MULTIPLE-CODE BENCHMARK SIMULATION STUDY OF COUPLED THMC PROCESSES IN THE EXCAVATION DISTURBED ZONE ASSOCIATED WITH GEOLOGICAL NUCLEAR WASTE REPOSITORIES

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Abstract: An international, multiple-code benchmark test (BMT) study is being conducted within the international DECOVALEX project to analyse coupled thermal, hydrological, mechanical and chemical (THMC) processes in the excavation disturbed zone (EDZ) around emplacement drifts of a nuclear waste repository. This BMT focuses on mechanical responses and long-term chemo-mechanical effects that may lead to changes in mechanical and hydrological properties in the EDZ. This includes time-de-pendent processes such as creep, and subcritical crack, or healing of fractures that might cause “weakening” or “hardening” of the rock over the long term. Five research teams are studying this BMT using a wide range of model approaches, including boundary element, finite element, and finite difference, particle mechanics, and elasto-plastic cellular automata methods. This paper describes the definition of the problem and preliminary simulation results for the initial model inception part, in which time dependent effects are not yet included.

1. INTRODUCTION

This paper presents an international, multiple-code benchmark test (BMT) simulation study of coupled thermal, hydrological, mechanical and chemical (THMC) processes in the excavation disturbed zone (EDZ) around an emplacement drift of a hypothetical nuclear waste repository. The study is part of the ongoing international DECOVALEX-THMC project, denoted as Task B (Rutqvist et al., 2006a). This simulation study focuses on mechanical responses and long-term chemo-mechanical effects that may lead to time-dependent changes in mechanical and hydrological properties in the EDZ. This includes processes such as creep, subcritical crack growth, and healing of fractures that might cause “weakening” or “hardening” of the rock over the long term. Five research teams are studying this BMT using a wide range of model approaches, including boundary element, finite element, finite difference, particle mechanics, and cellular automata methods (Table 1). An important part of this BMT is to investigate how these widely different approaches can be adapted and developed to include time-dependent processes to model the complex coupled THMC processes at various scales within or near the EDZ of an emplacement tunnel. Thus, this BMT is not a strictly defined problem for code-to-code comparison, but is rather designed to promote innovative model developments towards simulation of chemo-mechanical interactions with a future, fully coupled THMC modelling. The present paper describes the definition of the problem, and present and compares preliminary simulation results. Detailed simulation results for one individual research team are also presented in an accompanying paper by Lee et al. (2006).

2. SIMULATION TASKS

The coupled THMC processes of the EDZ are simulated for two sizes of model domains close to an emplacement tunnel (Figure 1); (1) a near-field model domain, and (2) a wall-block model domain. The near-field model domain extends a few meters into the rock from the drift wall and allows analysis of both the evolution and extent of the EDZ. The smaller sized wall-block model domain does not permit analysis of the extent of the EDZ, but rather it is used for detailed analysis of THMC processes within the EDZ. Various degrees of fracturing are considered according to Figure 2 and 3. The relatively small model domains adopted for this BMT allow a very fine discretization, which implies that detailed physics of the rock failure process can be studied.

The aim is to simulate, as closely as possible, the THMC environment of the near-field and the EDZ over a 100,000-year lifetime of a repository. Because the near-field and the wall-block model domains in Figure 1 only represent a small part of the repository system, the THMC environment has to be reproduced by specially designed, time-dependent boundary and interior conditions. For this BMT, the results from large-scale coupled THM and THC analyses conducted within the DECOVALEX-THMC project are utilised for assigning time-dependent boundary and interior conditions (Figure 4 and 5). Those large-scale analyses include complete THM and THC analyses of rock and bentonite buffer, to calculate the evolution of temperature, fluid pressure, bentonite saturation and swelling, thermal stresses, and evolution of chemical potential (See Rutqvist et al., 2006 and Xie et al., 2006). However, they do not include detailed modelling of the EDZ or chemo-mechanical couplings.

This BMT is divided into five modelling stages, starting with a well-defined linear thermal-hydro-elastic analysis, and then successively adding components of elasto-plastic and time-dependent mechanical behaviour. The following specific modelling stages are defined:

Stage 1—Linear thermal-hydro-elastic modelling: Model inception with linear elastic properties

Stage 2—Non-linear, elasto-plastic failure modelling: Extend model to include non-linear and elasto-plastic properties for failure analysis

Stage 3—Time dependent failure modelling: Extend model to include time-dependent changes in mechanical properties for analysis of creep and mechanical degradation

Stage 4—Chemo-mechanical modelling (optional): Extend model to include simplified chemical modeling of time-dependent pressure solution/stress corrosion, or other chemo-mechanical effects

Stage 5—Full THMC modelling (optional): Implement chemo-mechanical model developed under Stage 4 to link THC and THM models into a fully coupled THMC model

The primary purpose of the model inception (Stage 1) is for the research teams to familiarise themselves with the problem by performing one simulation in which all the properties are given, and no time-dependent changes in material properties are assumed (see Table 1 for basic mechanical properties in Stage 1). In Stage 2, the research teams should introduce nonlinear material properties and elasto-plastic material properties into their models to calculate actual development of failure. In Stage 3, the research teams would develop their models further to consider time-dependent effects. This may include development of models with time-dependent changes in continuum mechanical properties (e.g., by time-dependent damage parameters) or subcritical crack-growth modelling. After reaching Stage 3, the research teams should evaluate the need and potential, for extending their models to MC and THMC Stages 4 and 5.

Table 1. Research teams and numerical simulators.

Research Team	Numerical Simulator/Approach
DOE: U.S. Department of Energy's Research Team: Lawrence Berkeley National Laboratory (LBNL)	TOUGH-FLAC simulator using finite difference method (FDM)
	ROCMAS finite element (FEM) code
CAS: Chinese Academy of Sciences' Research Team	Elasto-plastic Cellular Automata (EPCA)
FRACOM: FRACOM Ltd, Finland	FRACOD boundary element (BEM) code with discrete fracture propagation
JAEA: Japan Atomic Energy Agency's Research Team, including Kyoto University	THAMES finite element (FEM) code.
SKI: Swedish Nuclear Power Inspectorate's Research Team: Royal Institute of Technology, Stockholm	PFC distinct element particle flow code

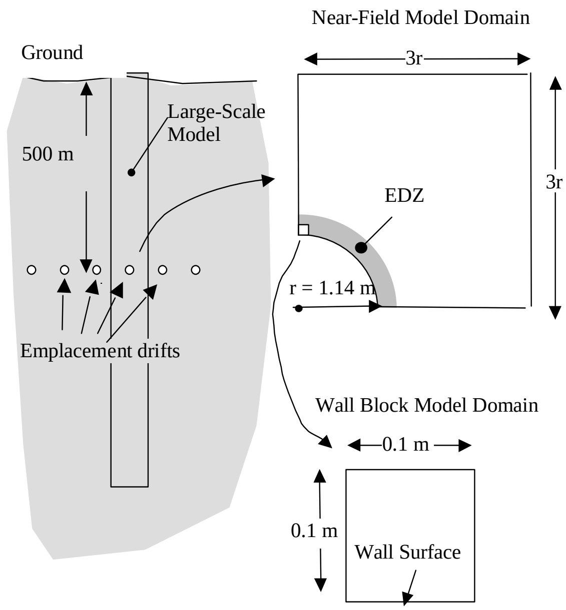


Figure 1. *Two model domains considered for detailed analysis of coupled THMC processes in the EDZ of a drift.*

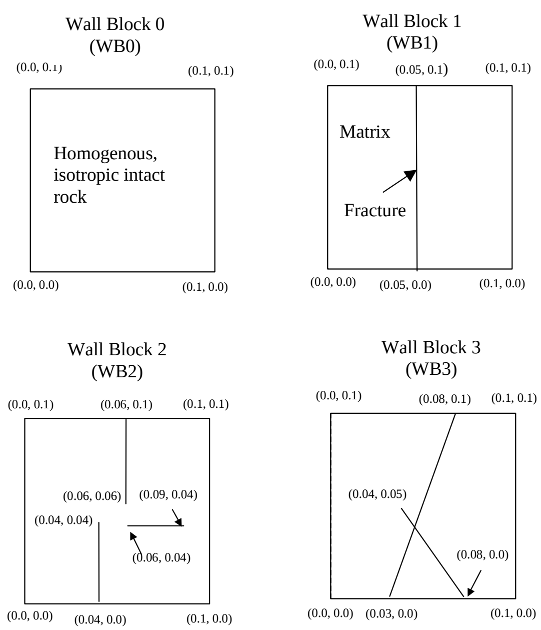


Figure 2. *Geometry of fracture system for four wall-block models (Rutqvist et al., 2006a).*

Table 2. Mechanical properties for Stage 1

Parameter	Value
Young's Modulus,	70 GPa
Poisson's ratio	0.3
Thermal expansion coefficient	$1 \cdot 10^{-5}$ °C^{-1}
Normal stiffness	2,000 GPa/m
Shear stiffness	200 GPa/m

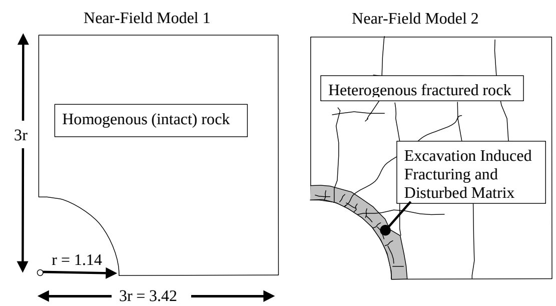


Figure 3. *Geometry of fracture system for two near-field models (Rutqvist et al., 2006a).*

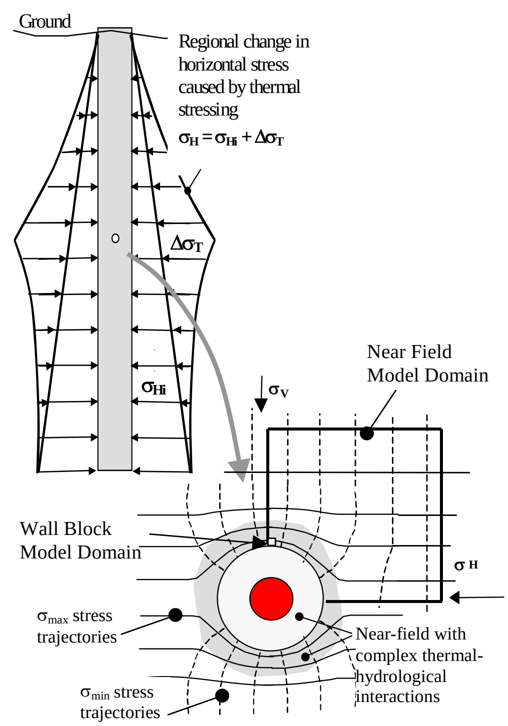


Figure 4. *Schematic of large-scale THM model used for deriving boundary and interior conditions for the near-field and wall-block model domains.*

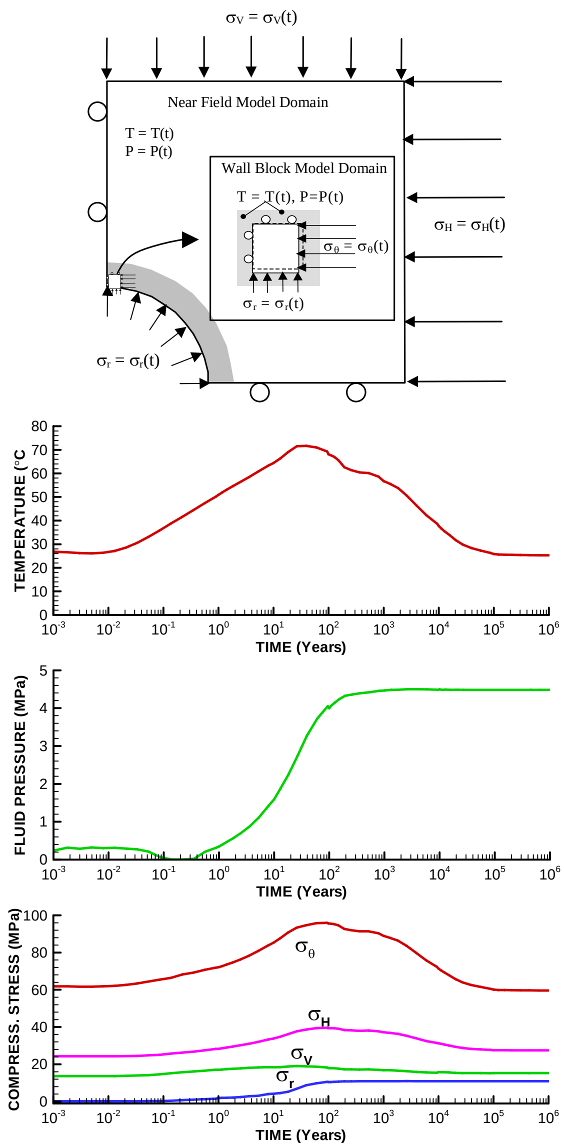


Figure 5. Time dependent THM boundary and interior conditions (Rutqvist et al., 2006a).

3. SIMULATION RESULTS

Preliminary results for Stage 1 for the near-field model and wall-block model domains, and the initial results from two research teams on Stage 2 are presented in the next two subsections.

3.2 Near-Field Model Domain

The results of the model inception of the near-field model domain (Stage 1), show that a relatively small model size of 3.42 by 3.42 meters leads to some unwanted stress concentrations at the lower right corner of the model (Figure 6). However, a comparison of vertical and horizontal stress profiles for different model sizes shows that within a distance of two meters from the drift wall, the small 3.42 by 3.42 meter model provides quite an accurate stress distribution (Figure 7). Since this BMT is focused on processes in the EDZ presumably within one meter of the drift wall, and a small model size is desired for allowing fine discretization, the small 3.42 by 3.42 meters model size is considered satisfactory.

The general results of the Stage 1 analysis of the near-field model indicate that tensile fracturing or opening of pre-existing radial fractures are likely to occur at the spring line, whereas the highest likelihood for shear failure occurs at the drift crown. The results of three research teams (DOE, FRACOM and CAS) are in reasonably good agreement regarding stress. The displacement distribution by FRACOM deviates somewhat since they do not consider thermal strain in their model (this will be further discussed below). The next step will be to introduce natural fractures to the analysis according to Near-Field Model 2 in Figure 3.

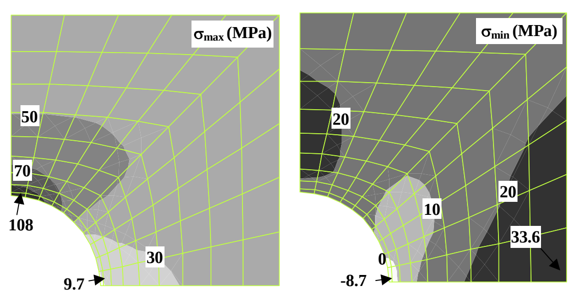


Figure 6. Simulation results by DOE's research team of maximum and minimum compressive principal stresses at 100 years for Stage 1.

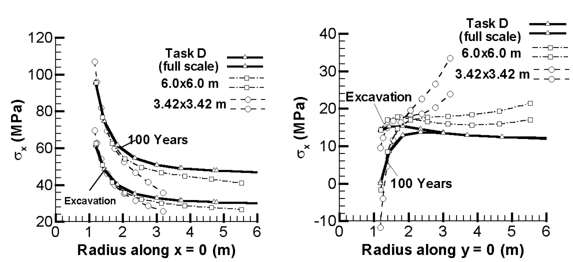


Figure 7. Simulation results by DOE's research team of stresses along two profiles

along x=0 and y=0 at 100 years for Stage 1.

3.2 Wall-Block Model Domain

Stage 1 simulation results for the wall-block model domain show that the stress distribution within the block depends on the presence and geometry of fractures. As an example, Figure 8 shows the results of maximum principal stress distribution at 100 years for Wall-Block Model 2 (WB2) calculated by three different models. Compressive stresses are concentrated in the central intact rock part where the maximum compressive stress exceeds 110 MPa at 100 years. However, the calculated maximum stress differs between different models as it is highly dependent on mesh discretization. A very fine mesh discretization is needed for an accurate calculation of the detailed stress distribution around the pre-existing fractures.

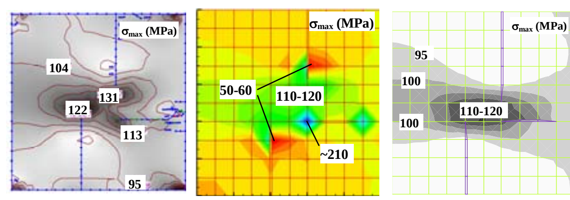
Figure 9 compares vertical and horizontal displacement profiles along the bottom (drift wall) surface of the WB0 and WB3. The results from DOE, CAS and JAEA are quite close, but not in perfect agreement. The calculated displacements for the WB0 (homogeneous rock) can be compared with the following analytical expression:

$$\frac{u_X}{L_X} = -\frac{(1-\upsilon^2)}{E}(\Delta\sigma'_X) + \frac{\nu(1+\nu)}{E}(\Delta\sigma'_Y) + (1+\nu)\alpha_T\Delta T \tag{1}$$

$$\frac{u_Y}{L_Y} = \frac{(1-\upsilon^2)}{E}(\Delta\sigma'_Y) - \frac{\nu(1+\nu)}{E}(\Delta\sigma'_X) - (1+\nu)\alpha_T\Delta T \tag{2}$$

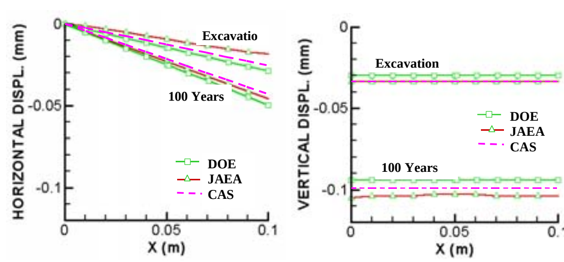
where compressive stress is positive. In Equations (1) and (2), u_x and u_y represent x- and y-displacements at the lower left corner of the block when L_x and L_y are set to 0.1 m. Figure 10 compares the simulated evolution of x and y-displacement at the lower left corner of WB0 with the analytical solution. The results indicate an excellent agreement with the analytical solution by the DOE results, whereas the CAS and JAEA results show a good but not perfect agreement. The discrepancies from the analytical solution in this case are likely to have been caused by different interpretations of the BMT definition of interior and boundary conditions. The calculated displacements by FRACOM (not shown in Figures 9 to 10) deviate from those of other teams, mainly because internal thermal expansion of the matrix is not considered in their BEM model. A sensitivity study by DOE and CAS shows that the internal thermal expansion of the matrix has a great impact on the calculated displacements, whereas it has little impact on the calculated stress distribution. It should be noted that the calculated displacements in this case are very small (on the order of 0.1 mm) and may not be practically relevant – other than for model comparison. Thus, for analysis of the stress distribution and failure process it might be possible to neglect the internal thermal expansion in this particular case.

Initial results from the FRACOM and CAS teams of Stage 2 (elasto-plastic) modeling are shown in Figure 11. The calculated initiation of discrete fracturing using the boundary element method (FRACOM) is roughly consistent with zones of induced plastic strain in the cellular automaton method (CAS). However, further refinement of mesh and modeling results of the other teams should be added for more detailed comparison among the different model approaches.

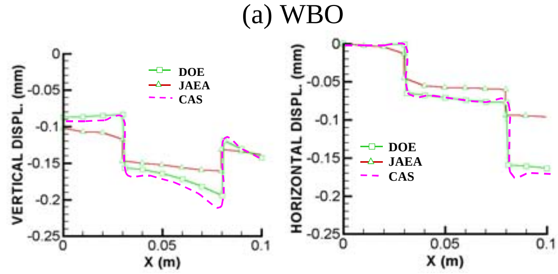


(a) (b) (c)

Figure 8. Distribution of maximum compressive principal stress after 100 years for WB2 calculated by (a) FRACOM's, (b) CAS's and (c) DOE's. research teams.



(a) WBO



(b) WB3

Figure 9. Comparison of calculated horizontal and vertical displacement along the bottom (drift wall surface) boundary of the wall block model WB0 and WB3.

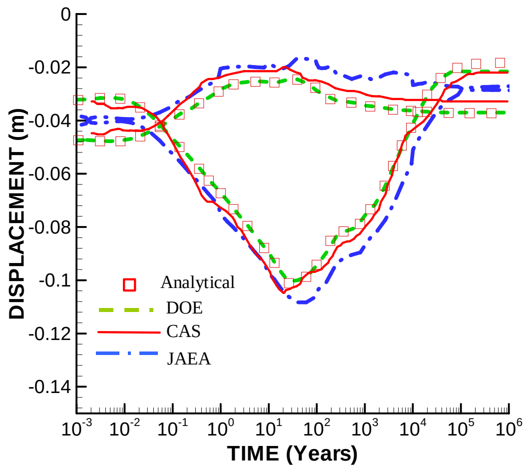
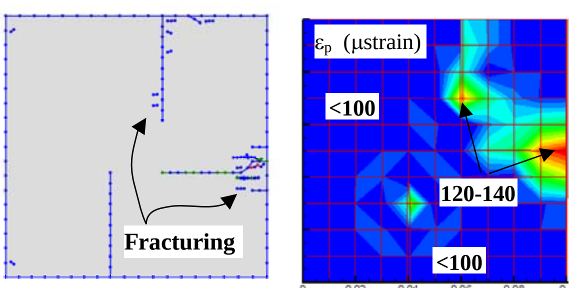


Figure 10. Comparison of calculated evolution of horizontal and vertical displacements of the lower left corner of WB0.



(a) (b)

Figure 11. Preliminary results for Stage 2 at 100 years. (a) Results of development of discrete fractures by FRACOM and (b) results of plastic strain by CAS.

4. CONCLUDING REMARKS

This paper presents the progress of an international, multiple-model benchmark test (BMT) study of coupled thermal, hydrological, mechanical and chemical (THMC) processes in the excavation disturbed zone (EDZ) around emplacement drifts. The results from a model inception stage show that the BMT description for the two model domains (near-field and wall-block model domains), including evolution of interior and boundary conditions, is appropriate, although some discrepancies may exist among the teams in the detailed interpretation of the description. The analysis of the near-field model shows that the maximum compressive stress peaks at about 100 MPa at the drift crown under a minimum compressive stress of about 10 MPa. Such stress magnitude is not likely to induce instantaneous failure in an intact granitic rock, for which the compressive strength exceeds 100 MPa. However, in this case, a high compressive stress on the order of 80 to 100 MPa is maintained for thousands of years, and stresses above 60 MPa will remain for the entire 100,000-year life-time of the repository. Such conditions may induce significant stress corrosion that could effectively weaken the rock and induce significant time dependent behavior. Moreover, the analysis of the wall-block model domain shows that existing fractures lead to further local stress concentrations, which may impact the failure processes significantly. Such effects will be further studied in the coming Stages 2 and 3 of this BMT, including much a refined mesh discretization to capture important heterogeneous failure mechanisms near pre-existing fractures.

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