Geomechanical/Geochemical Modeling Studies Conducted Within the International DECOVALEX Project

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Abstract – The DECOVALEX project is an international cooperative project initiated by SKI, the Swedish Nuclear Power Inspectorate, with participation of about 10 international organizations. The general goal of this project is to encourage multidisciplinary interactive and cooperative research on modeling coupled thermo-hydro-mechanical-chemical (THMC) processes in geologic formations in support of the performance assessment for underground storage of radioactive waste. One of the research tasks, initiated in 2004 by the U.S. Department of Energy (DOE), addresses the long-term impact of geomechanical and geochemical processes on the flow conditions near waste emplacement tunnels. Within this task, four international research teams conduct predictive analysis of the coupled processes in two generic repositories, using multiple approaches and different computer codes. Below, we give an overview of the research task and report its current status.

I. INTRODUCTION

An international cooperative project entitled DECOVALEX (an acronym for DEvelopment of COupled models and their VALidation against EXperiments) was established in 1992 by a number of national regulatory authorities and waste management organizations involved in nuclear waste disposal, to cooperate in developing and testing models capable of simulating coupled processes. Three multi-year project stages have been completed in the past decade, mainly focusing on coupled thermo-hydro-mechanical (THM) processes [1, 2]. Currently, a fourth multi-year project stage of DECOVALEX is under way, referred to as DECOVALEX-THMC. The new project stage expands the traditional geomechanical scope of the previous DECOVALEX stages by incorporating thermo-hydro-chemical (THC) processes important for repository performance. In this paper, we report on DOE's Task D (one of five research tasks in DECOVALEX-THMC), which aims at evaluating the long-term impact of geomechanical and geochemical processes on hydrologic properties and flow conditions near waste emplacement tunnels (drifts).

Geomechanical and geochemical processes may lead to changes in hydrological properties that are important for repository performance because the flow processes in the vicinity of emplacement tunnels will be altered from their initial state. 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.

To better understand these processes and their impact on performance, the international research teams participating in Task D were asked to conduct predictive analysis of the long-term coupled processes in generic repositories with simplified conditions and geometry. Participating research teams model the THM and THC processes in the fractured rock close to a representative emplacement tunnel as a function of time, predict long-term changes in hydrological properties, and evaluate the impact on near-field flow processes. Two generic repositories situated in different host rock types and featuring different emplacement conditions are analyzed for comparison.

Four research teams from China, Germany, Japan, and USA have conducted research activities regarding the geomechanical and geochemical research areas in Task D. As shown in Table 1, the research teams use different codes with different model characteristics. Since all teams model the same task configuration, research results from the participating teams can be directly compared.

In the next sections, we briefly review the basic repository concepts studied in Task D and describe the coupled processes expected to occur. We then explain the research tasks to be conducted and summarize the modeling progress to date, approximately 18 months after initiating the work. We also describe further modeling work to be conducted till the end of the project in 2007. The paper is concluded with some general remarks.

II. BASIC REPOSITORY CONCEPTS

Two generic repository types of similar geometry are analyzed in Task D of DECOVALEX-THMC (Figure 1). Both feature a multibarrier approach relying on an engineered barrier (e.g., waste, canister, buffer, and excavation) and a natural barrier (rock mass). Repository Type A is a simplified model of the Yucca Mountain site, a deep unsaturated volcanic rock formation with emplacement in open gas-filled drifts. In this case, the open drifts provide a natural capillary barrier that can limit liquid water entry from the densely fractured formation. Repository Type B is located in saturated crystalline rock; emplacement drifts are backfilled with a low-permeability buffer material such as bentonite (a concept considered in many European countries and in Japan). Since the sparsely fractured 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. There is also a difference in the amount of heat and temperature rise. Type A considers a heat load that will result in above-boiling temperatures within the tunnels and in the near field rock. In bentonite-backfilled repositories (such as Type B), the temperature is generally kept below 100°C to prevent chemical alterations of the bentonite material.

Research teams were encouraged to model both repository types to develop a broader understanding of the complex THMC behavior—and the related modeling challenges—in different emplacement conditions and host rock types.

Table 1: Research teams and simulators applied within DOE's DECOVALEX task

Research Team	Simulator	Coupling	Mechanical/Chemical Model	Hydraulic and Transport Model
DOE/LBNL	TOUGH-FLAC	THM	Elastic, Elastoplastic, Viscoplastic	Discrete, single or dual continuum; multiphase liquid and gas flow
DOE/LBNL	ROCMAS	THM	Elastic, Elastoplastic, Viscoplastic	Discrete or single continuum; unsaturated liquid flow; thermal vapor diffusion
BGR/Center for Applied Geosciences (Germany)	Geosys/Rockflow	THM	Elastic, Elastoplastic, Viscoplastic	Discrete or single continuum; unsaturated liquid flow; thermal vapor diffusion
CAS, Chinese Academy of Sciences	FRT-THM	THM	Elastic, Elastoplastic, Viscoplastic	Discrete or single continuum; unsaturated liquid flow; thermal vapor diffusion
JAEA, Japan Atomic Energy Agency	THAMES	THM	Elastic, Elastoplastic, Viscoplastic	Discrete or single continuum; unsaturated liquid flow; thermal vapor diffusion
DOE/LBNL	TOUGHREACT	THC	Equilibrium and kinetic mineral-water-gas reactions, HKF activity model	Discrete, single or dual continuum; multiphase liquid and gas flow; advection/ diffusion of total concentrations (sequential)
BGR/Center for Applied Geosciences (Germany)	Geosys/Rockflow with PHREEQC	THC	PHREEQC	Discrete or single continuum; unsaturated liquid flow; thermal vapor diffusion; advection/ diffusion of total concentrations (sequential)
JAEA, Japan Atomic Energy Agency	THAMES with Dtransu-3D-EL and PHREEQC	THMC	PHREEQC	Discrete or single continuum; unsaturated liquid flow; thermal vapor diffusion; advection/ diffusion of total concentrations (sequential)

III. DISCUSSION OF RELEVANT THM PROCESSES

Significant geomechanical alterations are expected to occur in response to the heat output of the decaying radioactive waste. The strongest effects coincide with the period of the highest temperatures; i.e., depending on the repository type, during the first decades or centuries after emplacement. For example, in Type A, 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 a few thousand years. In Type B, 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.

At the same time, thermally induced stresses act upon pre-existing fractures, which open or close depending on the local stress. One of the most 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. Inelastic mechanical responses, such as fracture shear slip, crushing of fracture asperities, microcracking, and subcritical crack growth, may change the fracture porosity and permeability in the near-field fractured rock.

IV. DISCUSSION OF RELEVANT THC PROCESSES

Increased temperature near emplacement tunnels results in mineral-water disequilibrium and increases the reaction rates of minerals with water, leading to enhanced mineral dissolution/precipitation with possibly permanent effects on hydrological properties. The impact of mineral precipitation on fracture porosity and permeability is particularly strong when temperatures are above boiling (Type A) because of a strong vaporization, condensation, and reflux cycle occurring near the drifts. In addition, changes in water and gas chemistry may affect the waste package environment and 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.

V. RESEARCH PROGRAM FOR TASK D

The research program developed for Task D of DECOVALEX-THMC involves separate geomechanical and geochemical sub-tasks that may be integrated at a later stage (in case THM and THC results suggest the need for a fully coupled THMC simulation). The geomechanical task builds on the substantial knowledge gained from a multiple team effort in modeling *in situ* heater experiments in a previous DECOVALEX project [2]. These experiments are the Drift Scale Test at Yucca Mountain (a setting similar to Repository Type A) and the FEBEX experiment at Grimsel in Switzerland (a setting similar to Type B). The previous DECOVALEX project also included a limited geochemical modeling work for the Drift Scale Test, with participation limited to two research teams [3]. Modeling of these short-term experiments (occurring over a few years) lead to an improved understanding of geomechanical and geochemical processes, which is now applied to the evaluation of long-term THM and THC conditions in generic repositories (with the compliance periods spanning thousands of years or more).

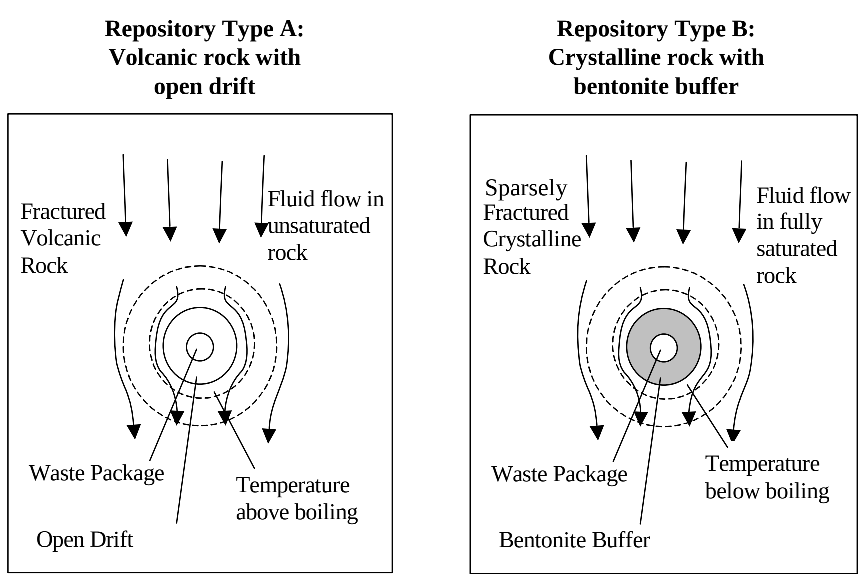


Fig. 1. Schematic showing the two repository scenarios (vertical cross sections perpendicular to drift axis)

The description for the THM and THC sub-tasks was designed such that the expected physical processes in the future repositories are incorporated in a realistic manner, yet allow for simplified modeling as the geometries and boundary conditions have been idealized (see Figure 1). Both repository types analyze 2-D vertical cross sections perpendicular to the axis of a representative emplacement drift. With the repository comprised of many parallel drifts (similar to the Yucca Mountain design), symmetry considerations allow limiting the model to one drift, with the lateral boundaries at the centerlines between 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 prescribed hydraulic head gradients (saturated flow) or by gravity (unsaturated flow).

Various sources of information were given to the research teams as a basis for developing rock property sets and *in situ* conditions. Data for Repository Type A are 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. Rock properties for Repository Type B are largely based on data from the Grimsel Test Site (GTS) and the FEBEX *in situ* experiment. In a few instances, data gathered in the Japanese and Swedish programs are used to complement the GTS/FEBEX data set. The crystalline host rock in Repository Type B is sparsely fractured, which would suggest that the fractures might be modeled using discrete approaches, if necessary. The THM and THC sub-tasks use the same repository geometries and identical thermo-hydro (TH) rock properties. See [4] for details.

V.A. THM Research Topics and Phases

Research teams participating in this THM task are asked to conduct predictive analysis of the long-term coupled THM processes for the two repository types. The main processes considered are heat and fluid flow, stress, deformation, and geomechanical alterations in hydrologic properties (e.g., porosity and permeability). Research topics of interest are:

- Comparative analysis of THM effects in different host rock types and repository designs
- Relative importance of thermal-mechanical changes to near-field hydrological properties and flow fields
- Evaluation of stress-permeability and stress-porosity relationships
- Assessment of uncertainties resulting from uncertain parameters, different conceptual models, and parameter heterogeneity

The simulation work is being conducted in three modeling phases that address 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 are defined as follows:

Phase 1. Model Inception

Phase 2. Preliminary Prediction and Sensitivity Study

Phase 3. Final Model Prediction with Uncertainty Range

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 explicitly provided. Thus, in this phase no data or model uncertainties are considered, and changes in hydrological properties are neglected. In Phase 2, the research teams are to develop their model and input material properties from available site data with the goal of predicting geomechanical changes in hydrological properties and their impact on flow patterns. In Phase 3, the research teams are asked to make final predictions, along with an evaluation of the related uncertainties. The teams are encouraged to use whatever modeling concepts they feel are appropriate for the task. For example, the fractured rock mass may be modeled with a continuum model using homogenous properties, a heterogeneous stochastic continuum model, or a discrete fracture model. Furthermore, different constitutive models may be used linking the mechanical conditions in fractures to changes in hydrological properties.

V.B. THC Research Topics and Phases

In this task, research teams conduct geochemical modeling analyses of the long-term coupled THC processes in the two generic repositories introduced above. 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. Research topics of interest are:

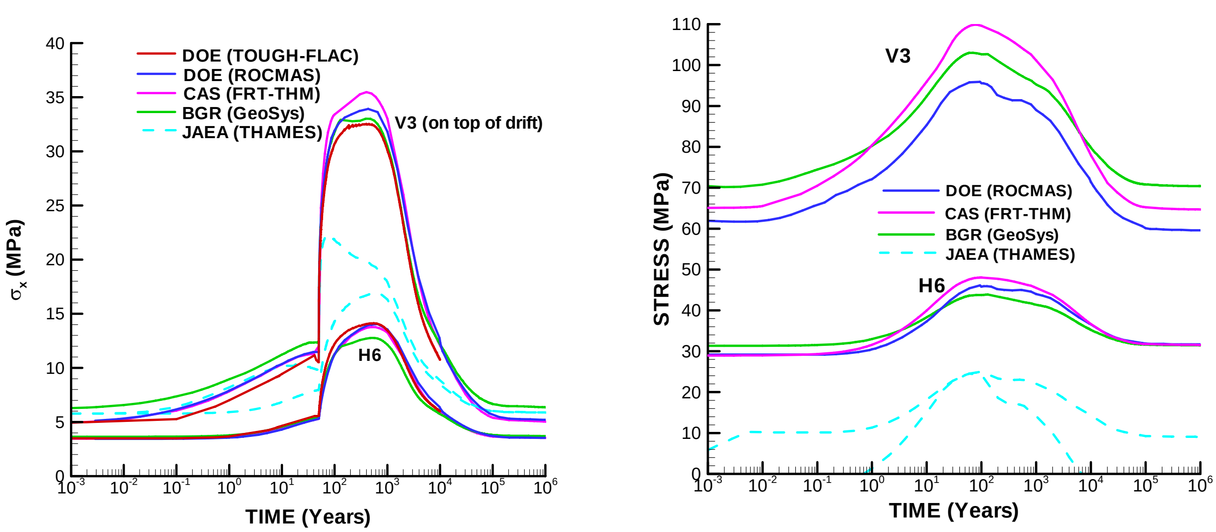
- Comparative analysis of THC effects in different host rock types and repository designs
- Relative importance of thermal-chemical changes on the near-field hydrological properties and flow field
- Mineral precipitation/dissolution in the near-field and in bentonite
- Evaluation of the relation between mineral alteration and hydrological properties
- Assessment of uncertainties

Similar to the THM task, THC modeling work is conducted in three phases, with increasing levels of complexity. In the Model Inception Phase (Phase 1), research teams are provided with all the geochemical properties for a limited set of mineral, aqueous, and gaseous species. The simulations focus on the evolution of temperature, gas and water composition, and mineral precipitation/dissolution (in fractures, matrix, and the bentonite) for a simplified geochemical system. In the next phase, a more complete geochemical system is considered, and parameter sets are to be derived using the available site data and various developed data. Also, the research teams focus on predicting permanent changes caused by mineral alteration. In Phase 3, the research teams are asked to make their final prediction, including estimation of the resulting uncertainties. Uncertainties are related to properties (e.g., thermodynamic and kinetic data, reactive surface areas) or model concepts (fracture representation, mineral representations, mineral textures, equilibrium vs. kinetic reactions, small-scale distributions of mineral precipitates, etc.).

VI. THM MODELING STATUS AND RESULTS HIGHLIGHTS

As listed in Table 1, four international research teams using five different simulators participate in the THM work for Task D. Currently, these teams have finalized the necessary model development and have provided results for the first modeling phase (i.e., assuming simplified geomechanical processes). In Phase 1, simple elastic models were used for simulation of the rock-mechanical behavior, consistent with the task definition. (However, all models are generally capable of simulating elasto-plastic behavior, which becomes necessary when stress-induced changes in hydrologic properties are to be considered in the next project phase.) With much more detail given in [4] and [5], we show example results (horizontal stresses) in Figure 2 for both repository types. All models predict a substantial stress increase with the increasing temperatures in the rock mass. Later, as the radioactive waste decays, its heat output decreases, and the heat- induced stresses return to pre-emplacement conditions in a very slow process. Generally good agreement is seen between all models except for one, which assumed different initial conditions because the task description was misinterpreted. The necessary revisions have been identified and will be conducted before starting research work on Phase 2.

Thermal-hydrological results such as fluid pressure, saturation, and vertical flux were also compared [4,5]. For Repository Type B, the five models were in reasonable agreement, despite the fact that different approaches were used to describe swelling pressure in the bentonite and that only one code solves for complex multiphase flow behavior of liquids and gases (TOUGH-FLAC). All teams used a single continuum representation of the crystalline rock mass in Repository Type B, which may change in later project phases, when the effect of sparsely distributed fractures is to be considered in a more rigorous manner. The comparison of hydrological model results was less good in case of Repository Type A, where the heat-induced flow perturbations are affected by a complex



(a) Repository Type A

(b) Repository Type B

Fig. 2. Evolution of horizontal stress in the rock mass just above the drift (V3) and laterally away from the drift at the mid-distance between two adjacent drifts (H6). Acronyms DOE, CAS, BGR and JAEA are explained in Table 1.

interaction between the abundant fractures and the rock matrix. Models that account for this interaction (such as a dual continuum model) capture such behavior adequately. However, only TOUGH-FLAC is currently capable of representing the fractured rock mass as a dual continuum; all other models approximate the fractured rock mass as a single continuum.

The next step for all teams is to move forward into the next THM modeling phase. As summarized earlier, Phase 2 involves the prediction of thermal-mechanical changes in hydrological properties including sensitivity analysis, the potential use of alternative conceptual models for flow in fractured rock (i.e., discrete vs. continuum), and the development of model data based on various reports and site data (instead of using pre-defined property values as in Phase 1). With respect to Repository Type A, some research teams will need to develop more rigorous models for fracture-matrix interaction (such as dual continuum models) in order evaluate THM related changes in near-field flow fields.

VII. THC MODELING STATUS AND RESULTS HIGHLIGHTS

Three research teams are involved in the geochemical modeling task, the BGR team from Germany, the JAEA team from Japan, and the DOE/LBNL team from the U.S. (Table 1). The teams from JAEA and BGR were mostly working on code and model development during the first year of the project. A fully coupled THMC code developed by JAEA is currently in its testing stage and has not yet been applied to the DECOVALEX test cases. BGR finalized the code development work on Geosys/ Rockflow with PHREEQC and conducted Phase 1 simulations regarding Repository Type B. These were compared with Phase 1 simulations performed by DOE/LBNL using the well-established TOUGHREACT code [6]. No results are available for Repository Type A yet. A detailed description of the respective simulation models as well as a comparative evaluation of results is provided in [4].

The thermal-hydrological part of TOUGHREACT is similar to TOUGH-FLAC. The code solves for complex multiphase flow behavior and allows for dual-continuum modeling, if necessary. In contrast, Geosys/Rockflow is a single continuum code that simulates variably saturated flow according to Richard's equation (assuming constant gas pressure). Vapor transport is treated in a simplified manner, by solving a diffusion problem with diffusivity dependent on pressure and temperature gradients. Despite these differences, the five models were in reasonable agreement regarding the thermal-hydrological processes in Repository Type B (TH results are not shown in this paper). There are model differences in the treatment of geochemical model as well, primarily related to the different thermodynamic databases used in the model simulations. For the first phase, only equilibrium reactions were considered in both models. Transport properties were also different, as discussed below, which likely accounts for the different magnitudes of the dissolved and precipitated phases.

Let as now compare the geochemical processes and selected model results for Repository Type B. Aqueous species concentration changes are dominated by diffusion and the influx of seawater during the rewetting phase (after peak temperatures have been reached and the system cools off slowly), somewhat 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 3 shows a comparison of Cl and Na concentrations 100 years after emplacement of waste. The chloride profile modeled by TOUGHREACT(solid green line) shows slightly greater diffusive exchange with the granite, owing to a larger tortuosity and porosity used in the DOE/LBNL study. 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 similar with slightly lower concentrations in the bentonite for the BGR simulation. These may be due to a slightly less dissolution of albite in the granite with diffusion into the bentonite.

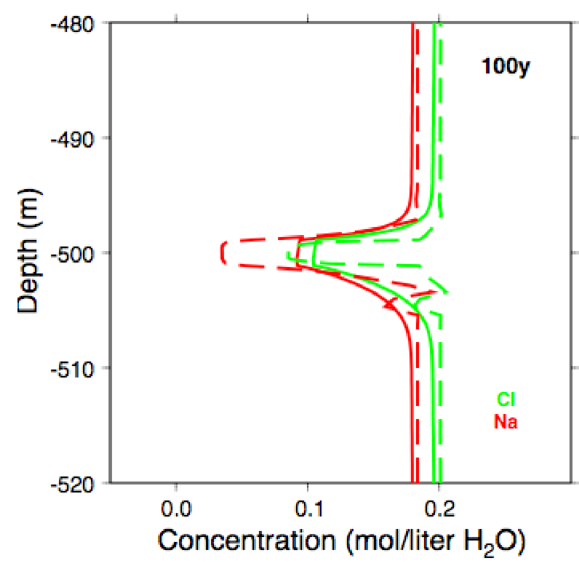


Fig. 3. Na and Cl concentrations along a vertical profile after 100 years for Repository Type B. TOUGHREACT results are shown as solid lines, and GeoSys/RockFlow results as dashed lines.

It appears that the models show good quantitative agreement regarding aqueous species concentrations, given some minor inconsistencies in input parameters and temperature evolution. While not presented in this paper, mineral alteration predictions have been in reasonable qualitative agreement between the two models. However, further comparison will be necessary to work out quantitative differences in the dissolution and precipitation patterns.

As the next step in the THC sub-task, research teams are expected to shift their focus towards the modeling of Repository Type A, the Yucca Mountain case. As pointed out before, one of the major conceptual difficulties with this task is the internal heterogeneity of the fractured porous rock, which significantly affects the geochemical behavior in the formation. Whereas the geomechanical processes can be reasonably well approximated with a single continuum model (as shown above), this is not the case with geochemical processes: a correct description of liquid and gas chemistry as well as mineral alteration requires a good representation of flow in the fractures and the rock matrix. Thus, one of the first steps of future research will be the joint development of simplified, yet realistic models for fracture-matrix representation, and implementation thereof into the BGR and JAEA codes.

VIII. SUMMARY AND DISCUSSION

This paper describes the ongoing research activities conducted in Task D of the international cooperative DECOVALEX-THMC program. The task aims at understanding and predicting the long-term impact of geomechanical and geochemical processes on hydrologic properties and flow fields near waste emplacement drifts. Four research teams from China, Germany, Japan, and USA participate.

Since the initiation of the program in 2004, good progress has been made in both geomechanical and geochemical research areas. All four teams working on THM processes presented results of the first modeling phase (assuming simplified geomechanical processes). Comparison of these results indicates a good overall agreement. The research teams participating in the geochemical tasks have mostly been working on code and model development. Preliminary simulation results show reasonable agreement for a simplified geochemical system. The work conducted so far provides the basis for adding another layer of model complexity in the next project phase, e.g., evaluating the changes in hydrological processes due to THM and THC changes, developing alternative model approaches, and estimating conceptual as well as data uncertainties.

True to the mission of the DECOVALEX project, the research work in Task D was performed in a collaborative manner with close interaction between the international research teams. This close collaboration is one of the major benefits of such international programs, because it (a) develops new insights in the understanding of geomechanical and geochemical processes in geologic systems and (b) provides valuable peer-review of the international modeling work conducted with respect to disposal of radioactive waste.

One important point in designing the Task D work scope was to evaluate two alternative repository settings, one a simplified model of the Yucca Mountain site, the other representative of the emplacement concepts considered in many European countries and Japan. Since participants were encouraged to model both scenarios (featuring many similarities, but also important differences), research teams developed a broader understanding and thus higher confidence in modeling of the complex THMC behavior near radioactive waste repositories. It was also demonstrated that the coupled processes codes TOUGH-FLAC and TOUGHREACT, proven to be capable of simulating the Yucca Mountain repository, are equally capable of simulating an alternative repository setting, thus adding confidence to their predictive capability.

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