

# Lawrence Berkeley National Laboratory

Lawrence Berkeley National Laboratory

## Title

Comparative simulation study of coupled THM processes near back-filled and open-drift nuclear waste repositories in Task D of the International DECOVALEX Project

## Permalink

<https://escholarship.org/uc/item/9d65k7hm>

## Authors

Rutqvist, J.  
Birkholzer, J.T.  
Chijimatsu, M.  
et al.

## Publication Date

2006-05-10

# COMPARATIVE SIMULATION STUDY OF COUPLED THM PROCESSES NEAR BACK-FILLED AND OPEN-DRIFT NUCLEAR WASTE REPOSITORIES IN TASK D OF THE INTERNATIONAL DECOVALEX PROJECT

J. Rutqvist<sup>1</sup>, J.T. Birkholzer<sup>1</sup>, J.T., M. Chijimatsu<sup>2</sup>, O. Kolditz<sup>3</sup>, Quan-Sheng Liu<sup>4</sup>, Y. Oda<sup>5</sup>, Wenqing Wang<sup>3</sup>, and Cheng-Yuan Zhang<sup>4</sup>

<sup>1</sup>) Lawrence Berkeley National Laboratory, Berkeley, USA

<sup>2</sup>) Hazama Cooperation, Tokyo, Japan

<sup>3</sup>) University of Tübingen, Tübingen, Germany

<sup>4</sup>) Chinese Academy of Sciences, Wuhan, China

<sup>5</sup>) Japan Atomic Energy Agency, Tokai, Japan

**Abstract:** As part of the ongoing international DECOVALEX project, four research teams used five different models to simulate coupled thermal, hydrological, and mechanical (THM) processes near underground waste emplacement drifts. The simulations were conducted for two generic repository types, one with open and the other with back-filled repository drifts, under higher and lower post-closure temperature, respectively. In the completed first model inception phase of the project, a good agreement was achieved between the research teams in calculating THM responses for both repository types, although some disagreement in hydrological responses are currently being resolved. Good agreement in the basic thermal-mechanical responses was also achieved for both repository types, even though some teams used relatively simplified thermal-elastic heat-conduction models that neglect complex near-field thermal-hydrological processes. The good agreement between the complex and simplified process models indicates that the basic thermal-mechanical responses can be predicted with a relatively high confidence level.

## 1. INTRODUCTION

This paper presents results from an international multiple-team simulation study on thermal, hydrological and mechanical (THM) interactions around underground waste emplacement drifts. The study is part of the international DECOVALEX-THMC project, denoted Task D\_THM (Birkholzer et al., 2006). Two generic repository types with horizontal emplacement tunnels are considered. The first type is a low temperature (below boiling) repository in a deep saturated crystalline rock formation with emplacement in back-filled tunnels, a concept considered in many European countries and Japan. The second type is a high temperature (above boiling) repository in a deep unsaturated volcanic rock formation with emplacement in open gas-filled tunnels, a concept considered by the United States.

The initial material properties for the two repository types are derived from measurements and previous DECOVALEX analyses of two major in situ experiments—the FEBEX In Situ Test (Alonso et al., 2005) and the Yucca Mountain Drift Scale Test (Rutqvist et al., 2005)—representing data and processes occurring at the two repository types.

Four international teams, from China, Germany, Japan, and USA are participating in this task. Altogether, five different numerical simulators for

coupled THM analysis are applied (Table 1). Among the five simulators, two main approaches can be distinguished. Three simulators—ROCMAS, THAMES, and FRT-THM—are based on single-phase fluid flow approach, whereas two simulators—TOUGH-FLAC and Geosys/Rockflow—include two-phase fluid flow (liquid and gas) approach. Several of these simulators have been applied in previous DECOVALEX projects for simulation of coupled processes in either one or the other of the two repository types.

In this study, the research teams conduct predictive analysis of the long-term coupled THM processes for the two repository types. The simulations are conducted on two-dimensional drift-scale models containing one horizontal emplacement tunnel, which for each repository type has different dimensions and thermal load (Figure 1). The simulations are conducted in three phases: (1) model inception, (2) preliminary model prediction and sensitivity analysis, and (3) final model prediction with uncertainty range.

This paper presents the results from model inception phase, in which all the properties are explicitly provided (Table 2) and changes in hydrological properties are neglected.

TABLE 1. Research teams and simulators applied in this study

Research Team	Numerical Simulator (Reference)
DOE U.S. Department of Energy's Research Team: Lawrence Berkeley National Laboratory (LBNL)	TOUGH-FLAC
	ROCMAS
BGR Bundesanstalt für Geowissenschaften und Rohstoffe's Research Team: University of Tübingen	GeoSys/ Rockflow
CAS Chinese Academy of Sciences' Research Team	FRT-THM
JAEA Japan Atomic Energy Agency's Research Team, including Hazama Cooperation	THAMES

TABLE 2. Some basic rock properties defined for Phase 1 (Model Inception).

Parameter	Type A (Tuff) <sup>1)</sup>	Type B (Granite)
Bulk Density, [kg/m <sup>3</sup> ]	2370	2700
Matrix Porosity [-]	0.13	0.01
Young's Modulus, [GPa]	15	35
Poissons ratio, [-]	0.21	0.3
Specific heat, [J/kg·°C]	985	900
Thermal cond., [W/m·°C]	2.29	3.0
Thermal exp. coeff., [°C <sup>-1</sup> ]	1.0×10 <sup>-5</sup>	1·10 <sup>-5</sup>
Bulk Permeability, [m <sup>2</sup> ]	3.3×10 <sup>-13</sup>	1×10 <sup>-17</sup>

<sup>1)</sup> The complete data set for welded tuff includes multiphase (e.g., retention and relative permeability data for gas and liquid) fluid flow properties for matrix and fracture continua.

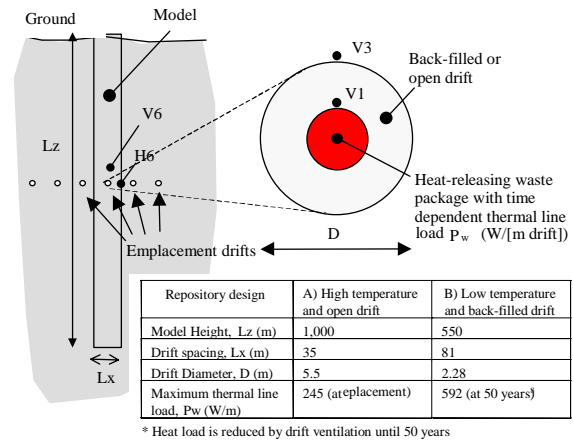


Figure 1. Schematic of main thermal-mechanical responses common for both Repository Type A and B.

## 2. THM SIMULATION RESULTS

### 2.1 Thermal-Mechanical Results

Figure 2 schematically illustrates the simulation results of coupled thermal-mechanical responses, which are induced by regional temperature changes (Figure 2a). A substantial increase in thermal stress in the horizontal direction occurs as a result of lateral confinement of the rock mass, whereas vertical stress is much less affected as the free moving ground surface allows for vertical expansion. The regional thermal stressing is amplified at the drift wall by stress redistribution causing highly compressive stress at the top and bottom of the drift and strong stress relief at the right and left side (Figure 2b).

Figure 3 shows comparisons of temperature and stress-evolution for the five different models. The figure shows a generally good agreement for temperature and stress evolution, especially in the case of Repository Type A (Figure 3a). The more significant deviations in temperature evolution for Point V1 for Repository Type B (Figure 3b) can be explained by differences in the evolution of saturation-dependent thermal conductivity in the backfill. The disagreement in thermal stress by JAEA from the simulations of other teams in Figure 3d, is a result of a misconception of the initial stress and excavation modeling.

The main difference between thermal-mechanical responses in Repository Type A and B, is related to the evolution of the heat-power and the thermal stress magnitude in comparison with the initial stress field. In Type A, the thermally induced

stresses are a little lower, but at the same time the initial stresses in that case are much smaller. Furthermore, in Type A, the thermal stresses cause the principal in situ stress field to rotate, from the initial maximum principal stress being vertical to becoming horizontal at the time of peak thermal stress. In Type B, on the other hand, the in situ stresses are initially already relatively high, with a horizontal maximum principal stress. In this case, the thermal stressing provides an additional increase in the horizontal stress, without a rotation of the principal stress field.

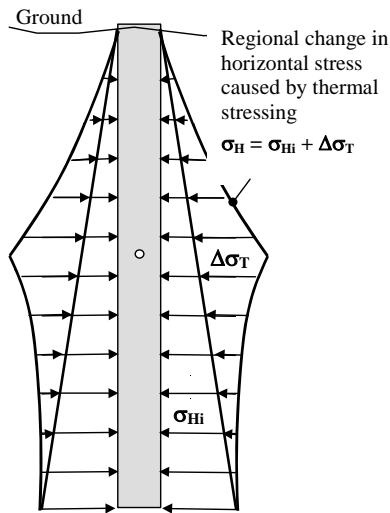
## 2.2 Thermal-Hydrological Results

Complex thermal-hydrological interactions occur in the near-field for both Repository Type A and B.

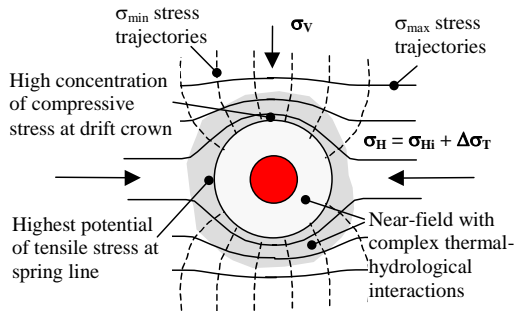
In the case of Repository Type A, high temperatures cause boiling and complex heat-pipe effects, which result in drying of the rock near the drift wall. A dryout zone is created, which extends as much as a few meters from the drift wall into the surrounding rock mass. The simulation results indicate that such a dryout zone would exist as long as the rock temperature near the drift exceeds the boiling points, between 50 and about 1,000 years.

In the case of Repository Type B, thermal-hydrological interactions are most prominent within the bentonite buffer. The bentonite buffer is installed and conditioned to an initial saturation of about 65%. During the early few years of heating, a relatively steep thermal gradient causes evaporation of liquid water near the waste canister, with migration of vapor along the thermal gradient towards cooler regions of the buffer, where it condenses as liquid water. However, this initial drying is later overcome by seepage of liquid water from the fully saturated drift wall into the partially saturated buffer, and the buffer becomes fully saturated in about 10 to 50 years.

Figure 4 shows a comparison of the evolution of liquid saturation at two selected monitoring points, Point V3 10 cm into the drift wall in Repository Type A and Point V1 at the canister-buffer interface in Repository Type B (see Figure 1 for locations of V1 and V3). Whereas the agreement between different models for Repository Type B is quite satisfactory, the results for Repository Type A are more complex. This is because the comparison for Repository Type A is complicated by the fact that the results of single continuum models (BGR, JAEA, CAS) are compared to that of a more rigorous dual-continuum model (DOE, TOUGH-FLAC). In general, Figure 3a shows that the total dryout time till rewetting is similar, while the time evolution of saturation is somewhat different. Better agreement is expected in future project phases, when more rigorous models (not just single continuum) will be used by all teams to simulate flow in fractures and matrix.

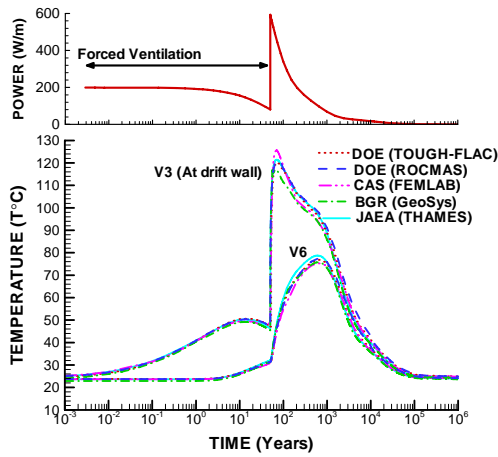


(a) Regional Changes in Horizontal Stress

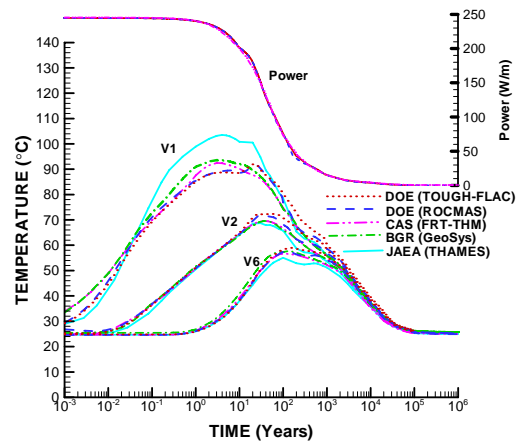


(b) Near-field stresses as a result of regional stress changes

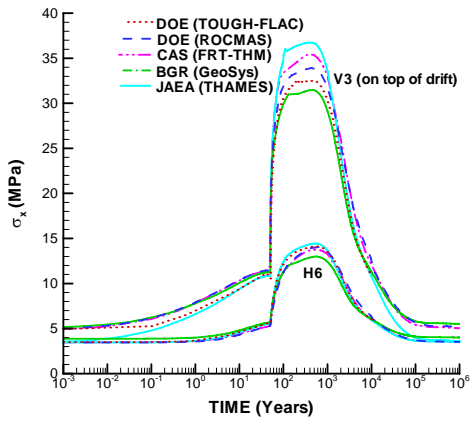
Figure 2. Schematic of main thermal-mechanical responses common for both Repository Type A and B.



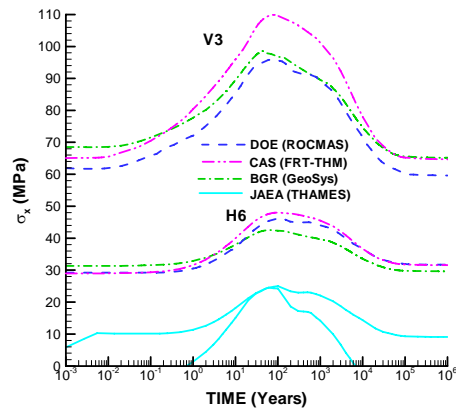
(a) Power and temperature for Repository Type A



(b) Power and temperature for Repository Type B

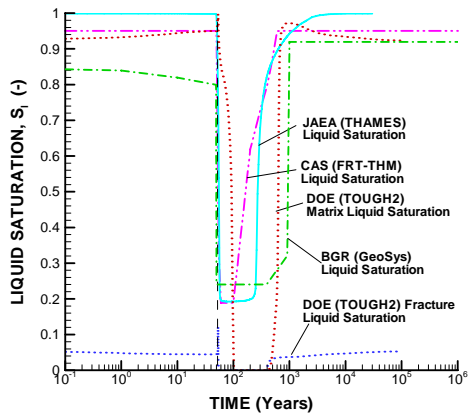


(c) Horizontal stress for Repository Type A

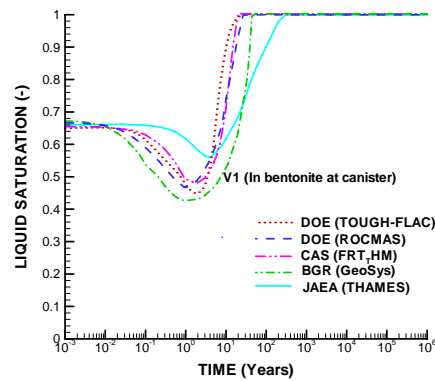


(d) Horizontal stress for Repository Type B

Figure 3. Evolution of thermal-mechanical responses. Approximate locations of Points V1, V3, V6, and H6 are shown in Figure 1.



(a) Repository Type A



(b) Repository Type B

Figure 4. Evolution of liquid saturation..

### 3. EVALUATION OF MODEL APPROACHES

Results of this study show that a reasonable good agreement was achieved in calculating THM responses for both repository types by various model approaches, thus demonstrating how different models and approaches can be adapted to both back-filled and open-drift systems. All models listed in Table 1 properly simulate the basic thermal-mechanical responses, including temperature and thermal stress evolution. All models are also capable of simulating coupled THM behavior under single-phase flow conditions in Repository Type B for the assumed simplified bentonite mechanical properties and equivalent continuum flow. At the moment, only the TOUGH-FLAC code with its capability for full multiphase dual-continuum fluid flow and heat transport can properly simulate fluid flow for Repository Type A. However, with the application of a dual-continuum or similar approaches that correctly account for fracture-matrix interactions, the results of other models could be much improved with regard to fluid flow, so that the remaining deviations in the evolution of saturation near the drift wall can be resolved.

Despite some differences in the evolution of near-field thermal-hydrological processes, the agreement in the predicted thermal-mechanical responses in the rock mass is good (see Figure 5). The near-field thermal-hydrological processes only affect the temperature evolution in the bentonite buffer and close to the drift wall, whereas these have a negligible effect on the regional temperature field. As a result, predictions of thermal-mechanical changes in the rock mass can be made with relatively simple models, without the need for detailed simulations of complex near-field thermal-hydrological processes. If the purpose were only to predict thermal-mechanical responses, a relatively simple thermo-elastic, heat-conduction model would be sufficient. However, to accurately predict the impact of thermal-mechanical responses on permeability and the flow field, a proper fluid flow model, which includes fracture-matrix interactions, is necessary.

### 4. CONCLUSIONS AND DISCUSSION

In this paper, we present the results of an international multiple-team study of coupled thermal, hydrological, and mechanical (THM) interactions associated with open and back-filled

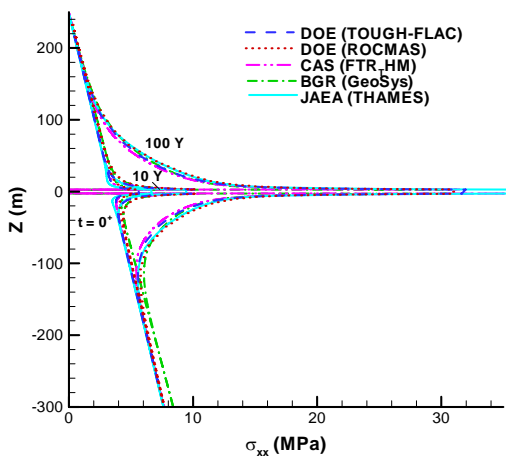
repository-drift designs in volcanic and crystalline rocks. A good agreement was achieved in the calculated THM responses for both repository types, although deviations related to multiphase fluid flow and matrix-fracture interactions should be resolved. The study shows that predictions of thermal-mechanical changes in the rock mass can be made with relatively simple models, without the need for detailed simulations of some of the complex near-field thermal-hydrological processes. This implies that the basic thermal-mechanical stresses can be predicted with a relatively high confidence level. The research teams are currently working on Phase 2, which is the preliminary model prediction and sensitivity analysis of long-term permanent (irreversible) changes, and the impact of those changes on the fluid flow field around the emplacement drift. Those calculations will require a fully coupled THM analysis with accurate modeling of the fluid flow field, including fracture-matrix interactions.

### ACKNOWLEDGMENTS

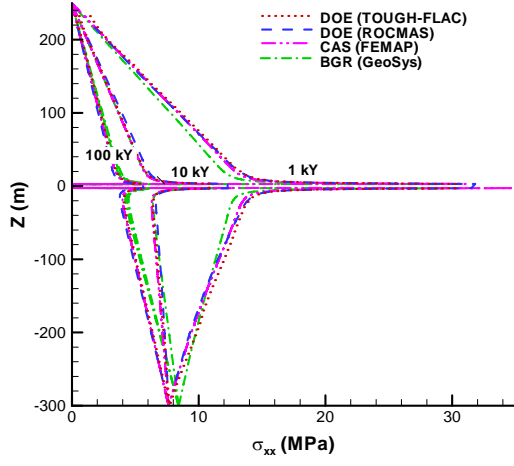
Funding for the LBNL authors was provided by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order QA-B004220RB3X between Bechtel SAIC Company, LLC and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab), provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC02-05CH11231.

### REFERENCES

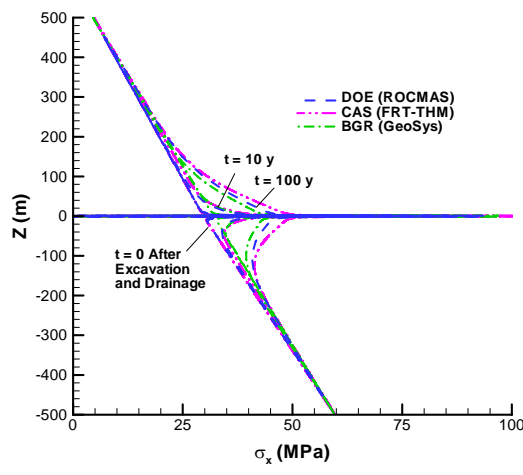
- Birkholzer J.T., Barr D., Rutqvist J., & Sonnenthal E. 2006. Motivation, Description, and summary status of geomechanical and geochemical modeling studies in Task D of the international DECOVALEX-THMC project. GeoProc 2006 Conference.
- Rutqvist J., Barr D., Datta R., Gens A., Millard M., Olivella S., Tsang C.F. and Tsang Y. 2005. Coupled thermal-hydrological-mechanical analysis of the Yucca Mountain Drift Scale Test – comparison of field results to predictions of four different models. *Int. J. Rock mech. & Min. Sci.*, 42, 680-697.
- Alonso E.E., et al, (26 co-authors). 2005. The FEBEX Benchmark test. Case Definition and comparison of modelling approaches. *Int. J. Rock mech. & Min. Sci.*, 42, 611-638.



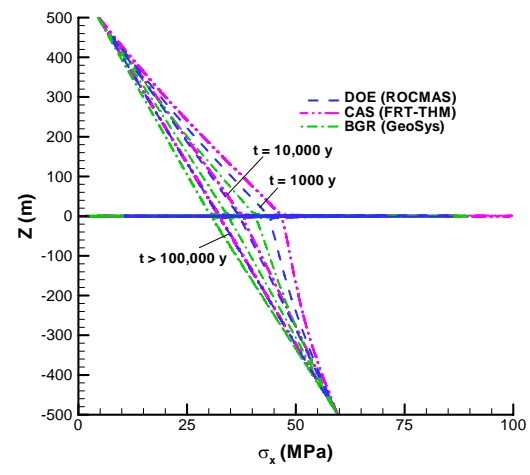
(a) Repository Type A (0 to 100 years)



(b) Repository Type A (0 to 100 years)



(c) Repository Type B (0 to 100 years)



(d) Repository Type B (0 to 100 years)

Figure 5. Comparison of simulation results for prediction of evolution of regional horizontal stress in Repository Type A (a and b) and Repository Type B (c and d).