MOL.20061204.0243

DT# 48416 QA:NA 8/2/06 CB

Results from an International Simulation Study on Coupled Thermal, Hydrological, and Mechanical (THM) Processes near Geological Nuclear Waste Repositories

J. Rutqvist[a,]*, D. Barr[b], J.T. Birkholzer[a], M. Chijimatsu[c], O. Kolditz[d], Quansheng Liu[e], Y. Oda[f], Wenqing Wang[d], and Chengyuan Zhang[e]

[a]*Lawrence Berkeley National Laboratory, Earth Sciences Division, MS 90-1116, Berkeley, CA 947 20, USA*
[b]*Office of Repository Development, U.S. Department of Energy, Las Vegas, USA*
[c]*Hazama Cooperation, Tokyo, Japan*
[d]*University of Tübingen, Tübingen, Germany*
[e]*Chinese Academy of Sciences, Wuhan, China*
[f]*Japan Atomic Energy Agency, Tokai, Japan*

* Corresponding author. Tel.: +1-510-486-5432, fax.: +1-510-486-5432
E-mail address: Jrutqvist@lb.gov (J. Rutqvist)

Version 5

Total number of figures: 8

Total number of tables: 2

Total number of pages: ~~35~~ 25 cb 10/16/06

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 waste emplacement drifts of geological nuclear waste repositories. The simulations were conducted for two generic repository types, one with open and the other with back-filled repository drifts, under higher and lower postclosure temperatures, 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 is currently being resolved. In particular, good agreement in the basic thermal-mechanical responses was achieved for both repository types, even though some teams used relatively simplified thermal-elastic heat-conduction models that neglected 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.

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, mainly focusing on coupled thermo-hydro-mechanical (THM) processes.[1] The general goal of the project is to encourage multidisciplinary, interactive, and cooperative research on modeling coupled processes in geologic formations, in support of performance assessment for underground storage of radioactive waste. Currently, a fourth multi-year project stage of DECOVALEX is underway, referred to as DECOVALEX-THMC, with the added C standing for chemical processes. Thus this project stage aims at the study and modeling of the four-way (THMC) coupled processes.

This paper presents results of an ongoing DECOVALEX-THMC research task, in which participating research teams were asked to conduct predictive analysis of the long-term impact of coupled THM processes in generic repositories with simplified conditions and geometries (without the C, which will be addressed later in the task). Examples of the multitude of coupled THM processes considered in this study are shown in Figure 1. However, the main coupled processes studied in this task are

1. Heating of the rock mass by the waste package, with associated thermally induced rock stresses

2. Changes in hydrological rock properties caused by the thermally induced rock stresses
3. Changes in the fluid flow distribution around waste emplacement drifts, caused by the thermally induced changes in hydrological properties

In the long term, coupled THM processes may lead to changes in geomechanical and hydrological properties that are important for repository performance, because the flow processes in the vicinity of emplacement tunnels will be altered from what they were initially. These changes can be permanent (irreversible), in which case they would persist after the thermal conditions have returned to ambient—that is, they would affect the entire compliance period.

Two generic repository types with horizontal emplacement tunnels are considered in this study:

Type A—A high-temperature (above boiling) repository in a deep unsaturated volcanic rock formation, with emplacement in open gas-filled tunnels, similar to the Yucca Mountain repository concept in the United States.

Type B—A low-temperature (below boiling) repository in a deep saturated crystalline rock formation, with emplacement in back-filled tunnels, a concept considered in a number of European countries.

The initial rock properties for the two repository types are derived from measurements and previous DECOVALEX analyses of two major *in situ* experiments. The first one, representing Repository Type A, is the Yucca Mountain Drift Scale Test, conducted at Yucca Mountain, Nevada.[2] The second one, representing Repository Type B, is the FEBEX *in situ* experiment, conducted at the Grimsel Test Site, Switzerland.[3] THM simulations of these two major field experiments under a previous DECOVALEX project stage have already demonstrated that the short-term (occurring over several years) coupled THM processes are well understood. In the present study, however, the models are used to predict coupled THM processes over tens of thousands of years.

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 I). Among the five simulators, two main approaches can be distinguished. Three simulators—ROCMAS, THAMES, and FRT-THM—are based on a single-phase fluid flow approach, whereas two simulators—TOUGH-FLAC and Geosys/Rockflow—are based on a 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 (see Table I for a short description of each numerical simulator with source references). In this research task, the codes are used to simulate coupled THM processes in both of the two repository types.

II. SIMULATION TASKS

Research teams participating in the research task are asked to 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 2). Participating research teams model the THM processes in the fractured rock close to the representative emplacement tunnel as a function of time, predict the changes in hydrological properties, and evaluate the impact on near-field flow processes. The simulations to be conducted include three phases:

Phase 1. Model inception

Phase 2. Preliminary model prediction and sensitivity analysis

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 one simulation in which all the properties are explicitly provided (Table II). Thus, in this phase no data or model uncertainties are considered, and changes in hydrological properties are neglected. The results of the research teams are compared at this stage to assure that they are starting the problem on a common basis before further complexities are added in Phases 2 and 3. In Phase 2, the research teams are to develop their model and input material properties from available site data, with the ultimate goal of predicting mechanically induced permanent changes. In Phase 3, the research teams are asked to make their final prediction and to evaluate the uncertainties in their predictions.

III. THM SIMULATION RESULTS

In the following two subsections, thermal-mechanical and thermal-hydrological simulation results from the different modeling teams are presented and compared. We present the results for the two repository types side-by-side, to find common observations and general conclusions that are valid for both repository types, which maybe applicable generally in other repository types as well.

III.A Thermal-Mechanical Results

Figure 3 schematically summarized the simulation results of coupled thermal-mechanical responses, which are induced by regional temperature changes (Fig. 3a). 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, since 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 (Fig. 3b).

Figures 4 and 5 show comparisons of temperature and stress evolution from simulations using the five different models. They show a generally good agreement for temperature and stress evolution, especially in the case of Repository Type A (Fig. 4a and 5a). The more significant deviations in temperature evolution for Point V1 for Repository Type B (Fig. 4b) can be explained by differences in the use of saturation-dependent thermal conductivity in the backfill. JAEA's disagreement in thermal stress in Figure 5b results from a misconception of the initial stress and excavation modeling, which can be easily corrected. One of the aims of the model inception (Phase 1) of this research task is to resolve such misconceptions in the modeling of basic thermal-mechanical responses before going to the next phase of the project.

The main difference between thermal-mechanical responses in Repository Type A and Type B is related to the evolution of the heat-power and the thermal stress 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.

III.B Thermal-Hydrological Results

Complex thermal-hydrological interactions occur in the near-field for both Repository Type A and Type B (Figure 3b). 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 point, 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 first 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 6 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 2 for locations of V1 and V3). Whereas the agreement between results from the different models for Repository Type B is quite satisfactory, the results for Repository Type A are appears to be mixed and less satisfactory. The comparison for Type A in Figure 6a looks less satisfactory partly because the results of single continuum models (BGR, JAEA, CAS) are compared to that of a more detailed dual-continuum model (DOE, TOUGH-FLAC). In general, Figure 6a shows that the total dryout times till rewetting for the different models are similar, while the time evolutions of saturation are 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 and their interactions.

IV. EVALUATION OF MODEL APPROACHES

Results of this study show that a reasonably 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 I properly simulate the basic thermal-mechanical responses, including the evolution of temperature and thermal stress. 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 the 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 regional thermal-mechanical responses in the rock mass is good (see Figure 7 and 8). The near-field thermal-hydrological processes affect the temperature evolution in the bentonite buffer and close to the drift wall, but 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. Thus, 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.

V. 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 among the teams was achieved in the calculated THM responses for both repository types, although there are deviations related to multiphase fluid flow and matrix-fracture interactions, which are understood and can 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 level of confidence. With a reasonably good agreement in the thermal-mechanical response, the next step will be to investigate whether these thermal stresses can result in 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. This effort is currently underway.

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

1. C.-F. Tsang, L. Jing, O Stephansson, and F. Kautsky, "The DECOVALEX III project: a summary of activities and lessons learned," *Int. J. Rock mech. & Min. Sci.,* **42**, 593-610 (2006).

2. J. Rutqvist, D. Barr, R. Datta, A. Gens, M. Millard, S. Olivella, C.-F. Tsang, and Y. Tsang, "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 (2005).

3. E. E. Alonso, et al., (26 co-authors), "The FEBEX Bechmark test. Case Definition and comparison of modelling approaches," *Int. J. Rock mech. & Min. Sci.*, **42**, 611-638 (2005).

4. J. Rutqvist, Y. S. Wu, C.-F. Tsang, and G. Bodvarsson, "A Modeling Approach for Analysis of Coupled Multiphase Fluid Flow, Heat Transfer, and Deformation in Fractured Porous Rock," *Int. J. Rock mech. Min. Sci.*, **39**, 429-442 (2002)

5. J. Rutqvist, and C.-F. Tsang, "TOUGH-FLAC: A numerical simulator for analysis of coupled thremal-hydrologic-mechanical processes in fractured and porous geological media under multi-phase flow conditions," *Proc. TOUGH symposium 2003*, Berkeley, California, May 12–14, 2003, Lawrence Berkeley National Laboratory (2003).

6. J. Rutqvist, and C.-F. Tsang, "Analysis of thermal-hydrologic-mechanical behavior near an emplacement drift at Yucca Mountain," *Journal of Contaminant Hydrology*, **62–63**, 637–652 (2003).

7. J. Noorishad, and C.-F. Tsang, "Coupled thermohydroelasticity phenomena in variable saturated fractured porous rocks—Formulation and numerical solution," In O. Stephansson, L. Jing,, and C.-F. Tsang, editors, *Coupled Thermo-hydro-mechanical Processes of Fractured Media. Developments in Geotechnical Engineering*, Elsevier, **79**, pp. 93–134 (1996).

8. J. Rutqvist, L. Börgesson, M. Chijimatsu, A. Kobayashi, T. S. Nguyen, L. Jing, J. Noorishad, and C.-F. Tsang, "Thermohydromechanics of Partially Saturated Geological Media – Governing Equations and Formulation of Four Finite Element Models," *Int. J. Rock Mech. Min. Sci.*, **38**, 105-127 (2001).

9. J. Rutqvist, L. Börgesson, M. Chijimatsu, T. S. Nguyen, L. Jing, J. Noorishad, and C.-F. Tsang,."Coupled Thermo-hydro-mechanical Analysis of a Heater Test in Fractured Rock and Bentonite at Kamaishi Mine – Comparison of Field Results to Predictions of Four Finite Element Codes," *Int. J. Rock Mech. Min. Sci.*, **38**, 129-142 (2001).

10. J. Rutqvist, M. Chijimatsu, L. Jing, J. de Jonge, M. Kohlmeier, A. Millard, T. S. Nguyen, A. Rejeb, M. Souley, Y. Sugita, and C.-F. Tsang, "Numerical study of the THM effects on the near-field safety of a hypothetical nuclear waste repository – BMT1 of the DECOVALEX III project. Part 3: Effects of THM coupling in fractured rock," *Int. J. Rock mech. & Min. Sci.,* **42**, 745-755 (2005).

11. O. Kolditz, S. Bauer, M. Beinhorn, J. de Jonge, T. Kalbacher, C. McDermott, W. Wang, M. Xie, R. Kaiser, and M. Kohlmeier, *ROCKFLOW - Theory and Users Manual, Release 3.9*, Groundwater Group, Center for Applied Geosciences, University of Tübingen, and Institute of Fluid Mechanics, University of Hannover (2003).

12. J. de Jonge, M. Xie, and O. Kolditz, "Numerical implementation of thermally and hydraulically coupled processes in non-isothermal porous media. In: Stephansson O, Hudson JA, Jing L, editors. Coupled T-H-M-C Processes in Geo-Systems: Fundamentals, Modelling, Experiments and Applications. Elsevier Geo-Engineering Book Series, Oxford, 205–210 (2004).

13. W. Wang, M. Xie, T. Nowak, H. Kunz, H. Shao, and O. Kolditz, "Modeling THM coupled problem of Task D of the DECOVALEX project," *Proc. GEOPROC2006 International symposium: 2nd International Conference on Coupled Thermo-hydro-mechanical-chemical processes in Geosystems and Engineering*, HoHai University, Nanjing, China, May 22-25, 2006, 226-232, HoHai University (2006).

14. M. Xie, W. Wang, T. Nowak, H. Kunz, H. Shao, and O. Kolditz, "Numerical simulation of a THC problem and its long-term effect on bentonite/granite FEBEX type repository," *Proc. GEOPROC2006 International symposium: 2nd International Conference on Coupled Thermo-hydro-mechanical-chemical processes in Geosystems*

and Engineering, HoHai University, Nanjing, China, May 22-25, 2006, 403-410, HoHai University (2006).

15. Q. Liu, C. Zhang, and X. Liu, "A practical method for coupled THM simulations of the Yucca Mountain and FEBEX case samples for task D of the DECOVALEX-THMC Project," *Proc. GEOPROC2006 International symposium: 2nd International Conference on Coupled Thermo-hydro-mechanical-chemical processes in Geosystems and Engineering*, HoHai University, Nanjing, China, May 22-25, 2006, 220-225, HoHai University (2006).

16. X. Liu, C. Zhang, and Q. Liu, "Analysis of uncertainty in coupled THM simulations of the FEBEX case example for Task D of the DECOVALEX-THMC project," *Proc. GEOPROC2006 International symposium: 2nd International Conference on Coupled Thermo-hydro-mechanical-chemical processes in Geosystems and Engineering*, HoHai University, Nanjing, China, May 22-25, 2006, 234-239, HoHai University (2006).

17. Y. Ohnishi, H. Shibata, and A. Kobayashi, "Development of finite element code for the analysis of coupled thermo-hydro-mechanical behavior of a saturated-unsaturated medium," In C.-F. Tsang, editor, *Coupled Processes Associated with Nuclear Waste Repositories*, Academic Press, 551–557 (1987).

18. Y. Ohnishi, and A. Kobayashi, "THAMES". In O. Stephansson, L. Jing, and C.-F. Tsang, editors, *Coupled Thermo-hydro-mechanical Processes of Fractured Media, Developments in Geotechnical Engineering*, Elsevier, **79**, 545–549 (1996).

19. M. Chijimatsu, T. Fujita, A. Kobayashi, and M. Nakano, "Experiment and validation of numerical simulation of coupled thermal, hydraulic and mechanical behaviour in the engineered buffer materials," *Int. J. Numer. Anal. Meth. Geomech.* **24**, 403–424 (2000).

20. M. Chijimatsu, T. S. Nguyen, L. Jing, J. de Jonge, M. Kohlmeier, A. Millard, A. Rejeb, J. Rutqvist, M. Souley, and Y. Sugita, "Numerical study of the THM effects on the near-field safety of a hypothetical nuclear waste repository – BMT1 of the DECOVALEX III project. Part 1: Conceptualization and characterization of the problems and summary of results," *Int. J. Rock mech. & Min. Sci.,* **42**, 720-730 (2005).

FIGURE CAPTIONS

Figure 1. Examples of coupled THM processes considered in this study.

Figure 2. Two-dimensional model geometry for analysis of the two repository types (A and B) and locations of some output points.

Figure 3. Schematic of main thermal-mechanical responses common for both Repository Types A and B.

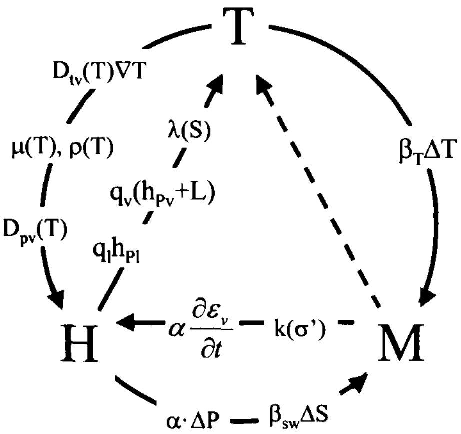
Figure 4. Evolution of calculated power and temperature for (a) Repository Type A and (b) Repository Type B. Locations of Points V1, V2, V3 and V6 are indicated in Figure 2.

Figure 5. Evolution of calculated horizontal stress for (a) Repository Type A and (b) Repository Type B. Locations of Point H6 is indicated in Figure 2.

Figure 6. Evolution of liquid saturation for (a) Repository Type A at Point V3 in the rock near the drift wall, and (b) Repository Type B at Point V1 in the bentonite near the waste canister.

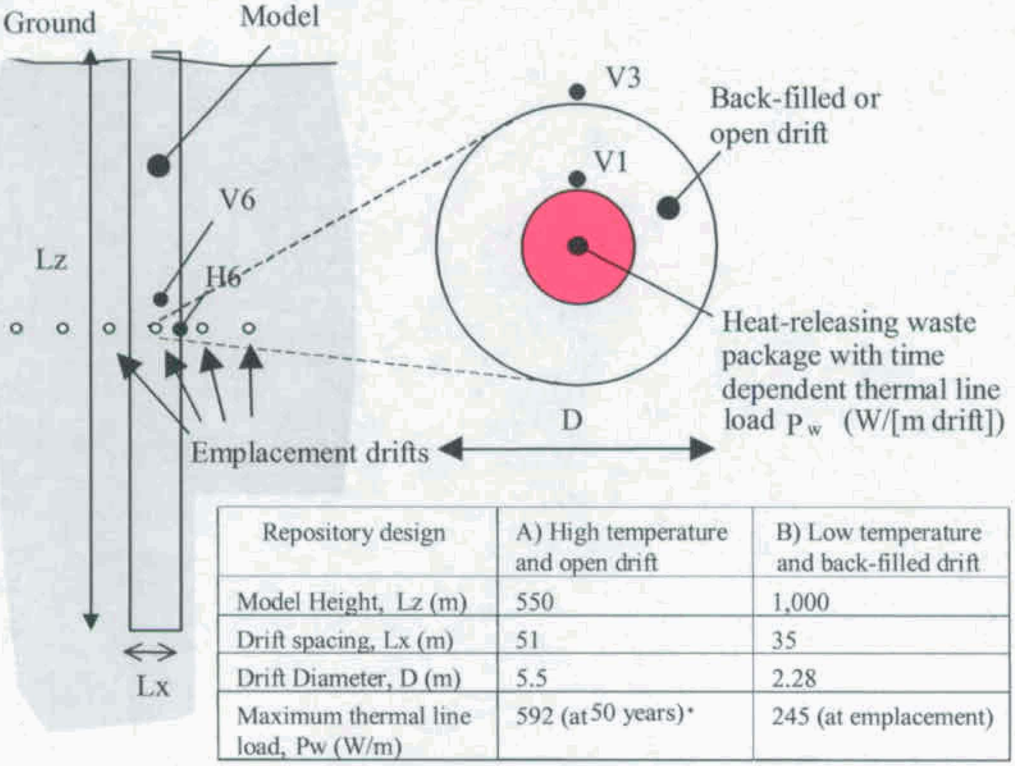
Figure 7. Comparison of simulation results for prediction of evolution of regional horizontal stress around Repository Type A: (a) 0 to 100 years, and (b) 1,000 to 1 million years.

Figure 8. Comparison of simulation results for prediction of evolution of regional horizontal stress around Repository Type B: (a) 0 to 100 years, and (b) 1,000 to 1 million years.



$D_{TV}(T)\nabla T$ = Vapor diffusion along thermal gradient
$\mu(T)$ = Temperature dependent fluid viscosity
$\rho(T)$ = Temperature dependent fluid density
$D_{PV}(T)$ = Temperature dependent vapor diffusion
$\lambda(S)$ = Saturation dependent thermal conductivity
$q_v(h_{pv}+L)$ = Heat convection with vapor flow
$q_l h_{pl}$ = Heat convection with liquid fluid flow
$\alpha \partial \varepsilon_v / \partial t$ = Poroelastic volume change
$k(\sigma')$ = Stress dependent permeability
$\alpha \Delta P$ = Effect of fluid pressure on effective stress
$\beta_{sw} \Delta S$ = Moisture (saturation) induced strain
$\beta_T \Delta T$ = Thermal strain

Figure 1



Repository design	A) High temperature and open drift	B) Low temperature and back-filled drift
Model Height, Lz (m)	550	1,000
Drift spacing, Lx (m)	51	35
Drift Diameter, D (m)	5.5	2.28
Maximum thermal line load, Pw (W/m)	592 (at 50 years)*	245 (at emplacement)

* Heat load is reduced by drift ventilation until 50 years

Figure 2

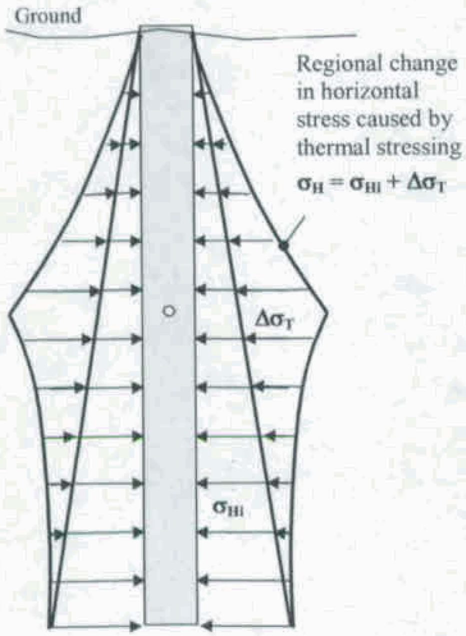


Figure 3a

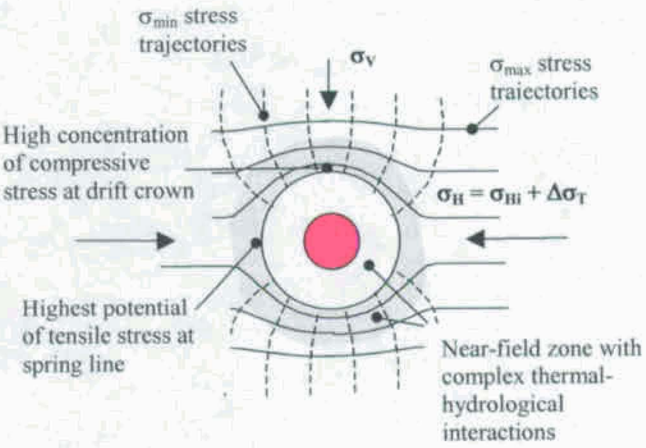


Figure 3b

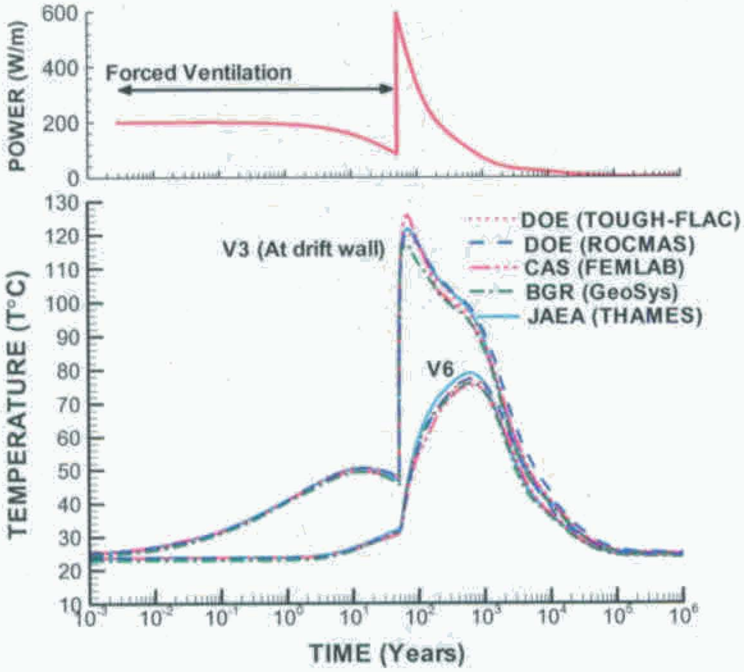


Figure 4a

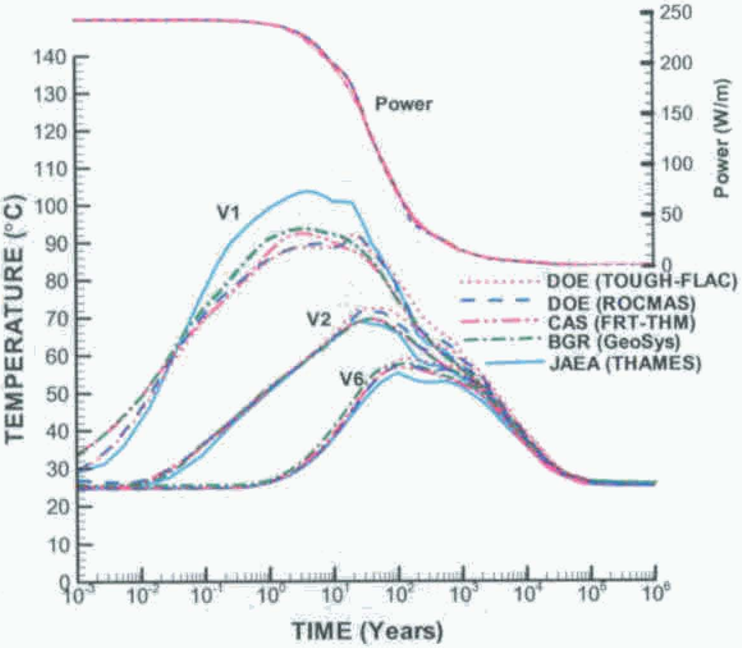


Figure 4b

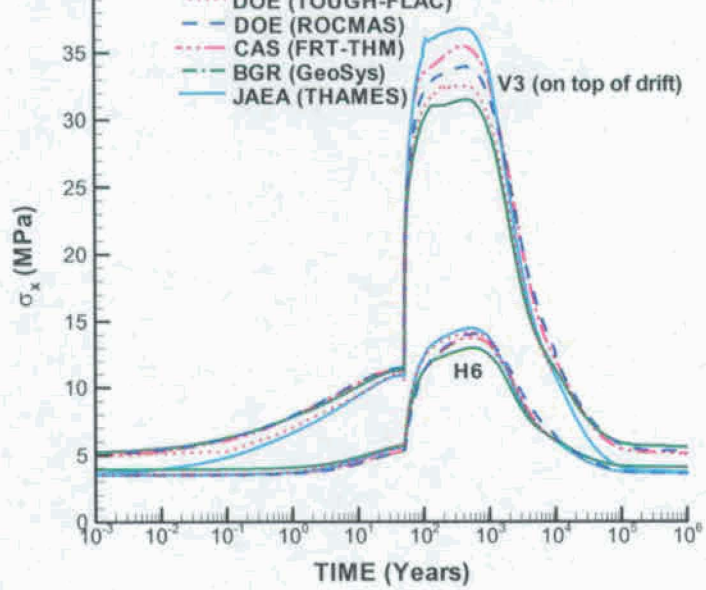


Figure 5a

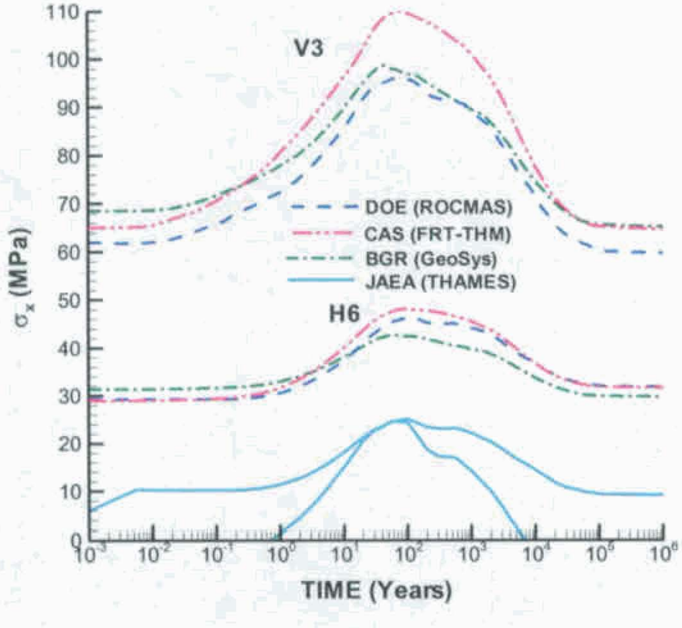


Figure 5b

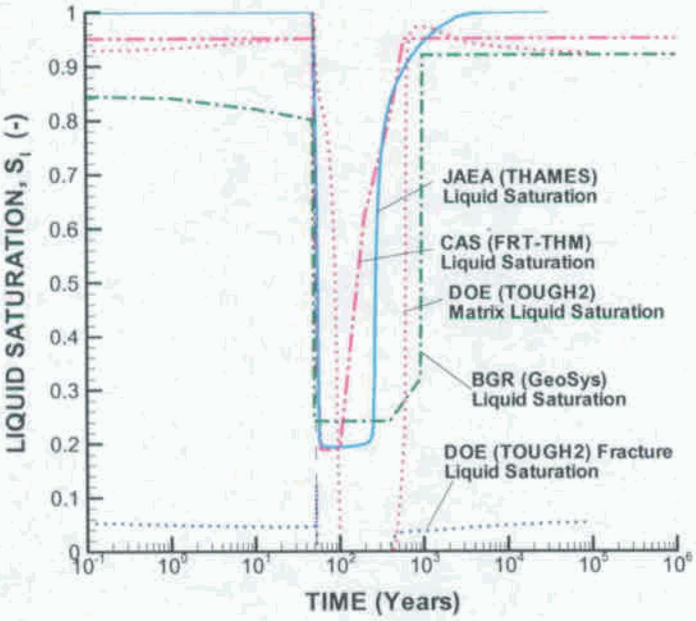


Figure 6a

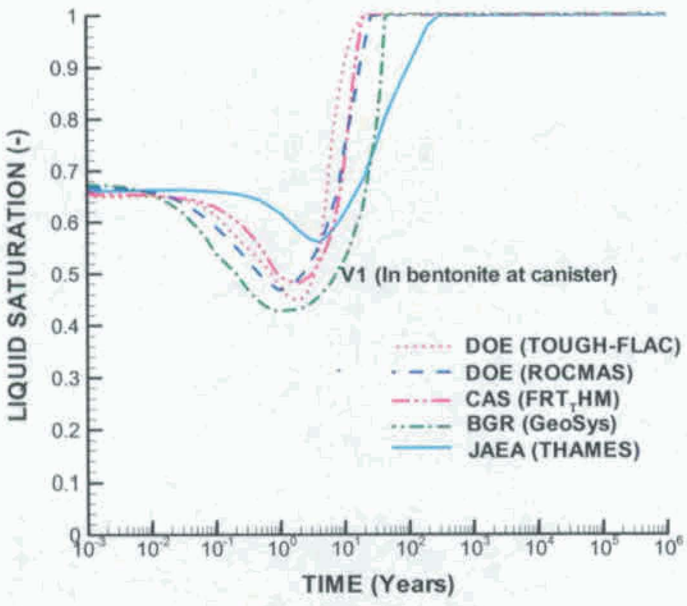


Figure 6b

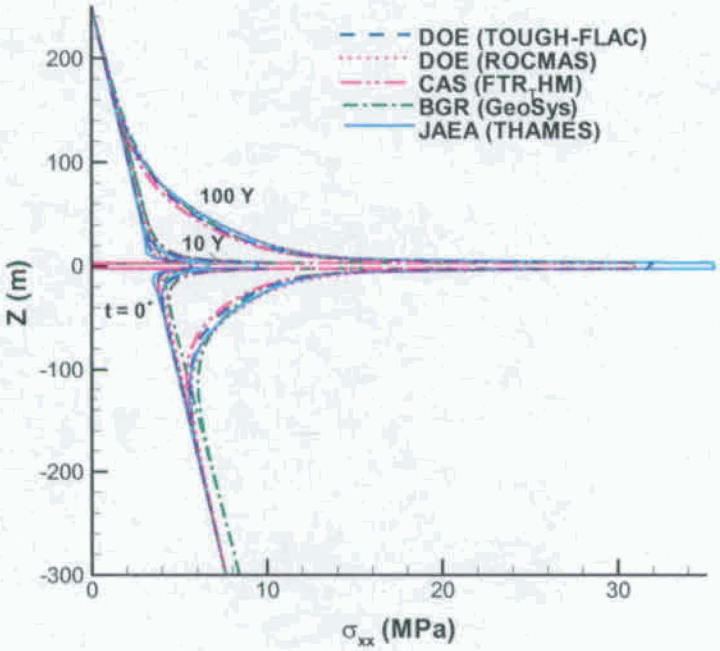


Figure 7a

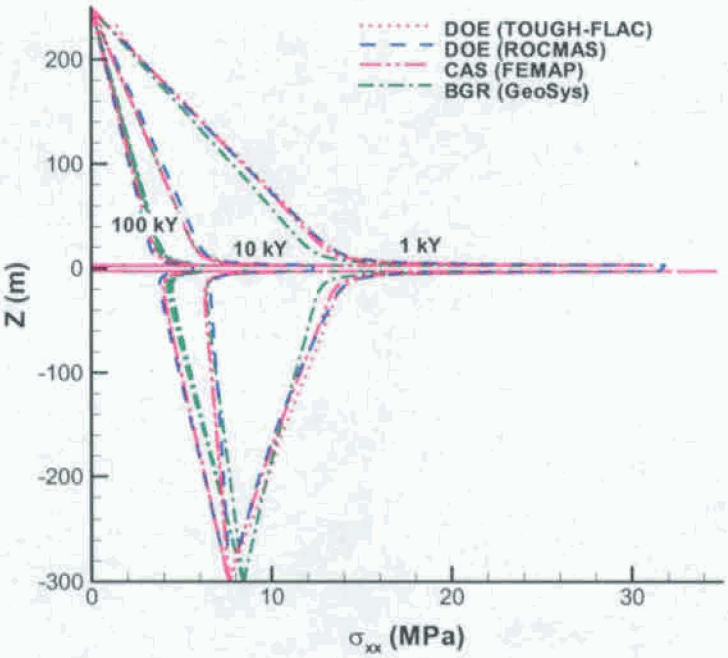


Figure 7b

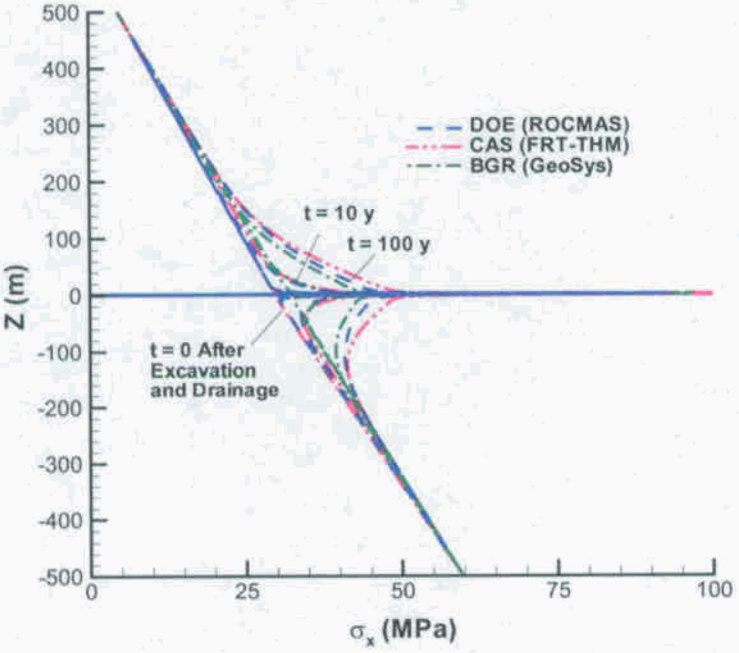


Figure 8a

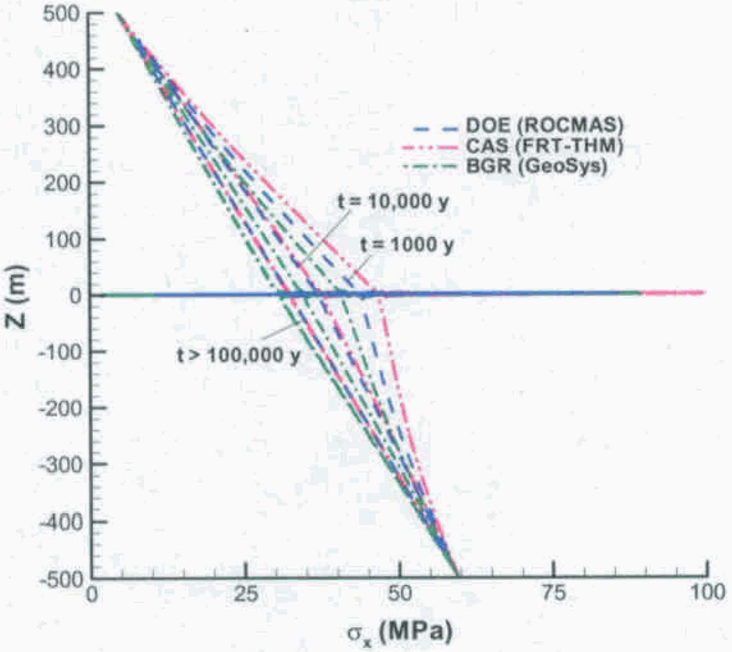


Figure 8b

TABLE I: Research teams and simulators applied in this study

Research Team	Numerical Simulator	Brief Description of Numerical Simulator
DOE U.S. Department of Energy's Research Team: Lawrence Berkeley National Laboratory (LBNL)	**TOUGH-FLAC**	TOUGH-FLAC is a simulator for analysis of coupled THM processes under multiphase fluid flow conditions developed at the LBNL in the last few years.[4, 5] The simulator is based on linking of the existing computer codes TOUGH2 and FLAC3D. It has been extensively used for analysis of coupled THM processes within the Yucca Mountain Project (e.g. ref. 3 and 6).
	ROCMAS	ROCMAS is a finite element program for analysis of coupled THM processes in porous and fractured rock developed at LBNL since the late 1980s. In the late 1990s, this code was extended to unsaturated media with single-phase liquid flow and vapor diffusion in a static gas phase.[7, 8] The code has been extensively applied in earlier phases of the DECOVALEX project for THM analysis in bentonite-rock systems (e.g ref. 2, 9, and 10).
BGR Bundesanstalt für Geowissenschaften und Rohstoffe's Research Team: University of Tübingen	**GeoSys/ Rockflow**	GeoSys/Rockflow is based on object-oriented programming and is developed at the University of Tübingen.[11] It was first applied in previous DECOVALEX phases for analysis of thermal-hydrological and thermal-mechanical processes[12] and has recently been extended to THM[13] and reactive chemical transport analysis[14]. For the present study, an unsaturated single-phase liquid flow and vapor diffusion is considered.
CAS Chinese Academy of Sciences' Research Team	**FRT-THM**	The FRT-THM (Fluid-Rock Transport simulator) being developed by the CAS is based on MATLAB and C language codes, in which FEMLAB is used as partial differential equation solver.[15] The approach being developed for the present study features an unsaturated single-phase fluid flow and vapor diffusion model approach.[15, 16]
JAEA Japan Atomic Energy Agency's Research Team, including Hazama Cooperation	**THAMES**	THAMES is a finite element program for analysis of coupled THM processes in porous and fractured rock developed at the Kyoto University since the late 1980s.[17, 18] The code has been extended to unsaturated media with single-phase liquid flow and vapor diffusion in a static gas phase.[19] The THAMES code has been extensively applied in earlier phases of the DECOVALEX project for THM analysis in bentonite-rock systems (e.g. ref. 2, 9, and 20).

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

Parameter	Type A (Tuff)[1]	Type B (Granite)
Bulk Density, [kg/m^3]	2370	2700
Matrix Porosity [-]	0.13	0.01
Young's Modulus, [GPa]	15	35
Poisson's ratio, [-]	0.21	0.3
Specific heat, [J/kg·°C]	985	900
Thermal conductivity, [W/m·°C]	2.29	3.0
Thermal expansion coefficient, [°C^{-1}]	1.0×10^{-5}	$1\cdot10^{-5}$
Bulk Permeability, [m^2]	3.3×10^{-13}	1×10^{-17}

[1] 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.