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Geomechanical/Geochemical Modeling Studies Conducted Within the International DECOVALEX Project

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INTRODUCTION

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 THMC processes in geologic formations in support of the performance assessment for underground storage of radioactive waste. THMC stands for **T**hermal, **H**ydrological, **M**echanical, and **C**hemical processes. Within the DECOVALEX project, DOE leads a modeling task on evaluating the impact of geomechanical and geochemical processes on the flow conditions near waste emplacement tunnels. The task is entitled “Long-term Permeability and Porosity Changes in the EDZ and Near Field due to THC and THM Processes for Volcanic and Crystalline-Bentonite Systems.” DOE coordinates and sets the direction for the cooperative research activities of four international research teams. Scientists at Lawrence Berkeley National Laboratory (LBNL) support DOE’s activities, as well as participate in the cooperative research effort. Below, we describe the modeling task defined by DOE, report the current status of the modeling work, and discuss the overall benefit of participating in the DECOVALEX project.

WORK DESCRIPTION

The DECOVALEX research program developed by DOE includes both geomechanical and geochemical research areas. 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.

The international research teams participating in DOE’s research task are 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. One repository is a simplified model of the Yucca Mountain site, 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 (Figure 1). A detailed task description with all necessary specifications for modeling work is given in Barr et al. (2005). Since all research teams model the same task configuration, research results from the participating teams can be compared.

RESULTS

Four international research teams from China, Germany, Japan, and USA participate in DOE's modeling task. As shown in Table 1, these teams are using different simulators with vastly different model characteristics. Since the initiation of the program in summer 2004, significant progress has been made in both geomechanical and geochemical research areas. 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 (see example for comparative evaluation in Figure 2). 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. A detailed description of simulation models and results as well as a comparative evaluation is given in a companion paper.

The good agreement between model results of different teams (that use different simulators) is valuable supporting evidence for the validity of DOE's predictive models simulating THM and THC processes. The work conducted so far provides a good 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.

CONCLUSIONS AND DISCUSSION

The first project year has demonstrated the merit of DOE's participation in the international DECOVALEX project. Research work was performed in a collaborative manner with close interaction between the international research teams. This close collaboration among top scientists and engineers is one of the major benefits of such international programs. First, discussion with top scientists helps to further the program's 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 DOE's modeling analyses in this field.

Pending future project phases, we have seen good agreement between model results from several international teams using very different computer codes. The value of analyzing two different repository sites is twofold: The first repository is a simplified representation of the geologic repository at Yucca Mountain, so that teams conducting model work for this site provide direct support for the DOE program. The second repository setting is representative of the possible emplacement conditions considered in many European countries and Japan. The geomechanical and geochemical processes expected in such a setting are different from those at Yucca Mountain. It was shown that DOE's models, 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.

REFERENCES

Barr D., Birkholzer J., Rutqvist J., Sonnenthal E., 2005. Draft Description for DECOVALEX-THMC Task D: Long-Term Permeability/Porosity Changes in EDZ and Near Field, due to THM and THC Processes in Volcanic and Crystalline-Bentonite Systems. Lawrence Berkeley National Laboratory Report, 2005.

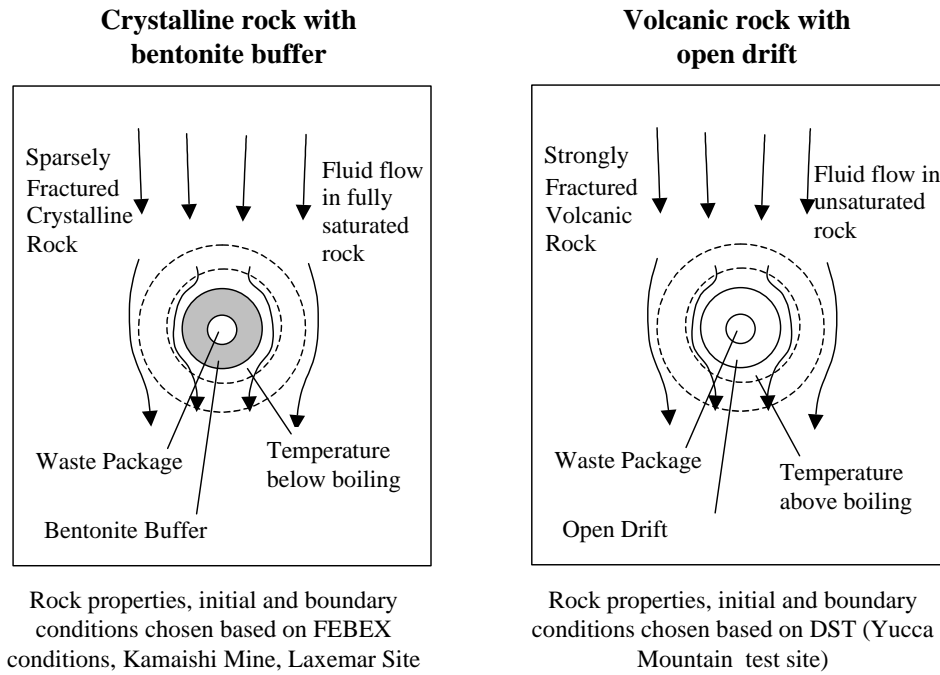


Figure 1. Schematic showing the two repository scenarios developed by DOE (vertical cross sections perpendicular to drift axis)

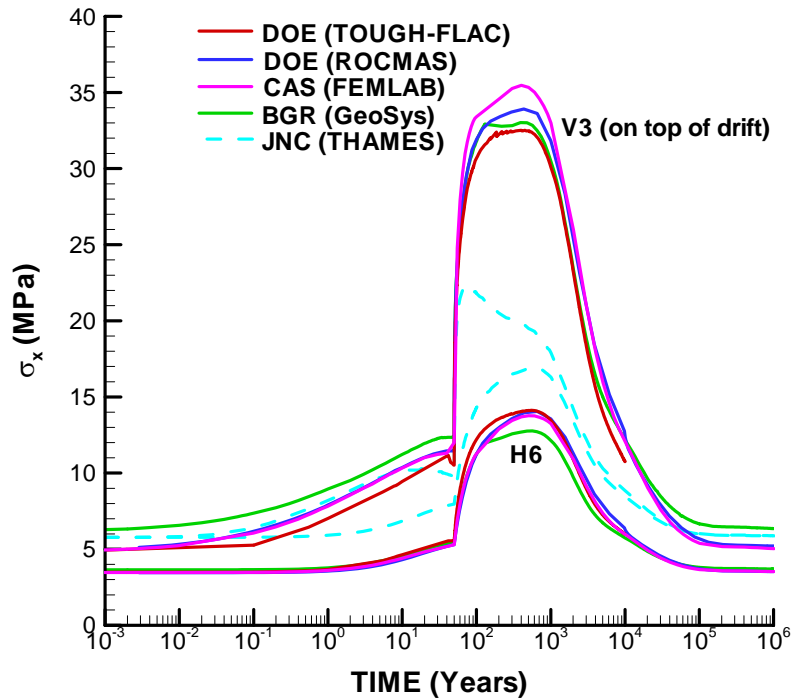


Figure 2. Evolution of horizontal stress at two representative locations using five different numerical models (for Yucca Mountain scenario). Discrepancies seen in the JNC-results are caused by differences in the initial stress field used for the simulation.

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

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 (Germany)	Elastic Elastoplastic Viscoplastic	Single continuum; unsaturated liquid flow; thermal vapor diffusion
FEMLAB	THM	CAS Chinese Academy of Sciences	Elastic Elastoplastic Viscoplastic	Single continuum; unsaturated liquid flow; thermal vapor diffusion
THAMES	THM	JNC Japan Nuclear Cycle Development Institute	Elastic Elastoplastic Viscoplastic	Single continuum; unsaturated liquid flow; thermal vapor diffusion
TOUGHREACT	THC	DOE/LBNL	Equilibrium and kinetic mineral- water-gas 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 (Germany)	PHREEQC	Single continuum; unsaturated liquid flow; thermal vapor diffusion; advection/ diffusion of total concentrations (sequential)
COUPLYS with THAMES, Dtransu-3D-EL and PHREEQC	THMC	JNC Japan Nuclear Cycle Development Institute	PHREEQC	Single continuum; unsaturated liquid flow; thermal vapor diffusion; advection/ diffusion of total concentrations (sequential)