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# CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

## TRIP REPORT

**SUBJECT:** DECOVALEX III Workshop III (20.01402.671)

**DATE/PLACE:** January 22–27, 2001
Mito, Japan

**AUTHOR:** Ronald T. Green

**DISTRIBUTION:**

**CNWRA**

W. Patrick
CNWRA Directors
CNWRA Element Managers
S. Hsuing
M. Hill
G. Ofoegbu
A. Ghosh
B. Dasgupta
D. Hughson

**NRC-NMSS**

J. Linehan
D. DeMarco
E. Whitt
B. Meehan
J. Greeves
J. Holonich
W. Reamer
K. Stablein
D. Brooks
M. Nataraja
J. Pohle
B. Jagannath

**SwRI Contracts**

T. Nagy (Contracts)
P. Maldonado

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**PERSONS PRESENT:** See attached list of participants.

## BACKGROUND AND PURPOSE OF TRIP:

The purpose of the trip was to participate in the third 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 results and plan future activities. Two new teams have joined the DECOVALEX III Project, Commisariat a l'Energie Atomique (CEA) and the German Federal Institute of Geosciences and Natural Resources (BRG), bringing the total number of teams to 15.

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 characterization information, 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. DOE has provided a description of the DST, characterization information, and stated what test result data are available; however, the test measurement data have not been disclosed to the DECOVALEX III Project. Typically, not all DECOVALEX teams participate in all Tasks.

## SUMMARY OF PERTINENT POINTS:

The workshop was organized into two days of task force meetings prior to three days of presentations and discussions following the structure of the DECOVALEX III Project and a one-day field trip to the Tono Geosciences Center. There are four Tasks in DECOVOLEX III: Task 1—FEBEX *in situ* experiments; Task 2—Yucca Mountain drift-scale test; Task—three benchmark tests (BMT) (BMT 1—resaturation, BMT 2—upscaling and homogenization, BMT 3—glaciation); and Task 4—forum and questionnaire on THM processes in performance assessment. NRC direct participation is limited to Tasks 2 and 4; however, comments on other Tasks are included in this report.

Opening remarks included a discussion of the DECOVALEX organization and introduction to the Japanese High-Level Waste (HLW) program. The Japanese HLW program consists of several research sites and candidate sites for long term disposal. The Kamiashi mine is the location of a crystalline rock underground research laboratory (URL). The Tono mine is the site of a sedimentary URL and is also a candidate for a crystalline (granite) HLW repository. The Horonobe site on Hoddiake Island is the candidate site of a sedimentary (bentonite clay/mudstone) repository. Construction at the Horonobe URL has been approved, but has not started. The field trip conducted as part of the DECOVALEX III workshop was to the Tono Mine URL at the Tono Geosciences Center.

There has been a reorganization in the Japanese HLW program with the passage of the Specified Radionuclide Waste Disposal Act in June 2000. The act resulted in the establishment of a new group, called Nuclear Waste Management Organization of Japan (NUMO) in October 2000, split from the Japan Nuclear Cycle Development Institute (JNC). NUMO will be responsible to implement the siting, license application, organization, and construction of the HLW repository. JNC will retain responsibility of the research components of the Japanese HLW program. It will be a challenge to identify a suitable site with respect to seismic and volcanic activity. The Japanese performance assessment assigns only 1,000 yr to the expected design duration of the engineered barrier system (EBS) overpack assembly. Regulatory overview has not yet been incorporated into the Japanese HLW program. There appears to be an intention to include this component in the future. The Japanese program hopes to have their HLW site selected by 2015 and in operation by 2032.

The DECOVALEX Secretariat announced that a second French team and a German team have been accepted into the DECOVALEX III project. The French team, representing CEA, joined in response to recent developments in the French HLW program to include interim storage in unsaturated consolidated media. This program modification has prompted interest by the French team in Task 2, THM analysis of the DST at Yucca Mountain.

Manfred Wellner represented BRG, the German team. Recent developments in the German program have encouraged their participation in DECOVALEX III. The German HLW program had earlier been committed to a salt medium. This commitment has been revoked. Consequently, until the medium of choice is selected by the German program, their interest has been broadened to include other potential media settings. The use of clay as the host medium or as a buffer material is now under consideration. Although none of the DECOVALEX III tasks have clay as the host medium, bentonite is used as the backfill or buffer material in Task 1, FEBEX, and BMT1, Kamiashi mine experiments.

**Task 1—FEBEX Mine Experiment**

Task 1 is the examination of the FEBEX *in situ* experiment at the Grimsel Test Site. A project status of the multi-national team working on FEBEX was made by J. Audstillo/ENRESA. A summary of the test was presented by F. Kautsky/Swedish Nuclear Power Inspectorate (SKI), managing director. The objectives of the FEBEX project are to understand (i) the EBS, (ii) THM processes, and (iii) thermal-hydrologic-chemical (THC) processes. The DECOVALEX III Task 1 update was given by E. Alonso of the Universidad Politecnica de Catalunya (UPC), the managing organization of Task 1. The objective of this set of analyses was to predict total inflow and pressure that was measured in a borehole near the heater canisters. Only two of the nine teams participating in Task 1 provided predictions of THM processes in time for preworkshop comparison, although the remaining teams presented prediction results at the workshop. The participants were asked to predict (i) the rate of water flow at one point in the tunnel, and (ii) water pressure in a borehole near the FEBEX tunnel as a result of excavation of the tunnel. The SKB results were very close (i.e., within 2 percent) to those measured by ENRESA. Results by all others varied by as much as one order of magnitude from the measured values. The approaches by the different teams varied considerably. Some teams used the characterization data explicitly. Other teams calibrated their models by allowing some data to vary while other data were held constant. This methodology was useful, particularly for data that appeared to be disparate.

L. Borgensson/Clay Technology AB presented results from the SKB team. The code ABAQUS was used in his analyses. The code was three dimensional and contained about 17,000 elements. Excavation of the FEBEX tunnel was discretized into nine steps. As mentioned, the SKB team results were within a few percent of the experimental measurements.

L. Costin/Sandia National Laboratories (SNL) presented the predictions by the DOE team. Their prediction was predicated on one-coupling on the mechanical effect on permeability, then the hydrological calculation was conducted. They used JAS3D to calculate the mechanical effect due to excavation. The DOE team then used TOUGH2 to make the hydrological calculation. Costin noted that his team would prefer to perform the fully coupled THM calculation using the coupled simulators ROCMAS/TOUGH2 rather than the decoupled calculations made using JAS3D and TOUGH2.

A. Rejeb/ISPN presented results for the ANDRA team. They employed interactive coupling of HYDREF to calculate pressures and VIPLEF to calculate mechanical stress. Only a few interaction couplings were required. The excavation was performed in four steps. Their results were sensitive to the orientation of the specified *in situ* stress field.

J. Rutqvist/Lawrence Berkeley National Laboratory (LBNL) presented results for the SKI team. ROCMAS was used for the analyses but only hydrologic-mechanical (HM) analyses were completed at this time. His prediction of stress (a decrease) was opposite of what was observed at FEBEX. There was an extensive discussion of the location of the measurement borehole relative to the location of the excavated tunnel, in particular, was the borehole located in a zone of compression or extension? Apparently, the borehole is located in the transition area between the two stress zones. Rutqvist noted that he needed to modify the *in situ* stress field to attain sign agreement. Other teams, most notably ANDRA, commented they encountered the same problem.

E. Alonso predicted total water inflow values close to values observed. Alonso noted that a three-dimensional (3D) fully coupled HM model is required to predict the evolution of the pore water pressure. One way coupling between hydrology and mechanical processes was assumed. Alonso noted that pore water pressure increases may be explained by 3D stress redistribution due to excavation. Consistent with Rutquist and Regel, he also noted that the orientation of the anisotropic stress field has influence on the pore water pressure evolution. Decreases in pore water pressure may be explained by dissipation in pressure due to the permeability of the host rock. In particular, the evolution in pore water pressure observed at point P4 (with low permeability) was not observed at point P3 (with high permeability). Alonso feels this interpretation requires additional analysis.

The next phase of Task 1, THM analysis of the bentonite backfill material of the FEBEX experiment, is to be initiated at the conclusion of this workshop.

**Task 2—Yucca Mountain Drift-Scale Heater Test**

DECOVALEX III Task 2, the DST, was discussed during the Task 2 Working Group meeting and during a formal session of the DECOVALEX III workshop. Following summaries synthesize the discussions from both sessions. R. Datta/CRWMS M&O provided a status report on the DST. Included in his report was a summary of the test design, construction, and operation to date. Heating power was reduced in March 2000 and again in May 2000 by 5 percent and in August 2000 by 3 percent to ensure that drift wall temperatures do not exceed 200 °C. Both the heater drift canisters and the inner and outer wing heaters were reduced at these times. This procedure is consistent with the pretest heating plan. R. Datta noted that the chemistry holes have not provided adequate chemistry data and that they have initiated a procedure to sample chemical alteration of rock near the heaters by side-wall sampling of rock from the boreholes. Results are not yet available from this sampling program. R. Datta responded to a question that heat flow by conduction through the 3- to 4-m long rock bolts has been dismissed, although the effect has not been explicitly modeled. L. Costin/SNL commented that heat flow by conduction through the rock bolts can be dismissed without explicit modeling because current models which neglect this effect have effectively replicated measured temperatures. R. Datta announced that a draft report for Task 2/DST activities is due from all team members by March 31, 2001.

The evolution of modeling heat and mass transfer through partially saturated fractured porous medium, with application to the DST, was summarized by R. Green/CNWRA at the task group meeting. The summary included a discussion of the evolution of the equivalent continuum model, the dual continuum model, and the active fracture model conceptualizations.

S. Olivella/UPC Spain described the development of the Spanish program to model the DST. Early attempts centered on a single continuum model of the single heater test. The name of his code is BRIGHTCODE. His model includes full coupling of THM processes, although infiltration at the upper boundary has not yet been incorporated. Fractures are to be represented with either the cubic law or an exponential law (to relate permeability to fracture aperture), or the Kozeny equation, which relates permeability to porosity. Early simulations by S. Oviella predicted a reduction in bulk porosity from 0.11 to 0.104 percent due to heating.

It was the intention by S. Oviella to extend the model to include two continua, matrix and fracture, under thermodynamic equilibrium conditions. In subsequent discussions during the task force meeting, he stated that his revised intention was to include the two continua, but not assume thermodynamic equilibrium. If so, BRIGHTCODE would have capabilities similar to MULTIFLO, TOUGH2, and NUFT with regard to dual continua conceptualization.

The CEA team represented at the workshop consisted of C. Grenier and E. Castilier and is led by S. Tillard. CEA joined DECOVAELX III as a result of the recent French decision to consider interim HLW storage in the unsaturated zone. The period of interim storage is unspecified, but could last as long as 30 yr. S. Tillard presented a summary of the recently formulated French program for the CEA to investigate heat and mass transport in the unsaturated zone. Final administrative approval of the proposed program is expected in May 2001 to ensure the preprogram is in place by the required date of 2006.

The CEA program, as envisioned, consists of theoretical investigations supported by nonisothermal laboratory- and field-scale experiments. The proposed testing program consists of a series of as many as five laboratory-scale experiments and three field-scale experiments in Cadrache, France. The laboratory-scale tests are to use silica sand for the media with a duration of one month each. R. Green noted difficulties experienced with using $SiO_2$ as test media under non-isothermal conditions and difficulties encountered when attempting to draw conclusions from experiments that do not attain steady state. The CEA team expressed interest in the CNWRA laboratory non-isothermal testing program and requested copies of relevant publications. The CEA program has planned two field-scale experiments for the vadose zone and one below the water table.

C. Grenier is the lead modeler of the CEA team. Current efforts have been to simulate the exploratory studies facility (ESF) single-heater test (SHT) using a mixed hybrid finite-element single continuum version of the CEA code, CASTEM, using the IDEAS mesh generator. C. Grenier has not yet included full THM coupling and is curious to see results of other modelers to determine whether full coupling of all three processes is necessary. At this time, C. Grenier has concerns with heat source homogenization and errors in meshing. Grenier stated that CEA wants to make some advancement with the SHT prior to addressing the DST.

J. Rutqvist presented the results of the SKI team on modeling the DST. It was his original plan to model the thermal-mechanical effects at the DST, however he modified his approach to use ROCMAS to simulate the entire THM coupled process. According to J. Rutqvist, ROCMAS is adequate to simulate sub-boiling nonisothermal problems, but does not include transport of gas by pressure gradients. J. Rutqvist used results from the ESF niche studies to establish the reduction in permeability that might be expected in the region above the area excavated relative to the area lateral to the excavated opening. In the niche studies, a 10- to 1000-fold reduction in permeability was experienced above the niches in contrast to no reduction in permeability to the side of the excavated niches.

R. Green presented the current status of the NRC/CNWRA team progress on modeling the DST. The NRC/CNWRA team was the only one to present actual thermal-hydrologic (TH) predictions of the DST. Green presented predictions of temperature at one year of heating. The results of sensitivity analyses were also reported. The effects of variations in infiltration rate, block size, and matrix/fracture interaction factor on ambient saturation were discussed. Once the basecase properties were identified, an additional sensitivity analysis was performed to assess the effect of changes in fracture permeability, thermal conductivity, matrix/fracture interaction factor, and the active fracture model conceptualization on TH predictions. The analysis results indicated that changes in the matrix/fracture interaction factor and the active fracture model had a minimal effect on temperature and saturation predictions. TH analyses, however, were somewhat sensitive to changes in thermal conductivity and significantly affected by changes (reductions) in fracture permeability. Temperature predictions were not compared with measured temperatures at the request of the Task 2 sponsor DOE.

M. Yui/JNC announced that JNC has not yet received approval to initiate modeling of the THCM component of the DST, but that approval is anticipated in FY01. JNC has interest in the generic problem of THCM processes between a bentonite buffer and an unspecified host rock in the presence of heat and moisture. They have interest in the DST because buffer materials are expected to remain unsaturated for long periods of time when heated. M Yui said that the JNC program would follow the approach of Glassley/LBNL at least at the onset of their analyses. M. Yui presented generic results which suggest a decrease in porosity/permeability may form from silica deposition in the area above the DST heater horizon. The JNC analyses are calculated using PREEQUE and a thermodynamic data base assembled by Yui.

**Task 3—Benchmark Tests (BMT)**

<u>BMT 1—Resaturation</u>

S. Nguyen/Canadian Nuclear Safety Commission is the lead of the BMT 1. The test site for BMT 1 is the Kamiashi mine experiment completed in 1998. In the first phase of the exercise, virtually all teams over-predicted resaturation of the bentonite overpack, when in reality, the overpack resaturated much more slowly. The next phase of the test will be to calibrate the models using limited data and then use the models to predict temperature, saturation and stress at locations different from those specified during the first phase.

BMT 2—Homogenization (Upscaling)

The Sellafield Site in England is used for the upscaling test. Unfortunately, subsequent to selection of Sellafield as the test site, the planned field-scale experiments were canceled, depriving the team participants of actual physical data. Teams were asked to calculate arrival time statistics for particles released from the proposed repository at three different times. Ground surface is the compliance boundary. Three performance measures for upscaling are identified: groundwater flux, transport time, and transport resistance (defined as the inverse of volumetric flux integrated over space). L. Costin/SNL reported that the DOE team will use sequential coupling (after each time step) of TOUGH2 and FLAC to finish complete upscaling. J. Gomez-Hernandez/University of Valencia reported for ENRESA results for a traditional upscaling using geometric averaging. He noted that increasing the block size from 5 m × 5 m to 100 m × 100 m reduced arrival times by half. Other teams are still performing calculations.

**Task 4—THM in Safety and Performance Assessment Applications**

J. Andersson discussed the current draft for Task 4. Participating team members (including DOE and NRC) have contributed responses to a questionnaire originally prepared by Andersson. The objective of the task is to build confidence in the linkage between thermal-hydrologic-mechanical-chemical (THMC) and performance assessment (PA). Andersson noted that the most current features, events, and processes (FEPs) of interest by the DECOVALEX III exercises address buffer materials and the host rock. He suggested that the FEPs also include overpack and some other aspects. Andersson broke PA into a short-term (< 100 yr up to 1,000 yr) period to develop monitoring to confirm modeling and prediction that was used in PA and a long-term period evidenced by degradation of the EBS and host rock and their effects on radionuclide migration.

J. Andersson included the following in monitoring: quality control, active control, surveillance, remedial work, passive control, and land use. He stated that the challenge of monitoring is to confirm that changes in the geotechnical environment are within acceptable limits. Monitoring should target all three zones of a repository: EBS, disturbed zone, and virgin zone.

L. Knight/NIREX noted that the first 100 yr after emplacement are becoming much more important to most national programs to support the credibility of the long-term predictive capabilities. C-F. Tsang/LBNL added that Carlsbad has a long-term tiered monitoring plan in effect. L. Knight also noted that failure criteria be identified at the onset on monitoring, otherwise, there will be possible indecision if surprise data are encountered.

The final Task 4 report will be initiated by participating teams in the Spring of 2001.

**SUMMARY OF ACTIVITIES:**

The NRC/CNWRA team participated in the Task 2 task force meeting, the full workshop, and the site visit to the Tono Geoscience Center. Many additional discussions were held, mostly with teams representing France and Spain during the week.

**Tono Geoscience Center Visit**

The Tono mine at the Tono Geoscience Center was visited on the Saturday following the workshop. The visit was hosted by JNC, the proprietor of the Tono Geoscience Center. The technical objectives of the Tono

Geoscience Center are to (i) characterize the subsurface of the site, (ii) investigate the long-term stability of the site, and (iii) develop techniques and tools to acquire data on the geological environment. There are two underground facilities at the Center—the existing Tono Mine URL in sedimentary rock overlying granitic basement rock and the planned Mizunami URL to be constructed entirely in granitic rock. Both are located next to the Tono Geoscience Center surface facilities. Current research in the Tono Mine URL includes measuring the effects of drill and blast versus boom header excavation methods, migration of U through sedimentary rock using packed off boreholes, monitoring groundwater stress and chemistry as seismic precursors, and analysis of groundwater flow through fractured crystalline rock. Research planned for the Mizunami URL includes fundamental investigation of rock and groundwater processes at depth, earthquake research, and additional studies such as a micro-gravity laboratory and research relevant to constructions on the moon.

**CONCLUSIONS:**

Developments in the German, French, and Spanish HLW disposal programs have led to increased interest in technologies developed to investigate heat and mass transfer at the proposed HLW repository at Yucca Mountain. The CEA contingent from France is particularly interested in past research and analysis activities at CNWRA because of the similarity of the newly defined French interim program to store waste in the vadose zone with the geologic setting of Yucca Mountain. The teams from Germany and Spain have increased interest in heat and mass transfer through partially saturated porous media because of uncertainty in the selection and design of their repositories.

**PROBLEMS ENCOUNTERED:**

None.

**PENDING ACTIONS:**

CNWRA publications documenting past investigations of heat and mass transfer through partially saturated porous media were requested by the French CEA team. The Spanish team requested copies of CNWRA publications that document the use of natural analogs in PA.

**RECOMMENDATIONS:**

It is recommended that the NRC/CNWRA continue their participation in DECOVALEX III. The modeling and analysis exercise provides an opportunity to critically compare numerical simulation results to a well-controlled, structured field-scale experiment. The NRC/CNWRA program can benefit from the advances of other national programs that address similar challenges facing the proposed repository at Yucca Mountain. Increased interest in THMC processes in unsaturated media by the French 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:**

Ronald T. Green, Principal Scientist
Geohydrology and Geochemistry

2/21/01
Date

**CONCURRENCE:**

Asad Chowdhury, Manager
Mining, Geotechnical, and Facility Engineering

2/22/2001
Date

Budhi Sagar
Technical Director

2/22/2001
Date

**ATTACHMENT**

# List of Participants

## DIII Workshop in Tokai, Japan, 22-27 January 2001
(Updated 2001-02-09)

Kiyoshi Amemiya.
Hazama Corporation
Nuclear Power Department
Kita-Aoyama 2-5-8, Minato-Ku, Tokyo, 107-8658, Japan
Tel: +81-3-3405-1124, Fax: +81-3- 3405-1814
amem@hazama.co.jp

Jordi Alcoverro
Universidad Politecnica de Catalunya, UPC
Civil Engineering School
Jordi Girona, 1-3 D2
08034 Barcelona, Spain
Tel: +34-93-4017248, Fax: +34-91-4017251
jordi.alcoverro@upc.es

Eduardo Alonso
Universidad Politecnica de Catalunya, UPC
Dep. de Ingenieria del Terreno
Jordi Girona, 1-3, Mod. D2,
08034 Barcelona , Spain
Tel: +34-93-401 68 62, Fax: +34-93-401 72 51
eduardo.alonso@upc.es

Johan Andersson
JA Streamflow AB
Korta gatan 7
171 54 Solna, Sweden
Tel: +46-70-622 21 32, Fax: +46-8-562 00 350
johan.andersson@streamflow.se

Philipp Blum
School of Earth Science
University of Birmingham
Edgbaston, Birmingham B15 2TT, UK
Tel:_+44-121-414-6165
pxb057@bham.ac.uk

William Boyle
U.S. Department of Energy (DOE)
Yucca Mountain Site Characterization Office
P.O. Box 30307
North Las Vegas, NV 89036-0307, USA
Tel: +1-702-794-5506, Fax: +1-702-794-5559
william_boyle@notes.ymp.gov

Lennart Börgesson
Clay Technology AB
Ideon Research Center
SE-223 70 Lund, Sweden
Tel: +46-46-286-2573, Fax: +46-46-134 230,
lb@claytech.se

Etienne Castelier
CEA CADARACHE
SAMRA/LGEM
Batiment 307
131 08 St Paul lez Durance, France
Tel: +33-4 42 25 62 44, Fax: +33-4-422532 06
etienne.caselier@cea.fr

Tin Chan
Atomic Energy of Canada (AECL)
C/o Ontario Power Generation (OPG) H16 E22
700 University Avenue
Toronto, Ontario, Canada M5G 1X6
Tel: +1-416-592-5296, Fax: +1-416-592-4485
chant@aecl.ca

Masakazu Chijimatsu
Hazama Corporation
Nuclear Power Department
Kita-Aoyama 2-5-8, Minato-Ku, Tokyo, 107-8658, Japan
Tel: +81-3-3405-1124, Fax: +81-3- 3405-1814
mchiji@hazama.co.jp

Rolf Christiansson
SKB
Pl 300
SE-572 95 Figeholm, Sweden
Tel: +46-491-767 802, Fax: +46-491-82005
rolf.christiansson@skb.se

Laurence Costin
Sandia National Laboratories
P O Box 5800.MS 0751
Albuquerque NM 87185, USA
Tel: +1-505-844 3367, Fax: +1-505-8447354
lscosti@sandia.gov

Robin Datta
Yucca Mountain Project, CRWMS M&O
1261 Town Center Drive
Las Vegas, NV 89134, USA
Tel: +1-702-295-5070, Fax: +1-702-295 3554
robin_datta@ymp.gov

Tomoo Fujita
Nuclear Waste management Organization of Japan (NUMO)
Shiba 4-1-23, Minato, Tokyp 108-0014, Japan
Tel: +81-3-4513-1513, Fax: +81-3-4513-1599
tfujita@numo.or.gp

Antonio Gens
Universidad Politecnica de Catalunya
Dep. de Ingenieria del Terreno
Jordi Girona 1-3 Edificio D-2
ES 08034 Barcelona, Spain
Tel: +34-93-401 6867, Fax: +34-93-401 7251
antonio.gens@upc.es

Jaime Gomez-Hernandez
Universidad Polítechnica de Valencia
Ingenieria Hidráulica Medio Ambiente
Camino de Vera Sin
46022 Valencia, Spain
Tel: +34-96-387 9614, Fax: +34-96-387 7618
jaime@dihma.upv.es

Ron T. Green
Center for Nuclear Waste Regulatory Analyses (CNWRA)
Southwest Research Institute
6220 Culebra
San Antonio, TX 78238, USA
Tel: +1-210-522-5305, Fax: +1-210-522-5184
rgreen@swri.edu

Christophe Grenier
Commisariat a l'Energie Atomique, CEA
Centre de Saclay
DRN/DMT/SEMT/MTMS
91191 Gif sur Yvette Cedex, France
Tel: +33-1-6908 9362, Fax: +33-1-6908 5242
christophe.grenier@cea.fr

Akira Ito
Japan Nuclear Cycle Development Institute (JNC)
Tokai works
Waste Management and Fuel Cycle Research Center
Waste Isolation Research Division
Barrier Performance Research Group
4-33, Muramatsu, Tokai-mura, Ibaraki, 319-1194, Japan
Tel: +81-29-287-3247, Fax: +81-29-287-3704
ito57@tokai.jnc.go.jp

Lanru Jing
Royal Institute of Technology
Engineering Geology
Teknikringen 72
SE-100 44 Stockholm, Sweden
Tel: +46-8-790-7053, Fax: +46-8-790 6810
lanru@aom.kth.se

Fritz Kautsky
SKI
SE-106 58 Stockholm
Sweden.
Tel: +46-8-698-8487, Fax: +46-8-661.9087
fritz@ski.se

Leslie Knight
NIREX
Curie Avenue
Didcot, Oxon, OX11 ORH, United Kingdom
Tel: +44-01235 825 447
les.knight@nirex.co.uk

Akira Kobayashi
Kyoto University
Graduate School of Agricultural Science
Div. of Science and Technology on Regional Environment
Kita-Shirakawa Oiwake-cho, Sakyo-ku
Kyoto 606-8502, Japan
Tel: +81-75- 753 6152, Fax: +81-75-753 6346
kobadesu@relief.kais.kyoto-u.ac.jp

Hiroshi Kurikami
School of Civil Engineering
Kyoto University
Kyoto 606-8501, Japan
Tel: +81-75-753 5127, Fax: +81-75-753 5129
Kurikami@geotech.kuciv.kyoto-u.ac.jp

Juan Carlos Mayor
ENRESA
Emilio Vargas 7
28043 Madrid, Spain
Tel: +34-91-566-82 17, Fax: +34-91-566 81 65
jmaz@enresa.es

Ki-Bok Min
Royal Institute of Technology
Engineering Geology
Teknikringen 72
SE-100 44 Stockholm, Sweden
Tel: +46-8-790-7067, Fax: +46-8-790 6810
kibok@aom.kth.se

Mysore Nataraja
US Nuclear Regulatory Commission
Mail stop 7-C-6, Two White Flint North
115 45 Rockville Pike
Rockville, MD 20852.2738, USA
Tel: +1-301-415-6695, Fax: +1-301-415-5398
msn1@nrc.gov

Son Nguyen
Canadian Nuclear Safety Commission, CNCS
P O Box 1046, Station B
280 Slater Street
Ottawa, Ontario, Canada K1P 5S9
Tel: +1-613-996-1436
nguyens@cnsc-ccsn.gc.ca

Auli Niemi
University of Uppsala
Dept of Earth Sciences
Villavägen 16
S 752 36 Uppsala, Sweden
Tel: +46-18-4712263, Fax: +46-18-551124
auli.niemi@geo.uu.se

Sebastia Olivella
ETSECCPB
Universidad Politecnica de Cataluna
Dep. de Ingenieria del Terreno
Jordi Girona 1-3, Campus Nord, Bldg/módulo D2
ES 08034 Barcelona, Spain
Tel: +34-93-401 7253, Fax: +34-93-401 72 51
sebastia.olivella@upc.es

Yuzo Ohnishi
Civil Engineering Systems
School of Civil Engineering
Kyoto University
Kyoto 606-8501, Japan
Tel: +81-75-753 5127, Fax: +81-75-753 5129
ohnishi@geotech.kuciv.kyoto-u.ac.jp

Amel Rejeb
IPSN/DPRE/SERGD
60-68 Avenue General Leclerc
BP 6
Fontenay-aux-Roses, FR 922 65, France
Tel: +33-1-465 480 09, Fax: +33-1-473 514 23
amel.rejeb@ipsn.fr

Jonny Rutqvist
Lawrence Berkeley National Laboratory (LBNL)
Earth Sciences Division, MS 90-1116
1, Cyclotron Road
Berkeley, CA 94720, USA
Tel: +1-510-486-5432, Fax: +1-510-486-5686
jrutqvist@lbl.gov

Ove Stephansson
Royal Institute of Technology
Engineering Geology
Teknikringen 72
SE-100 44 Stockholm, Sweden
Tel: +46-8-790 7906, Fax: +46-8-790 6810
ove@aom.kth.se

Hiroyuki Sugino
Japan Nuclear Cycle Development Institute (JNC)
Tokai works
Waste Management and Fuel Cycle Research Center
Waste Isolation Research Division
Barrier Performance Research Group
4-33, Muramatsu, Tokai-mura, Ibaraki, 319-1194 , Japan
Tel: +81-29-287-3247, Fax: +81-29-287-3704
sugino@tokai.jnc.go.jp

Yutaka Sugita
Japan Nuclear Cycle Development Institute (JNC)
Tokai works
Waste Management and Fuel Cycle Research Center
Waste Isolation Research Division
Barrier Performance Research Group
4-33, Muramatsu, Tokai-mura, Ibaraki, 319-1194 , Japan
Tel: +81-29-287-3247, Fax: +81-29-287-3704
sugita@tokai.jnc.go.jp

Sylvie Tillard
CEA CADARACHE
SAMRA/LGEM
Batiment 307
131 08 St Paul lez Durance, France
Tel: +33-4 42 25 35 88, Fax: +33-4-42 25 62 72
sylvie.tillard@cea.fr

Chin-Fu Tsang
Lawrence Berkeley National Laboratory (LBNL)
ESD, MS 90-1116
1, Cyclotron Road
Berkeley, CA 94720, USA
Tel: +1-510-486-5782
cftsang@lbl.gov

Manfred Wallner
Federal Institute for Geosciences and Natural Resources, BGR
Stilleweg 2
D-30655 Hannover, Germany
Tel: +49-511-643 2422, Fax: +49-511-643 3694
manfred.wallner@bgr.de

Mikazu Yui
Japan Nuclear Cycle Development Institute (JNC)
Tokai works
Waste Management and Fuel Cycle Research Center
Waste Isolation Research Division
Barrier Performance Research Group
4-33, Muramatsu, Tokai-mura, Ibaraki, 319-1194 , Japan
Tel: +81-29-287-1540, Fax: +81-29-287-3704
yui@tokai.jnc.go.jp

Johan Öhman
University of Uppsala
Dept of Earth Sciences
Villavägen 16
S 752 36 Uppsala, Sweden
Tel: +46-18-4717166, Fax: +46-18-551124
johan.ohman@hyd.uu.se