CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

TRIP REPORT

SUBJECT: DECOVALEX III Workshop (20.01402.671)

DATE/PLACE: June 11-12, 2002/Toronto, Canada

AUTHOR: Ronald T. Green

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PERSONS PRESENT: Representatives from the participating DECOVALEX III teams.

BACKGROUND AND PURPOSE OF TRIP:

The purpose of the trip was to participate in the regularly scheduled workshop of the international thermal-hydrological-mechanical (THM) modeling DECOVALEX III Project. DECOVALEX III is the third in a series of modeling projects initiated in 1992. The Nuclear Regulatory Commission (NRC) participated in DECOVALEX I, did not participate in DECOVALEX II because of budget constraints, and resumed participation in DECOVALEX III. A workshop or task group meeting is usually held twice a year to allow participants an opportunity to present and compare results and plan future activities.

The DECOVALEX III Project is divided into several test cases referred to as Tasks. Each Task has a sponsoring organization, typically the organization responsible for the conduct of the subject test case. It is the responsibility of the sponsoring organization to define the test case, provide required data, and define the target modeling objectives. For example, the DOE is the sponsoring organization of Task 2, the drift-scale heater test (DST) at Yucca Mountain (YM). DOE has provided a description of the DST, site characterization information, and some test results. Some test results have been withheld for use in checking validity of models. Typically not all DECOVALEX teams participate in all Tasks. The NRC, CNWRA, SKI, CEA, UPC, and JNC are participating in Task 2 of DECOVALEX III.

SUMMARY OF PERTINENT POINTS:

I arrived at the workshop at the start of the second day. Discussion of Task 1 (FEBEX) and Task 3C (BMT3 - Glaciation) was held on the first day.

Task 2 Session

The Task 2 Session was held on the second day. Bill Boyle/DOE presented opening remarks. Robin Datta/DOE-contractor described the sub-sections of Task 2 (2A, 2B, 2C, 2D), the Yucca Mountain Drift-Scale Heater Test (DST).

Johnny Rutquist/LBNL presented the status of SKI work on Task 2B/2C. Chin-Fu Tsang/LBNL is a co-author of this work. Coupled THM analyses have been conducted using a coupled simulator, TOUGH2-FLAC3D. An objective of the work is to evaluate the importance of the hydrology-mechanical (HM) coupling. My last recollection was that SKI was going to use the

THM coupled code ROCKMAS to perform this analysis. Although ROCKMAS was fully coupled, it was not capable of multi-phase flow (i.e., > boiling temperatures). The SKI team elected to use TOUGH2-FLAC3D, which does not have this limitation.

Rutquist reported recent progress on the analysis of air-permeability changes observed during pre- and post-thermal test periods. The first step was to formulate a model using the field measurements (both before excavation and after excavation) for stress-induced permeability changes (i.e., stress versus permeability or k/σ coupling). The second step was to validate/calibrate the model using experimental results. The last step was to predict future stress changes using the prepared model.

Results used in the validation/calibration process were taken from both laboratory and field k/σ experiments. These data were collected to help identify HM and THM effects versus depth and initial stress. The k/σ relationship was bounded by the intact rock relationship and large unmated shear fractures. Tension fractures were characterized as the mid-point between the two. Various THM experiments plotted at different (vertical stress) locations on this graph. The Yucca Mountain (at ~6 Mpa) was shallow, BMT2 (11–16 Mpa) was deeper, and BMT1 (17-30 Mpa) was deepest. Rutquist noted that at Yucca Mountain, hydraulic conducting fractures are spaced at 0.3 m but that high permeability fractures are spaced at 5 m.

Results from air permeability from YM Niche 3650 studies were used to give measurements of changes in permeability resulting from excavation. An interesting relationship was derived from these measurements. The change in permeability in response to excavation was greatest for fractures with initially low permeability and the least for fractures with initially high permeability.

The SKI THM model has a rectilinear grid. TOUGH2 provides analysis of fluid and heat transport. FLAC3D provides stress/strain analyses. The modeling components are fully coupled, with alternating TOUGH2 and FLAC3D analyses performed at each time step. Permeability is a function of both saturation and stress. Relative gas permeability versus saturation was represented using the Corey relationship.

Changes in permeability were predicted using a thermal-hydrological (TH)-only model and compared with results from the THM coupled model. THM analysis results predicted an increase in permeability in the region above the drift and decreased permeability to the side of the drift. No change in permeability was observed in the TH-only analyses. The THM analysis results were consistent with observed air-permeability measurements.

Rutquist concluded that matching measured air-permeability data is only possible if both saturation and stress-induced changes on permeability are incorporated. Future task objectives include: (1) loss of heat through the bulkhead, (2) incorporating displacement measurements from the extensometers, (3) refinement of the k/σ relationship, and (4) including the effects of cooling.

I presented the status of the NRC/CNWRA team project work. I first discussed the manner in which TH analyses will be loosely coupled with thermal-mechanical (TM) analyses. I then summarized the status of both the TH and the TM analyses. At previous workshops, we had presented temperature predictions using a 2D model with analyses performed using MULTIFLO. These analyses essentially fulfilled Task 2A requirements. During earlier discussions (i.e., at

previous workshop and task group meetings), limitations in the 2D model were noted: (i) three-dimensional heat loss may alter long-term (i.e., 4 yr) temperature predictions and (ii) the boundary condition at the drift wall did not allow for heat and mass loss experienced through the bulkhead. The NRC/CNWRA team decided to enhance the TH model to address these two limitations. The new 3D model with modified boundary conditions was described during the presentation. Temperatures at 3 months, 1 yr, and 3 yrs predicted with the 3D model will be used as input for the TM analyses. The ongoing TM analyses using FLAC 2D will be two dimensional at a vertically oriented plane located 21 m from the bulkhead.

Alain Millard/CEA presented results from earlier reported two-dimensional TM analyses. The analyses were conducted according to the following: (1) modeled a vertical slice perpendicular to the drift axis encompassing the wing heaters, (2) modeled the rockmass as a continuous medium with ubiquitous joints, (3) linear versus non-linear behavior evaluated, and (4) the ubiquitous joints were assumed orthogonal in xyz. The modeled zone was coincident with boreholes 154, 155, and 156 at 21 m from the bulkhead.

Alain Millard noted that IRSN was no longer funded to work on Task 2. Apparently Christophe Grenier/CEA had encountered difficulty in performing the coupled TH analyses within a short time frame. An important note: ISRN was formerly ISPN, a branch of CEA that performed regulatory analysis for the French HLW program. ISRN is now independent of CEA (and ANDRA funding). Millard stated there may be a restructuring in the French research program in the near future that would result in a re-alignment of locations where research is conducted (i.e., to become more centralized).

Three sets of analyses were reported by Millard/CEA: (1) elastic, (2) ubiquitous (elasto-plastic), and brittle. Both the ubiquitous and brittle approaches assumed pre-defined failure directions. A finite-element model was used to predict stress field. Results were displayed as contour plots at 100 and 500 days of the DST.

Conclusions by Millard were: (1) two-dimensional analysis was adequate, (2) measured temperatures should be smoothed, (3) some localized non-linear mechanical effects were observed, (4) more mechanical data are needed to improve computations (i.e., specific joint geometry). The current statistical description of joints is not considered sufficient. DOE representatives, the organization conducting the DST, noted that additional information of this nature was not available.

Chin-Fu Tsang/LBNL gave a presentation representing DOE work on coupled THM effects using results from the niche, the single-heater, and the drift-scale tests. This presentation was also, in part, supportive of Task 4, THM processes and performance assessment. The work was performed in collaboration with Johnny Rutquist. Based on these tests, the following processes are considered important at Yucca Mountain:

Heat transfer:
1 Conduction, convection
2 Counter current

Moisture redistribution
1 Fast vapor transport in fractures
2 Condensation

3 Imbibition into matrix
4 Gravity drainage in fractures
5 Dryout zone from heat
6 Rewetting during cooling

Mechanical

1 Changes in stress/strain
2 Changes in porosity
3 Changes in permeability

The coupled-process conceptual model in fractured rock is treated as a multiphase, non-isothermal, deformable medium. The coupled processes are simulated using TOUGH2-FLAC3D. This code has undergone quality assurance confirmation.

THM modeling entails calibration, process simulation, and calculation of seepage and humidity, the two factors important in performance assessment. The niche studies provided calibration information for this coupling. A key observation from the studies was that if permeability was small, then the increase in permeability after excavation was large. Likewise, if permeability was large, then the increase in permeability was small.

Tsang/LBNL presented drift-scale coupled THM prediction results at 10 and 1000 yrs for two heat loadings. These analyses were conducted with TH-only and THM coupling. Only post-excavation permeability predictions for full THM coupling matched those observed at the niche tests. Results indicated a reduction in both vertical and horizontal permeability near the drift in the short term and a reduction in vertical permeability only in the long term. Tsang summarized the LBL THM analyses:

1 Thermally induced stresses tend to close fractures to a residual value. This reduction and the residual value have potentially important implications to PA,
2 Joint normal stiffness at YM is the second key important factor,
3 Changes in permeability are a function of the initial value of permeability, smaller values of permeability tend to have larger THM-induced changes, and
4 Sensitivity analyses of these processes are planned.

Sebastia Olivella/UPC was not present. Robin Datta/DOE-contractor made a presentation of the status of the ENRESA/UPC project. Olivella et al. have been using their CODE_BRIGHT fully coupled THM model to perform their simulations. Current simulations are two dimension with the medium represented as a single porous medium. The heat source has been reduced by 30 percent to account for three-dimensional edge effects. Olivella had not yet had the opportunity to convert his conceptual model to a dual continuum.

R. Datta/DOE-contractor also provided a brief summary of the pre-test DOE simulations. The simulations were performed at LBNL using TOUGH2 and at LLNL using NUFT.

Task 2D, evaluation of coupled thermal-hydrological-mechanical-chemical (THMC) processes at the DST, has only one participant, JNC. The THMC evaluations are still preliminary at this time. Their interest in THMC stems from concerns with salt accumulation in bentonite buffers. They currently use what they refer to as a primitive THMC code, assembled by coupling THAMES with a mass transport code. They intend to introduce PHREEQUE into the analysis process. The

coupled code is to be used in performance assessment/safety analysis (PA/SA) analyses. R. Datta recommended that the JNC convert bentonite to rock in their model to be more representative of the DST.

R. Datta/DOE-contractor briefly summarized DOE THC modeling efforts lead by Eric Sonnethal and John Apps at LBNL. TOUGH_REACT, a dual continuum, non-isothermal, multi-species, multiphase reaction code, has been used to perform predictions of mineral dissolution and precipitation. Based on the results of these analyses, R. Datta commented that it appears that THC processes are potentially more important that THM processes, particularly over longer periods of time.

Task 2 scheduling was discussed. The draft for the Task 2A report is due to the secretariat on July 31, 2002. The draft for the Task 2B/2C is due to the secretariat on October 31, 2002. There is to be a Task 2 meeting at LBNL on December 3-4, 2002.

Task 4 Session

Johan Andersson/DECOVALEX-Secretariat led a discussion of Task 4, Coupled THM processes and performance assessment. Each task lead was asked to respond to the following PA related questions:

(1) Relevance of the task to the Safety Analysis
    a) how is your work relevant to the SA
    b) are there performance measures, if so, what are they
(2) Significance of couplings
    a) which couplings are important
    b) what is their relative importance
(3) Uncertainty
    a) are there uncertainties, is so, what are they
    b) what is their relative importance

Bill Boyle/DOE responded as follows for Task 2, the DST. His response was based on previous responses by the Task 2 participants: (1a) Task 2 involves the development of a good understanding of heat driven coupled processes. These coupled processes have limited direct impact on performance, however there still remains the need to demonstrate performance through 10,000 yrs. (1b) The performance measures are dose and the nature and quantity of seepage into drifts and their effect on performance. (2) There are no couplings of high significance. The TH coupling is of medium significance. All other couplings are of low significance. (3a) Uncertainties include spatial variability of properties, especially hydrological properties. Additional uncertainty is in the effective inclusion of THM processes and their phenomena. (3b) The relative importance of the uncertainties have not yet been completed. Bounding and sensitivity analyses are needed to assess these uncertainties.

Steering Committee Meeting

I attended the steering committee meeting as an observer in the absence of NRC staff. The steering committee meeting was held at the end of the workshop. There were 24 attendees representing the funding organizations and the Secretariat.

DECOVALEX III funding is secure. There are sufficient funds that the project completion date could be extended until September 2003 to allow its completion to coincide with BENCHPAR. The BENCHPAR project is aimed at improving the THM coupled processes content of radioactive waste repository Performance and Safety Assessments (PA/SA), to provide guidance to the EU Member States on how to improve this aspect of PA. However, it was noted that there is some uncertainty with the cost of report publishing. This uncertainty could result in a shortage of funds by the end of the project. C-F Tsang asked whether the funding organizations would be able to contribute an additional $5-10k to allow extending the project until September 2003 and insure that all publishing costs are met. Most organizations stated a willingness, however several organizations noted that their internal funding levels were already established and that additional funds may be difficult to procure. Task leaders were asked to estimate the number of reports that will be published for each Task and funding organizations were asked to estimate the number of reports they will need. This information is to be provided to the Secretariat. An estimate of final publishing costs is to be prepared by September 2002 to provide the basis for final project costs estimates prior to the next workshop.

All reports are to be completed by September 2003. Final reports are to be published in a special issue of Rock Mechanics. There will be a conference, titled GeoProc, which will target the work conducted as part of DECOVALEX. The conference is scheduled for October 13-15, 2003. There was discussion on how to coordinate the efforts of the special journal issue and the conference proceedings. Ove Stephansson and John Hudson are to resolve this issue.

There was an extended discussion regarding what project will follow the completion of DECOVALEX III. Topical areas of research for a follow-on project were discussed. The list of topics was vast, but the topics were summarized into the following categories: (i) chemical, (ii) shallow storage, (iii) short term-performance confirmation, (iv) long term–classical performance assessment, and (v) glacial. There was discussion that inclusion of chemical coupling into the scope of the project would change the mandate relative to the mandates of the past modeling endeavors (i.e., DECOVALEX, INTRAVAL, etc.). A task force was formed to explore the prospect of a follow-on project. Members to the task force are: Chin-Fu Tsang/LBNL, Les Knight/NIREX, Juan Carlos Mayor/ENRESA, Bill Boyle/DOE, Fritz Kautsky/SKI, Ove Stephansson/DECOVALEX-Secretariat, Johan Andersson/DECOVALEX-Secretariat, and Lanru Jing/DECOVALEX-Secretariat. Funding organizations will be sent the preliminary findings of the task group and asked to respond regarding suggestions and the level of interest by the funding organizations.

In addition, there is an effort under development by the European Union (EU) to coordinate European HLW disposal activities. The proposed endeavor is titled "Development of a THMC Toolbox for HLW disposal in different geologic environments". A draft proposal was submitted by a group of European countries to the EU on June 7, 2002. International participation by groups such as DOE, NRC, Ontario Power Generation (OPG), Canadian Nuclear Safety Commission (CNSC), and JNC is invited, although no interest has yet been indicated. A final proposal will be

due later in the year. Funding of $25M Euros for four years will be requested. None of the funds is anticipated to be allocated to non-European organizations. The steering committee agreed that DECOVALEX will assist in the preparation of the final proposal to the EU and will also continue to develop the potential for a follow-on project similar in scope to DECOVALEX.

The schedule of the next workshop was discussed. The venue will be Berlin, Germany and the dates will be January 27-30, 2003. There will be a field trip on January 31, 2003 to the Gorleben salt mine located near Hanover. There were previous underground investigative studies held at the mine, although all activity is currently halted.

There was discussion whether to coordinate a workshop in June 2003 with two other groups, one of which coordinates all European underground laboratories and the other is BENEPAR (performance assessment of the Spanish HLW program). The coordinated workshop would be sponsored by ENRESA and would probably be held in Spain. Further discussion of this coordinated workshop was tabled until the January workshop. There would also probably be a final DECOVALEX workshop held in conjunction with the GeoProc conference in October, 2003.

SUMMARY OF ACTIVITIES: I made a presentation that summarized the status and progress of DECOVALEX III modeling activities performed at CNWRA. I attended the DECOVALEX Steering Committee meeting as a non-voting participant in the absence of M. Nataraja, the official NRC representative to DECOVALEX III.

CONCLUSIONS: Participants to the DECOVALEX III project are making greater progress toward modeling goals compared with the first years of the project. With respect to Task 2 (modeling the DST), this is mostly due to recent advances in the codes used to model coupled THM processes. Comparison of final modeling results generated during the final year of the project will provide evidence to enable evaluation of the conceptual models used to assemble the models.

PROBLEMS ENCOUNTERED: None

PENDING ACTIONS: The upcoming conclusion of DECOVALEX requires that all participating teams complete their analyses sufficiently early to be included in project summary documents. The NRC/CNWRA team needs to schedule future activities to ensure these deadlines are met.

RECOMMENDATIONS: It is recommended that NRC/CNWRA continue their participation in DECOVALEX III and review the proposed follow-on project before deciding to participate in it. The modeling and analysis exercise provides an opportunity to critically compare numerical simulation results with other state-of-the-science coupled modeling codes. The NRC/CNWRA program can benefit from the advances of other national programs that address similar challenges facing the proposed repository at Yucca Mountain. Continued increased interest in THMC processes in unsaturated media by the French, Japanese, and Spanish teams increases the level of active interaction among research teams. This high level of interaction was not previously possible when the sole interest of other national HLW programs was restricted to saturated zone settings.

SIGNATURES:

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7/12/02
Date

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