/
Pardillo J., Campos R. and Guimera J. (1997). Caracterizacion geologica de la zone de ensayo FEBEX (Grimsel – Suiza). CIEMAT, 70-IMA-M-2-01, May 1997.	Download from LBNL web site: http://esd.lbl.gov/people/kavina/DECOVALEX/THM1_Phase2_Docs/
Pardillo J. and Campos R. (1996). FEBEX-Grimsel Test Site (Switzerland). Considerations with respect to the fracture distribution. CIEMAT, 70-IMA-L-2l05, Mar. 1996.	Download from LBNL web site: http://esd.lbl.gov/people/kavina/DECOVALEX/THM1_Phase2_Docs/
Guimera J., Carrera J., Marinez L., Vazquez E., Ortuno F., Fierz T., Bulher C., Vives L., Meier P., Median A., Saaltink M., Ruiz B. and Pardillo J. (1998). FEBEX Hydrogeological characterization and modelling. UPC, 70-UPC-M-0-1001, Jan 1998.	Download from LBNL web site: http://esd.lbl.gov/people/kavina/DECOVALEX/THM1_Phase2_Docs/
Fujita T., Sugita Y., Chijimatsu M. and Ishikawa (1996). Mechanical properties of fracture. Power Reactor and Nuclear Fuel Development Corporation (PNC), Technical note 06-95-06.	Download from LBNL web site: http://esd.lbl.gov/people/kavina/DECOVALEX/THM1_Phase2_Docs/
DECOVALEX III (2000). Task 1. Modeling of FEBEX in situ test. Part A: Hydromechanical modeling of the rock.	Download from LBNL web site: http://esd.lbl.gov/people/kavina/DECOVALEX/THM1_Phase2_Docs/
DECOVALEX III (2001). Task 1. Modeling of FEBEX in situ test. Part B: Thermo-hydro-mechanical analysis of the bentonite behaviour.	Download from LBNL web site: http://esd.lbl.gov/people/kavina/DECOVALEX/THM1_Phase2_Docs/
Alonso et al. (2004). Final report of DECOVALEX III, Task1: FEBEX in situ test. SKI report expected during 2004.	Download from Decovalex website: Login and go to Documents / Reports from DECOVALEX III and BENCHPAR / Final reports / **Task 1** /

Reports that may be used for D_THM2 are listed below, together with web sites where they can be retrieved.

Table 4.5: Supporting information for Phase 2 of D_THM2

Reference	Comment
BSC (Bechtel SAIC Company) 2003a. *Drift Degradation Analysis*. ANL-EBS-MD-000027 REV 02. Las Vegas, Nevada: Bechtel SAIC Company.	Download from: http://ocrwm.doe.gov/documents/amr/36086/index.htm
BSC (Bechtel SAIC Company) 2003b. *Calibrated Properties Model*. MDL-NBS-HS-000003 REV 01. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20030219.0001.	Download from: http://ocrwm.doe.gov/documents/amr/41503/index.htm
CRWMS M&O (Civilian Radioactive Waste Management System Management and Operating Contractor) 2000. *Statistical Analysis of Empirical Rock Properties by Lithographic Units*. CAL-GCS-GE-000001 Revc 00. Las Vegas.	Download from LBNL web site: http://esd.lbl.gov/people/kavina/DECOVALEX/THM2_Phase2_Docs/
CRWMS M&O (Civilian Radioactive Waste Management System Management and Operating Contractor) 1997. *Yucca Mountain Site Geotechnical Report*. B00000000-01717-5705-00043 REV 01. Two volumes. Las Vegas, Nevada.	Download from LBNL web site: http://esd.lbl.gov/people/kavina/DECOVALEX/THM2_Phase2_Docs/
CRWMS M&O (2000). Fracture Geometry Analysis for the Stratigraphic Units of the Repository Host Horizon. ANL-EBS-GE-000006 REV 00. Las Vegas, Nevada.	Download from LBNL web site: http://esd.lbl.gov/people/kavina/DECOVALEX/THM2_Phase2_Docs/
Datta et al. (2004). DECOVALEX III, Task 2, Final Report. (SKI report expected during 2004).	Download from LBNL web site: http://esd.lbl.gov/people/kavina/DECOVALEX/THM2_Phase2_Docs/
Hoek E., Carranza-Torres C. and Corkum B., (2002). Hoek-Brown Failure Criterion – 2002 Edition 5th North American Rock Mechanics Symposium and 17th Tunnelling Association of Canada Conference: NARMS-TAC 2002, July 7-10 University of Toronto, Toronto, Ontario, Canada.	Download from LBNL web site: http://esd.lbl.gov/people/kavina/DECOVALEX/THM2_Phase2_Docs/
Mongano G.S., Singleton W.L., Moyer T.C., Beason S.C., Eatman G.L.W. Albin A.L. and Lung R.C. (1999) Geology of the ECRB Cross Drift – Exploratory Studies Facility, Yucca Mountain Project, Yucca Mountain, Nevada. Denver Colorado U.S. Geological Survey.	Download from LBNL web site: http://esd.lbl.gov/people/kavina/DECOVALEX/THM2_Phase2_Docs/
CRWMS M&O (1998). Ge*ology of the Exploratory Studies Facility Topopah Spring Loop*. BAB000000-01717-0200-00002 REV 01. Las Vegas, Nevada	Download from LBNL web site: http://esd.lbl.gov/people/kavina/DECOVALEX/THM2_Phase2_Docs/
Olsson W.A. and Brown S. (1995). *Mechanical properties of fractures from drill holes UE25-NRG-4, USW-NRG-6, USW-NRG-7, and USW-SD-9 at Yucca Mountain, Nevada.* Sandia National Laboratories Technical Report, Sand 95-1736. Albuquerque New Mexico, Sandia	Download from LBNL web site: http://esd.lbl.gov/people/kavina/DECOVALEX/THM2_Phase2_Docs/
Brown S.R. (1985) Simple mathematical model of a rough fracture. J. Geophys. Res. 100, 5941–5952.	Download from LBNL web site: http://esd.lbl.gov/people/kavina/DECOVALEX/THM2_Phase2_Docs/

5. Task D_THC: GeoChemical Analysis

Three research teams are involved in modeling Task D_THC, from Germany, Japan, and the U.S. The CAS team from China has decided to primarily focus on geomechanical issues; however, it was indicated that they might join at a later stage. Overall, the progress made by the research teams has been good, considering that geochemical processes are new to the DECOVALEX project. While the DOE team has conducted geochemical modeling of the Yucca Mountain site for over 10 years, other teams have less experience with THC models. Section 5.1 below gives a brief summary on the current status of the geochemical modeling work. Each team has provided a status report, which describes the conceptual model approaches and discusses modeling results, if available. With some minor editing for format consistency, these status reports have been added as Appendices G through I of this letter report (see attached CD). To bring out similarities and discrepancies between different research approaches, the LBNL research team has conducted a comparative evaluation of the status reports with regards to the conceptual models used and the simulation results. This comparative evaluation is summarized in Section 5.2.1 (Conceptual Models) and Section 5.2.2 (Simulation Results). Note that the comparison was only conducted for Task D_THC1, since modeling results were not available yet for the Yucca Mountain task.

5.1. Summary Status of D_THC Research Work

For the teams from Japan and Germany, most of the initial project stages were devoted to code development and model testing. The JNC team from Japan started development of a code that can be used for a fully coupled thermal-hydrological-mechanical-chemical analysis (Table 5.1). The code uses a coupling system (COUPLYS) that links individual process codes for geomechanical analysis (THAMES), mass transport (Dtransu-3D-EL), and reactive geochemistry (PHREEQC). The code is currently in its testing stage and has not yet been applied to the D_THC test cases. JNC is also conducting a series of laboratory experiments (COUPLE-experiment) to better understand the geochemical evolution in a heated bentonite-rock system (see status report in Appendix H). The experiment, when finalized in March 2006, may provide valuable input data for the geochemical modeling of D_THC1.

Germany's BGR team has also been heavily involved in code development and testing. A THM code (GeoSys Rockflow) was combined with the reactive geochemistry code PHREEQC. Initial model simulations have been conducted for D_THC1, featuring the simplified FEBEX case as defined in the Model Inception Phase (see status report in Appendix I). As a next step, the BGR team will move into modeling of D_THC2.

DOE's team has conducted preliminary simulation work on D_THC1. Modeling of the Yucca Mountain case in D_THC2 would involve moderate revisions of the predictive simulations that have already been conducted for the Yucca Mountain Program (to adapt to the simplified setting and geometry). This task has not been completed, but will be finished during the next year as other teams also move into modeling of D_THC2.

The FEBEX case in D_THC1 required development of a completely new geochemical model by the DOE team. Prior to this modeling work, a significant amount of work was needed to construct the D_THC1 problem description, e.g., defining the bentonite and rock mineralogy, as well as the water chemistry. This model definition work for D_THC1 was conducted in close collaboration with the research teams in Japan and Germany. It should be noted that some definitions for D_THC1 are still somewhat preliminary and may need further refinement.

Table 5.1: Research teams involved in and numerical models applied within Task D_THC of DECOVALEX-THMC

Team	**Affiliation**	**Computer Code**	**Test Case Simulated**
DOE-Team	Lawrence Berkeley National Laboratory (LBNL) for DOE	TOUGHREACT	D_THC1
JNC-Team	Japan Nuclear Cycle Development Institute (JNC)	COUPLYS with THAMES, Dtransu-3D-EL and PHREEQC	NA
BGR-Team	Center for Applied Geosciences Tuebingen, for BGR	GeoSys/Rockflow with PHEEQC	D_THC1

All teams submitted reports on the current work status . These status reports suggest (a) that sophisticated THC codes have been developed by JNC and BGR that should soon be capable of simulating both D_THC1 and D_THC2, and (2) that the preliminary simulation results for D_THC1 (by DOE ‘s team and BGR’s team) are in reasonable agreement. However, more detailed comparison and further model revisions will be necessary in the future.

5.2. Repository Case D_THC1 FEBEX Type

5.2.1 Comparison of Model Approaches

The basic modeling approaches employed by the two international teams (DOE and BGR) modeling D_THC1 are summarized in Table 5.2. Both codes are capable of modeling thermal-hydrological-chemical (THC) coupling. At this point, both teams use a single continuum representation of the crystalline rock mass. This may change in later project phases, when the effect of sparsely distributed fractures may be considered in a more rigorous manner.

Note that TOUGHREACT simulates complex multiphase flow behavior, solving flow equations for both liquid and gas phases. In contrast, Geosys/Rockflow solves for variably saturated flow according to Richard’s equation (assuming constant gas pressure), but does not explicitly account for gas flow along a gas pressure gradient. However, recognizing the impact of vapor movement in a thermally perturbed setting with evaporation processes, the code accounts for transport of water vapor in a simplified manner, by solving a diffusion problem with diffusivity dependent on pressure and temperature gradients (e.g., see Appendix C, Equations 3.9 through 3.13).

Table 5.2: Comparison of basic modeling approaches used for D_THC1

Team	Numerical simulator	Couplings considered	Hydraulic model	Geochemical Model	Transport
DOE	TOUGHREACT	THC Sequential noniterative	Single continuum; multiphase liquid and gas flow	Equilibrium mineral-water reactions, using HKF activity model	Advection/ diffusion of total concentrations (sequential)
BGR	GeoSys/Rockflow with PHREEQC	THC Sequential noniterative	Single continuum, unsaturated liquid flow, no gas flow; thermal vapor diffusion	PHREEQC	Advection/ diffusion of total concentrations (sequential)

Comparison of Model Results

Some preliminary comparisons of the BGR and DOE results for THC1 are presented in this section. Two cases were run by each group; one assuming the bentonite and granite are fully water-saturated and another with the bentonite partly saturated.

5.2.1.1 Temperature History

Temperatures at point V1 in the bentonite adjacent to the canister are shown for the DOE (TOUGHREACT-TR) and BGR (GeoSys/RockFlow-GSRF) simulations. Temperatures for the BGR model quickly rise to higher values than that for the DOE simulation, with a peak value of 92.1 using GSRF and 85.4 with TR. Because TOUGH-FLAC and GSRF simulations show comparable temperatures (Figure 4.1), and TR uses the same modules for solving heat and fluid flow as TOUGH-FLAC, it is likely that there are set-up or gridding issues that give rise to the temperature discrepancies. The differences will have to be reconciled prior to the start of Phase 2. These temperature differences, though, are unlikely to result in significantly different geochemical behavior, because the system is below boiling and the differences become a few degrees or less after about 20 years.

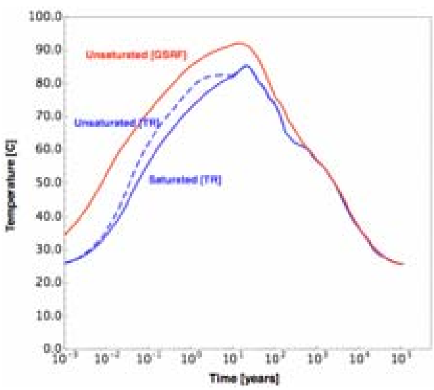


Figure 5.1: Temperature history at point V1 using TOUGHREACT (TR) and GeoSys/RockFlow (GSRF).

5.2.1.2 Drying/Rewetting History of Bentonite

The evolution of liquid saturation at point V1 using GSRF and TR is shown in Figure 5.2. The minimum liquid saturation is somewhat lower in the TR simulation, dries out later, and fully rewets much more rapidly. These differences are likely a result of slightly different capillary pressure-saturation relations (alternative formulations given in the task description), and the different treatments of vapor transport, since the temperatures are consistently higher in the GSRF simulation, and therefore it would be expected to result in a lower minimum liquid saturation.

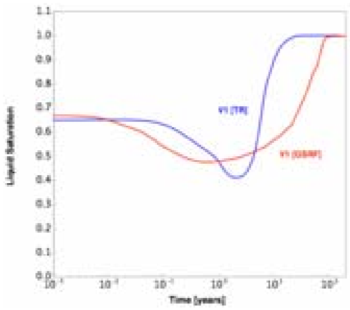


Figure 5.2: Saturation history at point V1 using TOUGHREACT (TR) and GeoSys/RockFlow (GSRF).

5.2.1.3 Water Chemistry Evolution

Aqueous species concentration changes in the unsaturated case are dominated by diffusion and the influx of seawater during the rewetting phase, and modified by mineral-water reactions. Chloride (Cl) is controlled solely by molecular diffusion and flow, and therefore these aspects of the model can be compared without added uncertainties from the thermodynamics of mineral-water-reactions. Figure 5.3 shows a comparison of Cl and Na concentrations after 100 years. The TOUGHREACT chloride profile (solid green line) shows slightly greater diffusive exchange with the granite, probably owing to a larger tortuosity and porosity used in the DOE simulation. A small peak in the Cl concentration in the granite below the drift in the BGR results is not seen in the DOE simulation results. Otherwise, the profiles are very close. The Na profiles are also very similar with slightly lower concentrations in the bentonite for the BGR simulation. This may be due to a slightly less dissolution of albite in the granite with diffusion into the bentonite.

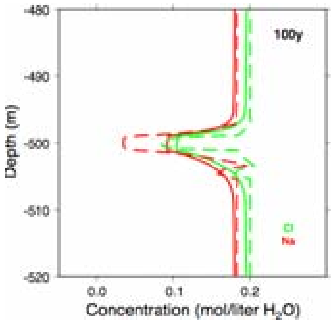


Figure 5.3: Na and Cl concentrations for the unsaturated case after 100 years. TOUGHREACT results are shown as solid lines, and GeoSys/RockFlow results as dashed lines.

5.2.1.4 Mineral Evolution

Changes in mineral abundances can be compared qualitatively in Figure 5.4. The main effects in the granite are albite dissolution and quartz precipitation in both GSRF and TR simulations. Once a factor of 10 is applied to the GSRF results for unit equivalency, the amount of albite dissolved is about three times that seen in the TR results. Precipitation of K-feldspar in the bentonite adjacent to the granite is also seen in both simulations. In addition both simulations show calcite precipitation adjacent to the canister; however it extends through the entire bentonite in GSRF results, but not in TR results. It appears that the models are giving similar results for the major phases, but further comparisons will be necessary to compare the differences more systematically.

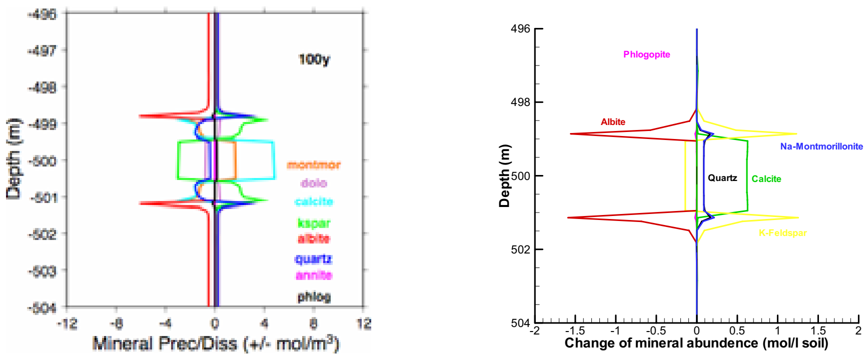


Figure 5.4: TOUGHREACT (left) and GeoSys/RockFlow (right) simulations of mineral abundances after 100 years for the unsaturated case. TR results show changes in moles per m^3 volume of rock, whereas GSRF results show moles per liter rock (0.1 m^3). A factor of 10 must therefore be applied to the GSRF results for direct comparison to TR results.

5.2.1.5 Summary

The preliminary comparisons of THC1 simulation results from DOE and BGR show similar profiles in aqueous species concentrations, given some minor inconsistencies in input parameters and temperature evolution. The mineralogical changes are similar in general, and future comparisons should look closely at the time evolution of each phase. Very strong changes over distances of a few cm at the contact of the bentonite with the granite indicate the necessity of highly resolved grids and small time steps to minimize numerical errors and oscillations in concentrations and mineral abundances. Yet, the cross diffusion of heat and mass can lead to zoning in mineral alteration that may be difficult to discern from numerical errors. Therefore, the comparison of results using different discretizations and numerical approaches will allow for better scrutiny of the results.

5.3. Future THC Workscope

Phase 1 (Model Inception Phase) activities will be ongoing during the next year of Task D research work. As pointed out before, the task description of D_THC1 may need some further revision or clarification in response to issues that came up in the initial simulations conducted for this task. We also expect that model simulations for D_THC1 will have to be adjusted in response to comparative evaluation between the research teams, as discrepancies may need to be resolved.

We also expect all research teams to shift their focus towards the modeling of Task D_THC2, which is the Yucca Mountain case. One of the major conceptual difficulties with this task is the internal heterogeneity of the fractured porous rock, with vastly differing permeabilities, moisture retention characteristics, and geochemical parameters in the fractures and the matrix, respectively. While dual continuum models are the best choice for D_THC2 (as discrete fracture-matrix continuum models or hybrid models are not feasible for the densely fractured formation), they require significant code development. Therefore, it is to be expected that some of the international research teams working on the Yucca Mountain case will *not* be using a dual continuum model. This raises the question of possible simplifications to the problem to avoid dual continuum modeling. In contrast to THM cases, however, a single continuum model of the fractured rock is not likely to produce reasonable geochemical results, because correct descriptions of liquid and gas chemistry require correct flux estimates of liquid and gas in fractures and matrix blocks. Even an effective continuum model (suggested for THM simulations) may not be sufficient. Thus one of the goals of future research within D_THC2 will be the joint development of simplified, yet realistic models for fracture-matrix representation.

6. Summary and Conclusions

In the international DECOVALEX-THMC project, DOE leads the modeling task entitled “Permanent Permeability/Porosity Changes in the EDZ and Near Field due to THC and THM Processes for Volcanic and Crystalline Rocks.” In its leadership role for this task (referred to as Task D), DOE has defined the research program and model scenarios, has coordinated and organized the cooperative research activities of international research teams engaged in Task D, and has conducted its own modeling work. Scientists at Lawrence Berkeley National Laboratory (LBNL) support DOE in organizational matters and conduct the respective modeling studies. The current report describes the activities conducted during the first year of the DECOVALEX-THMC project.

The research program developed for Task D of DECOVALEX-THMC involves both geomechanical and geochemical research areas. Coupled THM and THC modeling is conducted to evaluate long-term THM and THC processes in two generic geologic repositories for radioactive waste, with the ultimate goal of evaluating the impact of geomechanical and geochemical processes on hydrologic properties and flow patterns. The two repositories represent simplified versions of possible repository sites and emplacement conditions considered by the participating organizations. The first repository is located in saturated crystalline rock; emplacement tunnels are backfilled with a bentonite buffer material. The second repository is a simplified model of the Yucca Mountain site, featuring a deep unsaturated volcanic rock formation with emplacement in open gas-filled tunnels (Yucca Mountain type). DOE and LBNL produced a detailed report containing all necessary specifications for the geomechanical and geochemical modeling analyses of the two generic repositories (see Appendix A).

Four international research teams from China, Germany, Japan, and USA have started research activities for the geomechanical and geochemical scenarios of Task D. Work was performed in a collaborative manner with close interaction during meetings, visits, via email, and per telephone. This close collaboration among international top scientists and engineers is really one of the major benefits from DOE’s participation in DECOVALEX-THMC. Each team provided individual status reports on the progress of THM and THC modeling, included in Appendices C through I.

The research teams involved in modeling the geomechanical task have made significant progress during the first year of DECOVALEX-THMC. All teams finalized the model development work and presented results of the first modeling phase for both repository types. Comparison of these results indicates a good overall agreement between the research teams. Thus, DOE’s models, proven to be capable of simulating the Yucca Mountain repository, are equally valuable for the simulation of an alternative repository setting with different THM processes, at least for the problem considered in the first modeling phase.

Based on the good model agreement for the THM task, teams will move into the next, more complex modeling phase during the next project year. This second phase includes prediction of THM-related property changes with conceptual models chosen by the different research teams, sensitivity analysis with respect to THM property changes, application of alternative conceptual models for fractured rock (i.e., discrete, vs. continuum), and development of model data based on various reports and site data instead of using pre-defined values.

The two international research teams (Germany and Japan) participating in the geochemical tasks have mostly been working on code and model development during the last year. The BGR and DOE teams both conducted preliminary simulations for the first modeling phase of the FEBEX type repository task (D_THC1). Results from these simulations give great confidence in the transition to the more challenging Phase 2 and 3 analyses. Once the groups are satisfied with the magnitude and patterns of the geochemical changes, then the evaluation of changes to hydrological properties, i.e., porosity and permeability, will be a major goal of the simulations. In addition, more realistic treatment of bentonite-water reactions, including ion exchange, sorption, swelling and shrinkage, as well as kinetic rates of reaction, will be required.

D_THC1 was an ideal starting comparison for the groups because it allowed an excellent comparison of geochemical changes without the added effects of boiling and condensation, adding another layer of complexity and uncertainty. Now that the coupling of transport and water-rock reaction has been shown to give comparable results, then the transition to the Yucca Mountain type repository (D_THC2) can be made more smoothly in which alternate conceptual models of flow in unsaturated fractured rock must be evaluated (i.e., effective continuum, dual porosity, or dual permeability).

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