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CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

TRIP REPORT
October 30, 1990

SUBJECT: FIFTH INTRAVAL WORKSHOP
(Account No. 20-3704-051)

DATE AND PLACE: Cologne, Germany
October 15-19, 1990.

AUTHOR: Budhi Sagar

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CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

TRIP REPORT

SUBJECT: FIFTH INTRAVAL WORKSHOP

DATE AND PLACE: Cologne, Germany
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AUTHOR (S): Budhi Sagar

PERSONS PRESENT:

Participants came from several countries, principally from Western Europe, Canada, U.S.A., and Japan. A list of participants is attached. Traditionally, the host country (Germany for this workshop) has different people attending parts of the meeting at various times. Since the host country provides the chairman for the workshop, Peter Bogorinski of GRS was the chairman of this workshop.

AGENDA:

A copy of the agenda is attached. The workshop lasted five days (October 15 - 19, 1990), and was preceded by field trips to Konrad Mine on October 11, and the Asse Mine on October 12. Although I did not participate in these field trips, Tom Nicholson and Tim McCartin from NRC did attend both field trips.

SUMMARY OF PERTINENT POINTS:

Phase I of Intraval came to an end with this workshop and Phase II, to continue till 1993, was launched. Plans for completing the final report for Phase I were laid out in detail along with schedules. The final report from Phase I is expected to be printed in the Spring of 1992.

With the completion of Phase I, the VOIC was dissolved.

J. Andersson with the Secretariat re-articulated the objective of Intraval. Specifically, he said that the objective is to obtain basic understanding of flow and transport processes and not to validate specific models. This emphasis on "...not to validate specific models" in defining the objective may be the outcome of the difficulties faced in Phase I.

The next Intraval workshop will be held in Seattle, Washington from April 22-26, 1991.

Working Group 1 with Tom Nicholson in the lead will deal with the unsaturated test cases. Both the Las Cruces trench experiment and the Arizona Apache Leap experiments were retained for Phase II. In addition, the Canadian Twin Lake experiments at the Chalk River Laboratory were added to the preview of Working Group 1.

REPORT SUMMARY:

October 15, 1990

The workshop was opened by W. Thomas of GRS who gave a brief overview of the state of nuclear power and waste management in the Federal Republic of Germany. No new nuclear plants have been constructed in Germany since 1982. Germany produces about 500 tons of spent fuel every year. Reprocessing of part of spent fuel in France is included in the waste management strategy. Two sites are being investigated for HLW -- The Konrad Mine and the salt dome of Gorleben. Two shafts have been sunk at Gorleben salt dome. One of these was completed to the top of the salt dome. Because of recent elections in the region, the second shaft will be stopped at 345 meters as the Green party, a coalition partner in the new government is opposed to the site. Thomas' paper is attached.

J. Andresson from the Intraval secretariat indicated that a draft of the Phase I report will be ready by the spring of 1991 and the final report will be printed by the spring of 1992. For Phase II, it was recognized that validation is a difficult subject and to make advances one has to follow the entire problem, i.e., from the experimental stage to the modeling stage. To accomplish this, resources may have to be pooled in the second phase.

Each working group leader presented his report. Main points of these are summarized later (see reporting for October 18). A number of presentations on Phase I results that were submitted late were also made.

Steve Liew with CEC discussed plans to update a directory of available computer programs for assessing the HLW disposal in geologic formations. He encouraged INTRAVAL participants to send information about their programs for inclusion in the directory.

October 16, 1990

Phase I working groups met separately to review contributions of various teams to the draft report. I participated in Working Group 4, which was comprised of the unsaturated flow test problems and had the majority of the U. S. participants. The other working group with considerable participation from the U. S. was the one dealing with the salt related problems.

The entire day was spent in reviewing the first draft of the Working Group 4 report. Major revisions to the report were

suggested. Assignments for these revisions were made. Mr. Charlie Voss (Fax 206-882-5498, tel. 206-883-0777) at Golder Associates will be the coordinator for completion of the report. Major contributions for the report will come from the participants from the University of Arizona (Dan Evans and his group), New Mexico State University (Richard Hill and his group), the U.S.G.S. (Alan Flint and his coworkers), and the CNWRA (primarily Rachid Ababou). Rachid is to add a paragraph on BIGFLOW in Section 4.2. Contributors are to fax revised contributions to Charlie Voss by November 7. I agreed to write some general sections of the report also. A meeting of the main writers may be held in Las Vegas in early December, 1990. Draft copy of the Phase I report (without the appendices) is attached.

Alan Flint of USGS discussed some interesting aspects of measuring moisture content in the field. He contrasted the measurements from cores with those from in-situ neutron probes. Since the effective volume averaged by the neutron probe is considerably larger than the volume sampled in the cores, the saturation measurements looked very different even though both the measurements represented the same location. Through this example he was cautioning future investigators about interpretation of data. He was going to present a paper on this issue in a NEA workshop to be held in Paris in the week of October 22. A copy of this paper was obtained and is attached.

Linda Lehman from the State of Nevada submitted her critique of the INTRAVAL exercises. She wanted it to be included as an appendix to the Phase I report. However, since the appendices will include details of actual calculation, it was decided not to include it as a separate appendix, but to incorporate appropriate comments in the body of the report. In light of the discussions, Linda was asked to revise her comments. Her original submittal is attached.

<u>October 17, 1990</u>

The morning was spent in visiting a huge coal (lignite) mine in the vicinity of Cologne. It was an impressive site. Even more impressive was the planning horizon, i.e., the next mine is being planned for the year 2050! Apparently, the mining operations requires the relocation of entire villages. Once the mining license is granted, which may take from 20-30 years, the inhabitants are given up to 30 years to relocate.

INTRAVAL participants were given a tour of the city of Cologne in the first half of the afternoon. Working group meetings were held in the later part of the afternoon to complete the review of the Phase I report.

October 18, 1990

Each Working Group Leader presented conclusions from Phase I work. There were six working groups in Phase I. These have been reduced to four in Phase II. Working Group 1 dealt with problems related to simulation of laboratory experiments (test cases 1a, 1b, 2, and 9). Group 2 consisted of field-scale experiments and included test cases numbered 4 and 5. Natural analogues formed the subject for Group 3. Group 4 dealt with unsaturated flow and transport (both laboratory and field scale) problems which were numbered 10,11, and 12. Salt related cases (test case 13) was investigated by Group 5, and, finally, the synthetic data simulation (test case 6) was considered by Group 6. All the test cases are described in a bulletin issued by the NEA/SKI. This bulletin has some other interesting information also and is attached.

Peter Jackson of AEA, leader of Working Group 1 indicated that treatment of advection and dispersion did not present any problems in simulation. However, no firm conclusion about the importance of matrix diffusion could be reached. While sorption process was probably nonlinear and irreversible, standard linear approximation to sorption appeared to be adequate for simulating the experiments. He indicated that the most important use of the INTRAVAL was to use it as forum for obtaining technical review of models and experiments. He felt that issues related to performance assessment were not addressed as much as they should have been. Group 1 recommended that experiments that are designed with the explicit purpose of model validation should be conducted. The greater need for interaction between experimenters and modelers was also pointed out.

David Hodgkinson (Intera-ECL) and C. F. Tsang (LBL) presented the conclusions on behalf of Working Group 2. David talked about the Stripa 3-D experiment in which spatial heterogeneities were of main concern. Different modeling approaches were used to model the experiment. These included the channeling approach of Ivars Neretnieks, variable aperture channel concept of LBL, discrete fracture network and particle tracking of KTH and SKI, and the fractal network approach adopted by Nirex. Of all these approaches, the discrete fracture network seem to come closest to the observations. Notable variables were variability of injection rates, indirectly estimated porosities, non-fickian dispersion, scale dependence and channeling in the fractures. Chin-Fu Tsang discussed the results from the Finnsjon experiment in Sweden. He recommended that more experiments with better controls be conducted for model validation. He said that it could not be said that any thing was validated in the Phase I exercise. While preferred flow paths exist, it is difficult to correlate these to any physical properties and therefore difficult to specify.

Neil Chapman (Intera-ECL) presented the observations on behalf of Working Group 3. He indicated that simulation of natural analogues provided enhanced understanding of significant processes and their relative importance. Processes that were emphasized in these simulations included channeling, sorption, colloid formation and microbially mediated processes. The analogues provide a chance to test alternative conceptual models at a very large time scale.

Tom Nicholson (US NRC) presented the conclusions of Working Group 4. He suggested that one needs to validate not only the models, but the site characterization process and data also. The second point arose from the discussion of Alan Flint (USGS) who saw a great disparity in the measurement of saturation from cores and neutron probes. Tom also indicated that the validation exercises do provide for greater understanding of the processes, but that it is difficult to say that any model was validated. He indicated that the major purpose of the experiments was to figure out how to get large scale properties from small scale measurements.

Peter Glasbergen (RIVM) discussed the salt related problem which was a laboratory experiment. The main conclusion reached by this group was that dispersivity was a function of concentration and therefore a new constitutive equation was needed. A trial equation which required addition of non-linear terms to the Fick's equation was discussed. This matter will be investigated further in Phase II.

Richard Codell (US NRC) was the lead for Working Group 6. He indicated that not many teams participated in this working group and therefore this test case will not be continued in Phase II. However, the work of Gordon Wittmeyer at CNWRA on this problem will be included in the Phase I report. He indicated that the aim of this case was to identify the model structure. Since in this case, it was easy to generate data, one could have also tried to answer the question of how much is enough. U. Kuhlman (ETH) presented an application of the inverse methodology to the synthetic data.

The afternoon of October 18 was devoted to the presentation of proposals for INTRAVAL Phase II through poster presentations. These included posters on natural analogues, unsaturated flow experiments (Las Cruces Trench and the Apache Leap Tuff), WIPP Project, Mol tests on clay, and the Twin Lake experiment. The proposals were discussed in different working groups. This time only four working groups were identified. Working Group 1 was to consider the unsaturated flow and transport test cases; Group 2 was to concentrate on the crystalline rock experiments; Group 3 on Salt related test cases; and Group 4 on natural analogues. All the cases presented in the posters were selected for inclusion in Phase II.

October 19, 1990

The selection of test cases for Phase II were discussed in the combined session of all participants. Decisions made by the working groups were formally adopted by the entire body after some discussions of the merits of each of the test cases. Proposals on the unsaturated test cases are attached with this report.

A formal meeting of the INTRAVAL secretariat was held. The agenda for this meeting is enclosed. Mr. Kjell Andersson of SKI replaced Mr. Alf Andersson as the chairman of the coordinating group for INTRAVAL. The next workshop was announced to be held in Seattle from April 22-26, 1991. It was suggested that each working group should meet at least once in between the INTRAVAL meetings. The VOIC was dissolved.

IMPRESSIONS/CONCLUSIONS:

That "model validation" is a difficult subject was mentioned several times during this workshop. A consensus on what constitutes model validation at repository scales will probably not be reached in the context of INTRAVAL. Various national programs will eventually have to face up to the problem and set criteria in a legal framework. The differences between models designed to do performance (or safety) analyses, and those designed to predict, for instance, the detailed behavior of a contaminant plume would most likely require different validation criteria. Overall, the forum provided by INTRAVAL is of help in 1) providing access to experimental data that would normally not be available, 2) a chance to influence the conduct of ongoing experiments, 3) compare simulation results from codes developed independently, 4) provide some level of informal international review, and 5) a chance to influence (and be influenced by) international opinion on the subject.

PENDING ACTIONS:

Rachid Ababou is to complete his contribution to Phase I report.

Budhi Sagar to rework Table 1.1 and provide it to Charlie Voss.

RECOMMENDATIONS:

Because the NRC regulations are not specific to any site or type of geologic formation, it has legitimate interests in the outcome of all the test cases of INTRAVAL. However, active participation (i.e., actually working on the test cases) is an expensive proposition. The NRC and the CNWRA should, therefore, while maintaining a general interest in all the test cases, elect to actively participate in a few that are consistent with their

budgetary constraints. At the present time, for the obvious reasons, the U. S. has the greatest interest in the test cases that deal with unsaturated flow and transport. There are only two of these in Phase II of Intraval: the Las Cruces Trench and the Apache Leap, both conducted by the U. S. NRC. Unfortunately, these cases have not found much interest from investigators from countries other than the U.S. While other participants may join later, at the present, it appears that the U.S. DOE will participate in the Apache Leap test problems. It would, therefore be of value to actively participate at least in this set of test problems. At the present, only the NRC and its contractors (MIT, New Mexico State University, CNWRA, and Sandia) seem to be primarily interested in the Las Cruces Trench data. In view of this, some thought should be given to see if it would be more appropriate to deal with the Las Cruces test case outside of INTRAVAL, and include participation in one of the saturated crystalline rock test problems instead.

SIGNATURE:

Budhi Sagar — 10.31.90 Date
Manager - Performance Assessment

REFERENCES:

Participants list.
Agenda.
W. Thomas paper.
Draft copy of Phase I report.
A. Flint paper.
L. Lehman paper.
NEA/SKI Bulletin.
Unsaturated Test Case Proposals.
INTRAVAL Secretariat agenda.

CONCURRENCE SIGNATURES AND DATE:

Budhi Sagar — 10.31.90 Date
Manager - Performance Assessment

Allen R. Whiting — 10/31/90 Date
Director-Systems Engineering and Integration

Gesellschaft fur Reaktorsicherheit (GRS) mbH

INTRAVAL - WORKSHOP

Cologne, October 15-19, 1990

List of Participants

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DRAFT

FIFTH INTRAVAL WORKSHOP

Cologne, October 15-19, 1990
Gesellshaft für Reaktorsicherheit (GRS) mbH
Schwertnergasse 1
5000 Köln

PRELIMINARY AGENDA

Working hours

Monday	10.00 - 17.30
Tuesday - Thursday	09.00 - 17.30
Friday	09.00 - 13.30

Tuesday evening: VOIC meeting
Thurday evening: Conference dinner

MONDAY

10.00 - 12.00

Chairman: P. Bogorinski, GRS

Welcoming remarks
GRS

Opening of meeting
Alf Larsson, Chairman of Coordinating Group
SKI

Scope of workshop
Johan Andersson, SKI/Secretariat

Report from Working Group 1 (Test cases 1a, 1b, 2,)
C.P. Jackson, Harwell

Report from Working Group 2 (Test cases 4, 5)
C.F. Tsang/ David Hodgkinson

LUNCH

13.30 - 17.30

Chairman: David Hodgkinson

Report from Working Group 3 (Test cases 7, 8)
N. Chapman/ P. Duerden

Report from Working Group 4 (Test cases 10, 11, 12)

T. Nicholson

Report from working group 5 (Test case 13)
P. Glasbergen

Report from working group 6 (Test case 6)
Directory of Computer Programs, S. Liew
<u>Late Phase-1 papers</u>

Case 1b

Modelling test case 1b with various mechanisms and geometries. Jörg Haderman, PSI.

Modelling study on test case 1b. K. Hara, Y. Nakahara, A Shiga.

Case 5

Dipole results. A. Hautojärvi.

Case 6

U. Kuhlman (Interpretation of synthetic experiment)

Case 8

Test results of the simplified 2D modelling of the Koongarra system describing the preferential uranium pathways. C. Golian

Case 9

Preliminary results on Test case 9 by using Dual-Porosity simulation code, M. Kawanishi

Case 11

Two phase flow simulations in a heated tuff drillcore. M Lindgren and A. Rasmuson.

Case 13

A new appraoch to the RIVM experiment, P. Bogorinski, P.C. Jackson, J. Porter.

Working groups (1-6) meetings to discuss Phase-1 reports and conclusions.

Welcome reception at GRS (Tuesday at 6 PM)

<u>TUESDAY</u>

09:00 - 12:00

Continueed group meetings.

LUNCH

13:30 - 17:30

Continued group meetings.

15:00 - 17:30

Chairman: **Bertil Grundfelt**

Report (in plenum) from working group leaders - discussion.

WEDNESDAY

MORNING unit 15:00

Field trip in the vicinity of Cologne

15:00 - 17:30

Further working groups 1-6 meetings to discuss general INTRAVAL Phase 1 conclusions

Evening

Working group leaders meeting in order to coordinate general INTRAVAL Phase-1 conclusions. (Chairman: Claes Thegerström)

THURSDAY

09:00 - 12:00

Chairman: **Claes Thegerström**

General Phase-1 discussion.

LUNCH

13:30 - 15:00

Phase-2 poster session where all pilot groups should be represented at their respective poster.

15:00 - 17:30

Working group meetings to discuss INTRAVAL Phase 2 Test Cases and to start planning work.

Evening

Conference dinner

FRIDAY

09:00 - 11:00

Chairman: Chin-Fu Tsang

INTRAVAL Phase 2 Plenary discussion

11:00 - 13:00

INTRAVAL Coordinating group meeting. Decision on INTRAVAL Phase 2 Test Cases.

INTRAVAL WORKSHOP, COLOGNE, OCTOBER 15-19, 1990

Preliminary list of participants

K. Andersson, SKI
J. Andersson, SKI
P. Andersson, SGAB

P. Bogorinski, GRS

A. Cernes, CEA-IPSN
L. Chaturverdi, EEG/WIPP
N. Chapman, Intera/ECL

L. Dagerholt, Kemakta
P. De Preter, NIRAS/ONDRAS
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M. Durin, CHA.CEN SACLAY
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M. Eriksson, Kemakta
D. Evans, Univ. Arizona

E. Fein, GSF
S.J. Finley, SNL/WIPP

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C.T Kincaid, PNL/DoE
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U. Kuhlman, ETH

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S.K. Liew, WS Atkins

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Y. Nakahara, MAPI
I. Neretnieks, KTH
T. Nicholson, NRC

D. Perraud, CEA/ANDRA
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A. Ström, SKB

C. Thegerström, OECD/NEA
C.F. Tsang, LBL

J. Vira, VTT/TVO
C. Voss, USDOE / Golder Ass. Inc

J. Wollrath, Bundesamt Strahlenschutz
G.C. Wyland, RIVM

G. Uffink, RIVM

PHASE-1 REPORTING

FEB. 15, 1991 — WORKING GROUPS SUBMIT REPORT TO SECRETARIAT

MAR. 15, 1991 — WG REPORTS DISTRIBUTED TO ALL INTRAVAL PARTICIPANTS

APRIL 1, 1991 — FIRST DRAFT EXECUTIVE SUMMARY DISTRIBUTED

LATE APRIL, 1991 — DISCUSSIONS AT INTRAVAL MEETING

OCT, 1991 — WG REPORT + EXECUTIVE SUMMARY TO ALL PARTIES FOR ACCEPTANCE

DEC, 1991 — ACCEPTANCE OF ALL PHASE-1 REPORTS

EARLY SPRING — PRINTING!

5.INTRAVAL-WORKSHOP KÖLN, OCT. 15, 1990

NUCLEAR POWER AND WASTE MANAGEMENT IN THE FEDERAL REPUBLIC OF GERMANY

W. THOMAS, GRS MUNICH

Ladies and Gentlemen,

Nuclear power plays an important role in the energy supply of the Federal Republic of Germany. During the last year the West German utilities operated 20 nuclear power stations (13 pressurized water reactors and 7 boiling water reactors) with a total capacity installed of more than 22 GWe which provided approximately 40 percent of the total electricity. The first of these stations, the Power Station at Obrigheim, operating a pessurized water reactor of 340 MW, was commissioned in 1968 and the last one, unit 2 of the Power Station Neckar, also a pressurized water reactor of 1316 MW, in 1989. All these reactors operated very reliable and without any severe problems. Their availability averaged 83 percent. However, due to the arguments about nuclear power and to the fact that the energy demand levelled, no new facility had been ordered since 1982.

The feasibility of radioactive waste management and disposal is essential for the operation of nuclear power stations. Each year 500 tons of spent fuel arise from the operation of nuclear reactors. This can be reduced to 400 tons by increased burn-up. Reprocessing of spent fuel at the plants in La Hague, France, and Sellafield, UK, are accepted as part of the waste management concept.

Direct disposal of spent fuel is considered to be a second option. For certain types of fuel elements, e. g. those from the Thorium High Temperature Reactor it is the

only one. A pilot conditioning plant for spent fuel is planned in Gorleben, the first licence was issued.

However, the waste arising from the operation of the nuclear power plants as well as from reprocessing of spent fuel has to be stored in a safe way. According to our Atomic Law the federal government is responsible for safe disposal. This task was passed along to the Federal Agency for Radiation Protection (BfS) in Salzgitter. Deep geologic disposal is considered to be the only feasible option for final disposal of high-level as well as low- and intermediate-level waste or spent fuel within our densely populated country. Two sites were selected for this purpose.

The disused iron ore mine of Konrad, which some of you visited last week, is planned to be a repository for low- and intermediate-level waste of negligible heat production. It is in the licensing procedure with the Minister for the Environment of the State of Lower Saxony as the licensing authority. After the review of the safety analysis will have been finished by the authority's contracted experts - the GRS is involved in the long-term safety analysis - the documents will be laid open to start the public involvement. At the moment a definite date for that cannot be foreseen.

The salt dome of Gorleben is planned to host a repository for all types of waste, especially heat generating waste. During the past 10 years an extensive site

investigation programme was carried out. Some of you may use part of the data acquired in that programme to validate your computer models. Since most of the important information that could be collected by surface work is available now the program will be continued by underground exploration of the salt dome. For that purpose two shafts have been sunk since 1986. After a delay of more than a year, due to an accident in April 1987, the shaft Gorleben 1 reached the top of the salt dome some time ago. Work continues also with shaft 2 which now reached a depth of 190 m. However, as a result of the elections in Lower Saxony this spring the a new government was formed by a coalition that included the Green Party. Part of the coalition agreement is to abandon the plans for a repository at Gorleben for reasons of unsuitability of the salt dome. Therefore the sinking of the shafts will be stopped at a depth of 345 m. This depth is essential to ensure stable conditions.

Current theoretical studies that are based on the present knowledge of the internal structure of the salt dome derived from surface investigation deal with the comparison of the various options to dispose of waste from reprocessing as well as spent fuel.

The role of the GRS in the field of waste management and disposal is twofold. We are providing expertise in the field of operational safety for the Federal Agency for Radiation Protection as the developer of the repositories as well as in the field of long-term safety for

the Minister for the Environment of Lower Saxony as the licensing authority. Furthermore we support the Federal Minister for the Environment in his decisions concerning the various options of final disposal.

With the unification of West and East Germany we are facing a new challenge. According to our Atomic Law, the authorities have to assure that the nuclear installations in the part of our country that used to be the GDR are equally safe. This holds for the operating reactors in Rheinsberg and the 4 units in Greifswald as well as for those that are in their commissioning phase or under construction and also for the installations of the nuclear fuel cycle.

Safety assessments carried out during the last months by our Company resulted in a shut down of 3 of the operating units in Greifswald due to deficiencies in the safety systems. The last one will go off the grid towards the end of this year. In addition the commissioning of the unit 5 had been interrupted. Operation of these units will only be resumed after extensive backfitting measures.

The repository for low- and intermediate-level waste at Morsleben is operating since ten years. With the 3rd October responsibility for the disposal of nuclear waste in East Germany went over to the Federal Government. To support the decision of the Minister for the Environment whether to continue or to terminate operation

of the facility GRS is carrying out a safety assessment. This involves

- survey of the current state of the facility
- geology
- operational safety
- long-term safety
- operational experiences and control

The review will be finished towards the end of this year with an option to continue in those areas where more assurance of assumptions is needed.

To a large extent all these safety assessments rely on computer codes. Regardless of which code is used the models implemented have to be as good as possible to get reliable analyses. Code intercomparisons as well as comparisons with experiments - lab scale, field scale and natural analogues - are very useful means to assure that. Therefore a broad consensus on the phenomena involved and how to model them resulting from international projects like INTRAVAL is essential to build confidence in our predictions.

I wish you a very successful INTRAVAL-workshop here in Cologne. I hope that you will find some time to enjoy your stay in this 2000 year old city even if this week will be very busy for you.

Tom Nicholson

DRAFT

INTRAVAL Phase I Final Report

Unsaturated Zone Test Cases

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ABSTRACT

Three unsaturated flow and transport experiments are presented along with computer simulation efforts directed toward reproducing the experimental data. The three field sites investigated are the G-Tunnel located at the Nevada Test Site in Southern Nevada, the Apache Leap Tuff Site located in Central Arizona, and the Las Cruces Trench Site located in southern New Mexico. The G-Tunnel and Apache Leap experiments were conducted in unsaturated, fractured tuffaceous rock, while the Las Cruces experiments were conducted in unsaturated soil material. The G-Tunnel experiments were designed to investigate the relative influence of dry drilling on moisture content in the rock as opposed to wet drilling. The Apache Leap experiments were designed to investigate scale effects (laboratory vs. field data sets), spatial variability, non-isothermal effects, and coupled fracture-matrix flow processes. The Las Cruces experiments were designed to provide data to test stochastic and deterministic models for water flow in spatially variable unsaturated soils.

Simulation of the G-Tunnel results are limited to comparisons of material properties with the Apache Leap and Las Cruces results. Apache Leap simulations include nonisothermal modeling as well as coupled fracture-matrix flow and transport. Las Cruces simulation results include one-, two- and three-dimensional modeling of water flow and solute transport.

Recommendations from the experiments and simulations include the need to develop conceptual models and design experiments to test coupled processes (i.e., thermal, solute, pneumatic and hydraulic processes), examine sensitivity methods and experiments for assessing relative importance of parameters, develop scaling laws and experiments for examining spatial variability and heterogeneity, develop and test numerical and stochastic models for water flow and transport in spatially variable soils, and explore alternative models that describe fracture-matrix interactions. Outstanding validation issues include the need to investigate whether effective parameter approximation is valid and can be validated, and the need to determine appropriate acceptance criteria for use in validating models.

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B.3 "Two-Phase Flow simulations in a Heated Tuff Drillcore - INTRAVAL Case 11", by M. Lindgren & A. Rasmuson, KEMAKTA Consultants Co.

C. LAS CRUCES TRENCH EXPERIMENTS

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D. COMPARISON OF G-TUNNEL, APACHE LEAP TUFF AND LAS CRUCES TRENCH DATA

D.1 "Correlation of Saturated and Unsaturated Flow Parameters of Soil and Tuff" by J.S.Y. Wang, LBL

D.2 "INTRAVAL Review Comments", by L. Lehman, State of Nevada

0. EXECUTIVE SUMMARY

This document describes three INTRAVAL test cases related to unsaturated flow through porous media. The three unsaturated flow and transport experiments are presented along with computer simulation efforts directed toward reproducing the experimental data. The three field sites investigated are the G-Tunnel located at the Nevada Test Site in Southern Nevada, the Apache Leap Tuff Site located in Central Arizona, and the Las Cruces Trench Site located in southern New Mexico. The G-Tunnel and Apache Leap experiments were conducted in unsaturated, fractured tuffaceous rock, while the Las Cruces experiments were conducted in unsaturated soil.

Objectives

The G-Tunnel experiments were designed to investigate the relative influence of dry drilling on moisture content in the rock as opposed to wet drilling. The Apache Leap experiments were designed to investigate scale effects (laboratory vs. field data sets), spatial variability, non-isothermal effects, and coupled fracture-matrix flow processes. The Las Cruces experiments were designed to provide data to test stochastic and deterministic models for water flow in spatially variable unsaturated soils.

G-Tunnel Summary

[To be provided by US DOE]

Apache Leap Summary

Field experiments are conducted at the Apache Leap Tuff Site in tuffaceous rock (dated approximately 19 m.y. B.P.) near Superior, Arizona, located approximately 160 km north of Tucson, and 100 km east of Phoenix. At the experimental site, the tuff formation is approximately 600 m thick and grades from a densely welded unit near its base to a slightly welded tuff which has a total porosity of 17 percent. The unsaturated zone extends to great depth due to topography and to pumping associated with a nearby underground mine. Vertical and horizontal fracture traces are evident on the land surface and can extend for several hundred meters. Laboratory experiments and measurements are conducted using cores obtained during borehole drilling at the field site and using shaped blocks removed from the field site.

Las Cruces Trench Site Summary

A series of experiments were performed at the New Mexico State University College Ranch, 40 km northeast of Las Cruces, NM. A trench was dug in the undisturbed soil to provide a large number of soil samples for site characterization and to provide horizontal access to irrigated areas adjacent to the trench. The soil samples were used to determine the spatial variation in soil-water retention characteristics and the saturated hydraulic conductivities for the site. In addition, borehole permeameters

were used to estimate the spatial variation of *in situ* saturated hydraulic conductivity. Water containing tracers was applied to two areas adjacent to the trench to provide data on water flow and transport through a spatially variable, but well characterized, unsaturated soil. These areas were heavily instrumented with arrays of neutron probe access tubes, tensiometers, and solute samplers. Data from these experiments are presently available in database format and can be accessed through Internet, a national computer network.

Summary of Modeling

Simulation of the G-Tunnel results are limited to comparisons of material properties with the Apache Leap and Las Cruces results. Apache Leap simulations include nonisothermal modeling as well as coupled fracture-matrix flow and transport. Las Cruces simulation results include one-, two- and three-dimensional modeling of water contents and tracer tests. Conclusions from the experimental and simulation groups are reported, as well as recommendations for further studies.

Summary of Validation Efforts

Scientists from the Center For Nuclear Waste Regulatory Analysis at the Southwest Research Institute; HydroGeoLogic, Inc.; KEMAKTA Consultants Co.; Massachusetts Institute of Technology, New Mexico State University; Pacific Northwest Laboratory; and Sandia National Laboratories have used the Las Cruces data to test transient models for water flow and solute transport through unsaturated soils. These models range from two-dimensional deterministic simulations of water flow and transport through uniform isotropic soils to three-dimensional simulations of water flow through fully heterogeneous, anisotropic soils. Stochastic models include one-dimensional simulations of water flow using Monte-Carlo methods and two-dimensional simulations of mean water flow using the effective model of Mantoglou and Gelhar (1987). Graphical comparisons are made between the observed field data and the model predictions for water content, solute concentration, and their spatial moments as a function of time.

Summary of Recommendations

Phase I activities have resulted in recommendations to develop conceptual models and design experiments to test coupled processes (i.e., thermal, solute, pneumatic and hydraulic processes), examine sensitivity methods and experiments for assessing relative importance of parameters, develop scaling laws and experiments for examining spatial variability and heterogeneity, develop and test numerical and stochastic models for water flow and transport in spatially variable soils, and explore alternative models that describe fracture-matrix interactions.

Additionally, experimental methods must be reexamined to develop characterization, sampling, monitoring schemes that quantify the complexity of a site while meeting modeling demands and the identification of effective parameters in a parsimonious manner. *In situ* instrumentation must be

developed for measuring solute concentrations, unsaturated hydraulic conductivities, matric suctions and water contents in fractures. Experimentalists need the ability to determine parameters *in situ* in response to boundary conditions and induced stresses. It is also important to determine hydraulic and transport properties *in situ* for multiphase flow and transport systems for various matric suctions and water contents.

Necessary additions to the Las Cruces data acquisition include: (1) The determination of the extent of small-scale anisotropy in hydraulic conductivity by taking horizontal as well as vertical soil cores; (2) The need to obtain coincident (space and time) water content and concentration data in 3-D; and (3) The measurement of necessary transport parameters (e.g., dispersivity) directly, for instance, using columns of varying length to determine influence of travel distance, if any.

With regard to numerical solution techniques, efforts should be directed toward: (1) The development of numerical tools for modelling field scale system while accounting for effects of small scale heterogeneities; (2) Investigating alternative descriptive models of unsaturated flow and solute transport; and (3) Developing coupled process models that can account for interactive stress, pressure, temperature, and concentration conditions for hydro-thermo-chemo-mechanical systems. Outstanding validation issues include the investigation of whether effective parameter approximation is valid and can be validated, and the determination of appropriate acceptance criteria for use in validating models.

1. INTRODUCTION

1.1 Test Case Summaries

Three test cases are being examined as part of the U.S. INTRAVAL program. All of the cases focus on unsaturated flow and transport in geologic media. Two of the test cases are related to flow in unsaturated fractured rock (G-Tunnel in Nevada, and the Apache Leap Site in Arizona), while the third examines flow in unsaturated soil materials (Las Cruces Trench in New Mexico).

1.1.1 G-Tunnel

[To be provided by US DOE]

1.1.2 Apache Leap

The Apache Leap Tuff Site is located near the extreme western edge of the Pinal Mountains, which rise to over 2100 m in elevation. Lying immediately east of Superior, Arizona is the Apache Leap which forms a 600 m west-facing escarpment that exposes a volcanic zoned ash-flow tuff sheet and an underlying carbonate. The Apache Leap Tuff Site is approximately one km to the east of the escarpment at an approximate elevation of 1200 m. The rocks exposed at the site are the uppermost unit of a sequence of ash-flow tuff sheets. The tuff is a consolidated deposit of volcanic ash, with particle diameters less than 0.4 mm, resulting from a turbulent mixture of gas and pyroclastic materials of high temperature about 19 million years ago. The ash-flow deposits at one time covered an area of approximately 1000 km^2 with a maximum thickness of 600 m but have been eroded in some places to about 150 m in thickness.

Atmospheric precipitation has been recorded near the site, with the long-term average estimated to be approximately 538 mm/year. Most of the precipitation occurs during two periods, from mid-July to late-September, and from mid-November to late-March. Summer storms are characterized by high-intensity, short-duration thunderstorms during periods of high temperature and evapotranspiration demand. Winter storms are of longer duration and lower intensity during cooler periods with much lower evapo-transpiration demand.

Regional ground water levels below the site have been substantially modified by dewatering activities at the nearby Magma mine which extends to a depth of 1500 m below the site. The water levels have been drawn down to levels below the tuff unit. Perched water has been observed at several locations near the site, notably in shallow alluvial aquifers along major washes and from seeps near washes. Noticeable increases in inflows to the main haulage tunnel for the Magma mine are observed within days following streamflow in Queen Creek, which is located approximately 100 m above the haulage tunnel. Observations in mine workings at deeper levels demonstrate increased inflows up to several weeks following streamflow events.

Twelve inclined and three vertical boreholes have been installed at the site in five sets of boreholes. Each set consists of three boreholes drilled in a plane. The inclined boreholes are not of the same length, with the lengths of the boreholes being 15, 30 and 45 m. This design results in the bottom of each borehole in a series lying along the same vertical line. Two inclined borehole sets are parallel to each other and the other two inclined sets are oriented 90° and 180° to the first two sets. A plastic cover has been placed over the rock surface to cover an area of approximately 30 x 50 m. The cover is designed to prevent evaporation from the rock to the atmosphere as well as to prevent precipitation from infiltrating into the rock.

1.1.3 Las Cruces Trench Site

The Las Cruces Trench site is located on the New Mexico State University College Ranch, about 40 km northeast of Las Cruces, New Mexico. The site is on a basin slope of Mount Summerford at the north end of the Dona Ana Mountains. The Dona Ana Mountains form a domal uplift complex of younger rhyolitic and the older andesitic volcanics intruded by monzonite. Climate in the region is characterized by an abundance of sunshine, low relative humidity and an average Class A pan evaporation of 239 cm per year. Average annual precipitation is 23 cm (Wierenga et al. 1987).

A trench 26.4 m long by 4.8 m wide by 6.0 m deep was excavated in the undisturbed soil to provide horizontal access to the irrigated plots and to provide approximately 600 core and 600 disturbed soil samples for site characterization. Irrigation systems were installed on two plots (denoted Plot 1 and Plot 2) adjacent to the trench. The irrigated plots and the surrounding area were covered with a pond liner to prevent infiltration from rainfall and local runoff and to minimize evaporation. To monitor water flow during the experiments, neutron probe access tubes were installed along several vertical planes extending through the irrigated area. In addition, two-dimensional arrays of solute samplers and tensiometers were installed through the trench walls to allow solute concentration and tension to be monitored as a function of time.

During the Plot 1 experiment, water containing tritium was applied at a rate of 1.82 cm/day to an 4 by 8 m area through a closely spaced grid of drip emitters for 10 days. Water without tritium was applied for an additional 76 days. During the Plot 2 experiment, water was applied to a 1.2 by 12 m area at a rate of 0.43 cm/day for 11.5 days with tritium and bromide and for an additional 64 days without the tracers. The movement of water and the tracers were carefully monitored during infiltration and redistribution.

1.2 Validation Objectives

1.2.1 G-Tunnel

[To be provided by US DOE]

1.2.2 Apache Leap

The ultimate objective of the Apache Leap experiments is to predict water flow and solute transport through unsaturated fractured rock under field conditions. Specific objectives leading to the ultimate objective are:

- To further assess appropriate technology for characterizing and monitoring water flow and transport through unsaturated fractured rock, including interaction between the rock matrix and the fracture system.
- To examine relevant hydraulic, pneumatic, thermal and solute transport processes, singularly and coupled, at laboratory scales (1 to 60 cm) and at field scales (1 to 30 m).
- To generate data sets, for simple, uncoupled systems as well as more complex, coupled flow and transport systems, for use in the validation of unsaturated flow and transport models related to the INTRAVAL program.
- To assess, cooperatively with other INTRAVAL participants, various experimental and modeling approaches and their limitations in predicting flow and transport through unsaturated fractured rock.

These objectives are related to the assessment of characterization methods based primarily on soil science techniques for determining the hydraulic, pneumatic, thermal, and solute transport properties of rock matrix cores, and the comparison with transport properties determined from *in situ* experiments. These objectives include the evaluation of the use of moisture characteristic and unsaturated transmissivity and conductance curves for fractures. They are also related to the examination of relevant processes at selected scales.

Relevant processes include hydraulic, pneumatic, thermal, and solute transport components, which may be coupled using experiments conducted over several length scales, on unfractured tuff cores measuring 6 and 10 cm in length, on rock blocks with a single discrete fracture measuring approximately 50 cm in length, and on *in situ* measurements taken over distances of from 1 to 30 m. Time scales also vary, from the order of minutes for small core samples, through months for discrete fracture block experiments, to years for large-scale field experiments.

Coupled processes are examined using non-isothermal core experiments, as well as field heater experiments under conditions of partial liquid saturation. The determination of the significance of material heterogeneities and multiple discontinuities will be made at the field site. Due to presence of multiple porosities (including various microporosities, fractures, and vugs), hydraulic properties can vary seven orders of magnitude as a function of position as well as water content.

The objectives will incorporate the evaluation of the predictive ability of various alternative modeling strategies (including the equivalent porous medium representation of fractured flow, as opposed to discrete fracture network flow representation within a porous matrix) for their ability to accurately represent fluid flow and solute transport processes in unsaturated fractured rock. NUREG/CR-5097 by Yeh et al. (1988) discusses the

various conceptual models being considered along with a review of possible numerical codes for providing simulation results prior to performing the experiments.

Validation of model forecasts is important due to the reliance on these models for performance assessment. Predictions of solute transport from a high-level waste repository to the accessible environment are uncertain due to the possible exclusion of relevant processes and the inability to correctly identify and estimate material properties which are highly variable. This INTRAVAL study is designed to evaluate the relative significance associated with excluding various processes, and to evaluate scale dependent procedures used to estimate material properties. Extrapolation of laboratory tests conducted over short distance and time scales with simple analytic solutions to field tests conducted over longer distance and time scales using complicated stochastic models will be used to guide validation activities.

The approximation of multiple porosities and multiple dimensional flow using an effective porosity and dimensionality must be validated prior to application of effective parameters for predictive purposes. Performance assessment issues include the influence of high permeability zones of reduced dimensionality (i.e., one-dimensional channels within fractures) on the ability to contain high-level waste, and the importance of non-isothermal conditions on near field hydraulic conditions. From the proposed experiment, useful performance assessment related information can be extracted directly. Modeling of the experimental results is an important validation aspect, and is the principal reason for conducting the tests. Ideally, the tests will be designed using calibrated models, with calibration data sets having been obtained using laboratory and field tests. Once calibrated, the model will be validated by proposing a perturbation of the system not related to calibration experiments for the purpose of evaluating the assumptions inherent in the model.

Specific validation exercises will be conducted with respect to the conceptual models described in the experimental plan, below. The validation exercises include:

- Use of an equivalent porous medium model for characterizing the rock matrix properties with respect to hydraulic, pneumatic, thermal and solute transport;
- Evaluation of various parametric relationships between material properties and water content, relative saturation and matric potential;
- Assessment of the ability to properly parameterize and conceptualize flow through a discrete fracture bounded by a porous matrix;
- Identification of relevant processes related to non-isothermal flow through an unfractured porous tuff rock; and
- Ability of existing numerical and analytic methods to predict flow and transport through nonisothermal, unsaturated fractured rock.

The validation data sets will not be limited to these exercises alone, and can be expected to yield additional value as other validation exercises are identified.

1.2.3 Las Cruces Trench Site

The overall goals of the Las Cruces Trench experiments were to provide data to test stochastic and deterministic models for water flow and transport in spatially variable, unsaturated soils and to examine site characterization methods for very dry sites. To meet the goal of model testing, the experiments were designed with the following objectives in mind:

- The hydraulic properties for the site were characterized in sufficient detail so that the site can be modeled using deterministic and stochastic models. To meet this objective, the site was characterized using a large number of soil samples and *in situ* saturated conductivity measurements taken over a dense grid in a vertical plane immediately adjacent to the experimental plots.

- The boundary conditions on water flow and solute transport were carefully controlled to minimize the ambiguities associated with model validation. Water and solutes were applied through carefully controlled drip irrigation systems. In addition, the irrigated and surrounding area were covered with a pond liner to inhibit evaporation and rain induced infiltration.

- The movement of water and solute through the soil profile during infiltration and during redistribution was monitored in sufficient detail so that the effect of spatial variability can be defined. Water content was measured as a function of time along several vertical planes (3 for Plot 1 and 4 for Plot 2). Neutron probe observations were made on a grid with a horizontal spacing of 1 m (2 m for Plot 1) and vertical spacing of 0.25 m. Solute concentrations and tensions as a function of time were monitored in several vertical two-dimensional arrays (1 for each plot) with horizontal and vertical grid spacings of 0.5 m.

- The temporal and spatial scales of the experiments were sufficient so that the effects of spatial variability can be addressed. The temporal scales of the characterization and the Plot 1 and 2 experiments range from hours to years. The spatial scales range from core size to tens of meters.

The development of methodology to characterize and monitor a LLW site and to test and validate (or invalidate) models for water flow and transport require that many relevant scientific and performance assessment issues be addressed. These include the following:

- How should a LLW site be characterized to adequately describe spatial variability? The characterization of hydraulic properties for the unsaturated zone are typically performed using core samples. How many samples should be taken and what hydraulic parameters should be estimated? What experimental techniques should be used to measure these parameters? What models should be used to extrapolate the core

scale characterization parameters to field scale models describing spatial variability?

- How should water flow and transport models incorporate the models describing the spatial variability of the hydraulic properties? What is the role of dimensionality in water flow and transport.

- In view of the uncertainties associated with spatial variability, how should stochastic and deterministic water flow and transport models be tested and validated against field data? What is the impact of these uncertainties on predicting water flow and transport at LLW sites and on site monitoring.

Several of these issues were address during Phase I of the Las Cruces INTRAVAL experiments. Others will be addressed during Phase II.

1.3 Common Validation Issues

Table 1.1 presents the scientific and performance assessment issues that are common to the three test cases:

Table 1.1: Validation issues common to G-Tunnel, Apache Leap, and Las Cruces Trench test cases.

Scientific Issues

1) Strongly nonlinear processes related to unsaturated flow and transport

2) Scale effects

3) Heterogeneous materials

4) Multi-dimensional flow

5) Evaluation of characterization methods

6) Fracture flow

7) Measurement of field parameters

Performance Assessment

1) Examination of unsaturated flow processes relevant to radioactive waste disposal

2) Examination of experimental and field characterization techniques

3) Determination of level of characterization detail required for modelling

4) Examination of conceptual models for the prediction of flow and transport

5) Examination of numerical and analytical solution techniques

6) Examination of uncertainty (including both geologic variability and measurement uncertainty) in characterization strategies

7) Examination of effects of uncertainty on model results

8) Examination of adequacy of Richard's equation for flow characterization

9) Examination of adequacy of advective-dispersive equation for solute transport characterization

2. CONCEPTUAL MODELS

2.1 Geometric Models

2.1.1 G-Tunnel

[To be provided by US DOE]

2.1.2 Apache Leap

The tuff matrix at the Apache Leap Tuff Site is composed of three pore classes which can be identified by a multimodal distribution. The largest matrix pore class consists of vugs and voids with an opening side ranging from 1 to 10 cm along the long axis. Two microscopic pore classes have been identified using mercury intrusion methods. The larger of the pore size distributions averages approximately 3 μm and comprises about half of the microporosity. The smaller of the pore classes averages approximately 0.07 μm and accounts for the other half of the microporosity.

Fractures at the site are ubiquitous, and average approximately 0.77 per meter, with an average dip of 64.5° and a strike of 214.4° (southwesterly). From hydraulic tests two types of fractures are evident; a smaller, more frequent set of fractures with lower fracture permeability, and a larger, more conductive set of fractures. Flow through fractures is idealized as a multi-dimensional phenomenon dependent upon the scale of observation. For tests over short distances flow through channels of high permeability within a single fracture is expected. Over larger distances within a single fracture a network of such one-dimensional channels is formed which results in a two-dimensional flow network. As the scale is enlarged still further, networks of intersecting fractures will be tested which will display three-dimensional properties.

Models which reproduce the interstitial geometry must consider the multi-dimensional, multiporous nature of the rock at the Apache Leap Tuff Site. Lacking the ability to parameterize all aspects of the physical system, simplified models must be used depending upon the scale of measurement and the degree of precision required. A porous medium equivalent is assumed for small, unfractured rocks without large voids, as well as to initially describe mesoscale (i.e. over tens of meters) field tests. For fractured block tests in the laboratory, dual porosity and discrete fracture network models are employed. Field data can also be interpreted using percolation network and stochastic continuum models.

To investigate spatial and temporal variability, the core and borehole sampling strategy is to repetitively measure material properties at the same interval. Comparisons of matrix and bulk properties can then be compared to infer the influence of heterogeneities, and scale effects. Various temporal scales are employed at the different physical scales, ranging from minutes for core experiments to years for field experiments.

2.1.3 Las Cruces Trench Site

Water flow and solute transport is conceptualized to be transient and multidimensional at the Las Cruces field site. For the modeling work presented here, water flow is assumed to be through an unsaturated porous media with a lack of significant preferential flow induced by fractures, root channels, or cracks. The models used to describe the spatial variability of the hydraulic properties range from simple deterministic, isotropic, uniform soil models to three-dimensional heterogeneous, anisotropic, stochastic models. The conceptual models used to describe water flow and transport range from one-dimensional transient deterministic models to multidimensional transient stochastic models.

2.2 Process Models

2.2.1 G-Tunnel

[To be provided by US DOE]

2.2.2 Apache Leap

Hydraulic processes are governed by Richards' Equation which includes Darcy's Law. The Van Genuchten model for determining the water content as a function of the matric suction is also used. Darcy's Law is also used for predicting air flow, with modifications for slip flow using the Klinkenberg model and moisture-dependent pneumatic permeability. The heat conduction equation is used to describe thermal transport, with the inclusion of a moisture dependent thermal conductivity and specific heat.

2.2.3 Las Cruces Trench Site

Richards' equation is used to model water flow through the unsaturated porous media. Water retention is modeled by van Genuchten's relationship with both the Mualem-van Genuchten model and the exponential model used for the unsaturated hydraulic conductivity. In addition, several of the models for water flow utilize a pressure head dependent, anisotropic, unsaturated, hydraulic conductivity expression which is based on stochastic theory (e.g., incorporating anisotropy through statistical correlations). The advective-dispersive equation is used to model solute transport.

3. EXPERIMENTAL TECHNIQUES

3.1 Measured Parameters

3.1.1 G-Tunnel

[To be provided by US DOE]

3.1.2 Apache Leap

A multistage experimental plan is used to estimate parameters related to hydraulic, pneumatic, thermal, and solute transport. The effect of variable fluid saturation of the parameters will be evaluated for a wide range of matric suctions, from oven-dry to saturated. Also, the effect of fractures on bulk properties at various scales will be determined. Table 3.1 presents the stages, scales and processes to be incorporated.

Table 3.1: Experimental stages designed to predict fluid flow and solute transport through unsaturated fractured rock. Each stage introduces additional complexity.

Stage	Scale	Medium	Processes
I	cm	Matrix (core)	- Liquid, Gas, Thermal Flow - Gas Diffusion
II	cm	Matrix/Fracture (block)	- Matrix, Fracture Flow - Solute Transport
III	m	Matrix/Fracture (*in situ*)	- Matrix, Fracture Flow - Solute Transport
IV	cm	Matrix (core)	- Nonisothermal matrix flow - Coupled liquid, vapor, air, solute, and heat flow
V	m	Matrix/Fracture (*in situ*)	- Nonisothermal matrix/fracture flow - Coupled liquid, vapor, air, solute, and heat flow

Specific parameters from rock core segments (Stage I experiments) include:

- Rock physical properties, including porosity, bulk and grain density, total and incremental pore surface area, and pore size distributions.
- Moisture characteristic curves.
- Saturated and variably saturated rock matrix hydraulic, pneumatic, and thermal conductivity curves.

Parameters from fractured blocks (Stage II experiments) include:

- Fracture surface roughness, aperture, and characteristic curves.
- Fracture transmissivity as a function of matric suction.
- Solute transport properties of individual fractures.

Parameters estimated from *in situ* borehole measurements (Stage III experiments) include:

- Hydraulic, pneumatic and thermal conductivities at the same three meter intervals used to determine rock matrix properties (Stage I experiments).
- Ambient borehole water contents obtained at three meter intervals.

Laboratory core heater measurements (Stage IV experiments) will be used to estimate parameters including coupled liquid, vapor, air, thermal energy, and solute transport coefficients for the rock matrix. Some of these coefficients will be estimated independently before or after the experiments on the sample or on rock immediately surrounding the core samples. Others will be estimated during the course of the experiment.

Field heater measurements (Stage V experiments) will be used to determine the effects of fractures on coupled liquid, vapor, air, thermal and solute transport coefficients. The effect of material property heterogeneity on field scales will be examined with respect to the change from estimates based on laboratory samples.

3.1.3 Las Cruces Trench Site

The parameters measured at the Las Cruces Trench experiments can be categorized into two classes. The first class consists of measurements made to characterize the hydraulic parameters for the site. The second class consists of measurements made to monitor the dynamic variables (pressure, water content, concentration) during the execution of the experiments. These measurements are summarized in Table 3.2. Additional details are presented in Appendix C and in the references cited in the table.

Table 3.2: Parameters measured for the Las Cruces Trench Experiments.

Characterization Variables

Parameter	Scale	Technique	Reference
K_{sat}	Core	Measured flow across saturated cores	Elrick et al., 1980 Wierenga et al., 1989
K_{sat}	Core	Borehole permeameter	Reynolds et al., 1984 Wierenga et al., 1989
$\theta_r, \theta_s, n, \alpha$	Core	Cores and constant pressure apparatus with parameter estimation	Wierenga et al., 1989
Particle size distr.	Core	Soil sieves and modified pipet method	Gee and Bauder, 1986 Wierenga et al., 1989

Dynamic Variables

Parameter	Scale	Technique	Reference
θ	≈0.5 m	Neutron Probe	Wierenga et al., 1990
h	cm	Tensiometers	Wierenga et al., 1990
Concentration of ^3H and Br^-	cm	Solute samplers	Wierenga et al., 1990

3.2 Experimental Setup

3.2.1 G-Tunnel

[To be provided by US DOE]

3.2.2 Apache Leap

The multistage experimental plan described earlier is being conducted to incrementally increase complexity from simple systems to complicated ones. The ultimate concern of the study focuses on two related field experiments, one with and the other without imposed temperature gradients and in similar geologic settings (slightly welded unsaturated fractured tuff). The

experimental site with an undisturbed thermal regime has been under study for three years. Fifteen boreholes were installed and used for *in situ* site characterization, while the obtained cores are used for logging the fractures and characterizing the rock matrix. Preliminary water and gas injection-recovery tests were made at the site to determine temporal and spatial responses as well as other flow characteristics. A long-term water injection-recovery experiment is being planned for initiation in the summer of 1990.

Additional experiments in an abandoned road tunnel and mine haulage tunnel will also provide important data in welded tuff. Comparison of parameters between sites should allow models developed at one site to be verified at another. Regional geochemical experiments are being performed which provide supplementary data sets. Natural analog experiments are recommended to extend the time scales of current analyses, but are beyond the scope of the present study. Nonisothermal studies in the G-tunnel at Yucca Mountain (Daily and Ramirez, 1989) also provide complementary data sets for comparison with experiments proposed here.

3.2.3 Las Cruces Trench Site

A trench 26.4 m long by 4.8 m wide by 6.0 m deep was excavated in the undisturbed soil to provide horizontal access to adjacent irrigated plots and to provide core and disturbed soil samples for site characterization. Drip irrigation systems were installed on two plots, denoted Plot 1 and Plot 2, immediately adjacent to the north and south trench faces (the 26.4 m sides). The systems irrigated a 4 by 9 m area for Plot 1 and a 1.2 by 12 m area for Plot 2. The irrigated plots and the surrounding area were covered with a pond liner to prevent infiltration from rainfall and local runoff and to minimize evaporation.

To monitor water flow during the experiments, neutron probe access tubes were installed in several vertical planes extending through the irrigated area. The access tubes were used to take water content measurements at 0.25 m increments down to 6 m. A total of 18 tubes were installed in Plot 1 and 43 tubes for Plot 2. An additional 5 tubes were installed to a depth of 1.5 m in Plot 1. An array of tensiometers was installed on the trench walls adjacent to each experimental plot. The tensiometers were installed at a slight incline 0.5 m into the soil formation. A total of 79 tensiometers were installed for the Plot 1 experiment and 49 tensiometers for the Plot 2 experiment. Two arrays of solute samplers were also installed through the trench walls for the Plot 1 and 2 experiments (one each). A total of 24 solute samplers were installed for the Plot 1 experiment and 49 samplers for the Plot 2 experiment. Nine of the tensiometers from the Plot 2 experiment were replaced with the solute samplers after the wetting front had passed.

During the Plot 1 experiment, water containing tritium was applied at a rate of 1.82 cm/day for 10 days. Water without tritium was applied for an additional 76 days. During the Plot 2 experiment, water was applied at a rate of 0.43 cm/day for 11.5 days with tritium and bromide and for an additional 64 days without the tracers. The movement of water was moni-

tored during infiltration and redistribution for both experiments. Tracer movement was monitored during infiltration for the Plot 1 experiment and during both infiltration and redistribution for the Plot 2 experiment. Addition information is provided in Appendix C. Details of the experimental setup are provided in Wierenga et al. (1990).

3.3 Available Experimental Results

3.3.1 G-Tunnel

[To be provided by US DOE]

3.3.2 Apache Leap

Data sets related to Stage I activities (i.e., matrix properties) have been completed and are currently available in draft form. Data sets for Stage II activities (i.e., block experiment) are partially completed and additional data sets will be completed by August 1990. Stage III activities (i.e., field injection tests) are also partially completed with additional experiments planned for Summer 1990. Prototype experiments for Stage IV activities (i.e., non-isothermal core experiments) are currently underway, with a final experiment contemplated for completion by August 1990. Stage V activities (i.e., field heater experiment) are only at preliminary stages. The experimental plan related to Stage V activities will consider a preliminary experiment conducted in the road tunnel, for which some data sets are available. The plan should be completed by October 1990 with borehole construction and instrument emplacement scheduled for completion by October 1991.

It is expected that as additional knowledge becomes available with regard to processes important to the modeling of variably saturated non-isothermal flow, complementary experiments and data collection will be required. In such circumstances the Pilot Group and its contractor will be available for designing, constructing and conducting the necessary experiments and collecting any and all data of interest to the Project Teams, subject to budgetary constraints.

3.3.3 Las Cruces Trench Site

The experimental measurements discussed in Section 3.1.3 are stored in the Las Cruces Database which is installed on a Digital VAX, The database is accessible through the national computer networks using FTP. The database includes both raw and processed data from the characterization, Plot 1, and Plot 2 experiments. The database files are in ASCII format, have the same general tabulated structure, and are easily readable by FORTRAN using unformatted reads. Hardcopy of the site characterization and dynamic data is available in Wierenga et al. (1989) and in Wierenga et al. (1990), respectively. The database is discussed in more detail in Appendix C.

4. COMPUTER PROGRAMS

4.1 Inverse Modeling

The objective of inverse modeling is to provide estimates of parameters using experimental data sets, or to calibrate models to provide optimal fits of observed data. Inverse modeling is normally performed once data sets have been collected. The inverse models are evaluated in terms of the standard error estimate of the estimated parameters, or the ability of the model to estimate known parameters accurately.

4.1.1 G-Tunnel

[To be provided by US DOE]

4.1.2 Apache Leap

Two computer programs were used to estimate hydraulic parameters from laboratory experiments. The first, named VGFIT, was used to estimate the parameters of the Van Genuchten equation (Van Genuchten, 1978, 1980) of the form:

$$S = (1 + (\alpha\psi)^n)^{-m} \tag{4.1}$$

where

- S relative saturation, dimensionless;
- α scaling parameter, kPa^{-1};
- ψ matric suction, kPa;
- n fitting parameter, dimensionless; and
- m fitting parameter, dimensionless, equal to 1-1/n.

Pressure extraction and thermocouple psychrometer data were used to provide the least squared error estimate of relative saturation assuming a constant value of n and m for all samples, and no residual saturation.

The second program, named KFIT, was used to estimate the unsaturated hydraulic conductivity of rock core samples. Input to the program was provided from data obtained using the outflow technique (Klute, 1964). Klute (1964) presents an analytic solution for the outflow method when the hydraulic diffusivity is a constant over each pressure increment. For the samples and pressure increments employed in this analysis, however, the hydraulic diffusivity can not be assumed constant. Instead, an exponentially decreasing hydraulic conductivity is assumed over each pressure step:

$$K(p_f) = K(p_i)\ \exp[a(p_f - p_i)] \tag{4.2}$$

where

- K hydraulic conductivity at pressure p, m/s;
- p_f, p_i final and initial pressures, Pa, respectively; and
- a regression coefficient, 1/Pa.

Using the saturated hydraulic conductivity at zero pressure to begin the procedure, the equation above provides stepwise estimates of the unsaturated hydraulic conductivity. Lacking an analytic solution for the outflow method using this technique, a nonlinear least squares finite element program provided by Kool and Parker (1987) was modified to estimate the unsaturated hydraulic conductivity at each pressure step. The revised program, named KFIT, uses the least squared error in outflow volumes during each pressure outflow step as the objective function.

4.1.3 Las Cruces Trench Site

The NLIN procedure of SAS (SAS Institute Inc., 1985) was used to find least-squares estimates of the parameters α and n in van Genuchten's water retention model for each core location (see Section 4.1.2). In addition to estimating the hydraulic parameters that appear in van Genuchten's water retention model for each core sample, estimates for these parameters were obtained for a layered soil model and for a uniform soil model. The layers in the layered soil model correspond to the 9 soil layers identified at the site (Wierenga et al., 1989). The water retention data from all 50 samples from a given layer were used to estimate α, n, θ_r, and θ_s for a single water retention curve for that layer. The water retention data for all 450 sample locations were simultaneously used to estimate single values for each of the parameters α, n, θ_r, and θ_s in a least-squares sense which resulted in a single water retention curve (i.e. uniform soil model) for the entire site.

4.2 Predictive Modeling

Predictive modeling is normally employed to forecast experimental results either prior to conducting the experiments, or independently of the experimental results. The predictive models are evaluated in terms of the error between the model outputs and the experimental results.

4.2.1 G-Tunnel

[To be provided by US DOE]

4.2.2 Apache Leap

Huang and Evans (1985) have published a discrete fracture network (DFN) computer model. The model requires as inputs fracture geometrical information including densities, orientations, areal extent, and transmissivities. Extensions by Rasmussen et al. (1985), Rasmussen (1986, 1987, 1988) and Rasmussen and Evans (1989) have extended the original model by allowing discretization within the plane of the fracture, as well as the bounding matrix blocks using the boundary integral method. The model, as modified, is restricted to uniform material properties within each subdomain. Variable saturation has been included by assuming a constant capillary potential within each fracture, and a discrete air-water interface. Solute transport is modeled using calculated travel times along streamlines.

Laboratory experiments on heat flow through a rock core have been modeled by T. McCartin (NRC) using TOUGH. T. McCartin has also modeled field scale injection and redistribution data using SUTRA and VAM2D. D. Codell presented a particle tracking model to evaluate solute transport at the Third INTRAVAL Workshop at Helsinki. Flow through a fractured rock block has been modeled by P. Davis and N. Olague at Sandia National Laboratories using VAM2D. The following table summarizes modeling activities.

Table 4.1: List of modelers involved with Apache Leap Tuff Site Test Case.

Stage		Simulation Modeling Groups
I	Core	- UAz, NRC, LBL
II	Fractured Block	- UAz, NRC, LBL, SNL, CNWRA, PNL
III	Field Imb./Redist.	- UAz, NRC, LBL
IV	Nonisothermal Core	- UAz, NRC, LBL, MIT
V	Field Heater	- UAz, NRC, LBL, CNWRA

UAz - Dept. of Hydrology & Water Resources, Univ. of Arizona, Tucson, AZ
NRC - U.S. Nuclear Regulatory Commission, Washington, D.C.
LBL - Earth Sciences Div., Lawrence Berkeley Laboratory, Berkeley, CA
SNL - Division 6415, Sandia National Laboratories, Albuquerque, NM
CNWRA - Center for Nuclear Waste Regulatory Analyses, San Antonio, TX
PNL - Pacific Northwest Laboratories, Richland, WA
MIT - Massachusetts Institute of Technology, Boston, MA

4.2.3 Las Cruces Trench Site

Water flow and solute transport at the Las Cruces Trench Site were modeled using a variety of numerical algorithms. A summary of the modeling efforts is presented in Table 4.2. Detailed discussions of these modeling efforts are provided in Appendix C.

Table 4.2: Modeling of the Las Cruces Trench Experiments

Group	Model	Comments
CNWRA	BIGFLO	Finite difference code for water flow. Modeled a 3-D, randomly heterogeneous and stratified, soil with boundary conditions similar to Plot 1 but with wetter initial conditions.
HGL	VAM2D	Finite element code for water flow and transport. Modeled Plot 2 with several levels of heterogeneities (isotropic and anisotropic) in 2-D.
KCC	TRUST,TRUMP	Integrated finite difference code for water flow and transport. Modeled Plot 2 as a homogeneous and a layered soil in 2-D.
MIT		Finite element code for water flow using modified Picard iteration. Modeled Plot 1 using 3-D effective media stochastic property models in a 2-D simulation.
NMSU		Water content based finite difference code for water flow and transport. Modeled Plot 2 as a homogeneous soil in 2-D.
PNL	UNSAT2	Finite element code for water flow.
	TRACER3D	Finite difference code for water flow and transport. Modeled Plot 1 water flow with several levels of heterogeneities in 2-D.
SNL	VAM2D	Finite element code for water flow and transport. Monte-Carlo simulation of 2-D water flow using VAM2D with multiple realizations of a uniform soil model.

CNWRA - Center For Nuclear Waste Regulatory Analyses
HGL - HydroGeoLogic, Inc.
KCC - KEMAKTA Consultants Co.
MIT - Massachusetts Institute of Technology
NMSU - New Mexico State University
PNL - Pacific Northwest Laboratory
SNL - Sandia National Laboratories

5. VALIDATION METHODS

Evaluating models for their ability to describe flow and transport processes related to the permanent geologic disposal of HLW requires that an assessment of the performance of the models be performed with respect to laboratory and field data sets. The assessment must be made using rigorous tests of model reliability and accuracy. Table 5.1 presents a proposed process for model validation. An important requirement of model validation is the characterization of the uncertainties associated with the conceptual models, governing equations and parameters. The uncertainties are used to evaluate the reliability of model forecasts. Estimates of parameter uncertainty due to measurement and spatial variability must be determined using field and laboratory tests. The tests are also useful for verifying the validity of the governing equations and identified processes and mechanisms used to construct the conceptual model.

Table 5.1: Proposed model validation process

STEP	
1	A conceptual model is developed in which the dominant interstitial, hydraulic, pneumatic, chemical, mechanical and thermal mechanisms, processes and interrelationships are determined. All possible components are included initially and processes not relevant to site characterization are removed as characterization progresses.
2	The governing equations and parameters which describe the dominant mechanisms and processes are identified.
3	Representative values of parameters are estimated from laboratory and field testing programs, from natural analog studies, or from geochemical information. Uncertainties due to geologic variability and measurement error are estimated. Covariances between parameters are determined.
4	Forecasts of site performance with respect to performance parameters are generated using site specific information. Confidence intervals on the forecasts are reported.
5	Confirmatory experiments are conducted to evaluate the predictive capability of the forecast models. Errors in forecasts are quantified to determine risks associated with forecast uncertainties.

Comparisons of data sets obtained using various techniques spanning a wide range of conditions and implicit assumptions concerning flow processes are an integral part of site characterization. Potential biases may not be resolved without confirmatory data sets from diverse sources, including information from short-term field tests along with geochemical and natural analog information. The inability to resolve potential biases may result in the false acceptance of a site that would not be suitable for long-term LLW and HLW isolation.

5.1 Experimental Design

The ability to test the proposed model rests on the ability to design an experiment which adequately tests the forecasting ability of the model. While experimental design is only one component of model validation, it is probably one of the more critical in terms of allowing modelers, experimentalists, and policy makers to determine the form of the validation test.

5.1.1 Parameter Estimates

Initial parameter estimates are required in order to use models for experimental design purposes (Step 3 in Table 5.1). At all of the test sites, initial estimates of water content and matric suction are available. Material properties are also available.

5.1.2 Acceptance Criteria Definition

Of all the issues related to model validation, the determination of acceptance criteria is the most difficult. Heuristic techniques are generally used, because quantitative estimates of the goodness-of-fit are difficult to obtain. As discussed in Chapter 7, it is recommended that more attention be focused on devising appropriate acceptance criteria.

5.1.3 Uncertainty Measures

Uncertainties result from natural geologic variability, from improper measurements, from inaccurate instruments or from factors that are not controlled. The effect of the uncertainty is to reduce the confidence in a proposed conceptual model or to result in the incorrect specification of a conceptual model. Sources of uncertainty must be characterized with regard to the degree of uncertainty introduced in data collection and interpretation as well as the influence of the uncertainty on system performance.

Because uncertainties may arise due to natural variability in the subsurface, the influence of natural variability can be difficult to distinguish from instrument error. Changing the scale over which a parameter is measured often can change the interpreted value of a parameter, especially for heterogeneous materials. Averaging over larger volumes may result in more stable parameter estimates but at the cost of predictive capability over smaller regions.

Measurement errors can be estimated by using replication, duplication and redundancy. Replication seeks to estimate measurement error by repeating a measurement on the same sample using the same instrument. The mean and variance of the parameter are then estimated. To determine whether the instrument is providing a biased estimate, a different instrument can be employed to duplicate the experiment. If the method itself is providing a biased estimate, then changing the instrument used to measure the parameter will not be sufficient. Rather, an entirely different procedure must be employed. This redundancy is another means to estimate sample bias.

Geologic variability is estimated by assuming that total parameter variance is the sum of the variance due to measurement error and variance due to geologic variability. This assumption implicitly requires that the measurement error is uncorrelated to geologic variability. The methods employed to characterize parameters includes procedures for minimizing correlations between measurement error and spatial variability.

5.2 Comparison of Model Results with Experimental Data

5.2.1 Qualitative

Wang (Appendix D.1) used measured core data from the three sites (G-Tunnel, Apache Leap, and Las Cruces) to evaluate similarities and differences in hydraulic property distributions. Parameters from the various sites measured at various scales were compared.

For the Apache Leap Tuff data sets, various comparisons were made for each experiment. Computer simulation models of the fractured block experiments were compared to measured data for observed water intake rates, measured suctions and chloride concentrations both in the matrix and in the fracture. Simulations of the nonisothermal core experiments were compared with measurements of temperature, water contents and the final solute concentrations.

Visual comparisons between the observed and predicted wetting front motion were made for the Las Cruces Plot 1 experiment. In addition, spatial distributions of water content, matric suction, and solute concentrations were compared to numerical predictions for the Plot 1 and Plot 2 experiments. In one case, the detailed three-dimensional structure of a strip-source moisture plume was analyzed with emphasis on dimensionality and anisotropy effects.

5.2.2 Quantitative

Statistical tests were performed by Sandia National Laboratories using the Las Cruces characterization data to determine if the laboratory and the *in situ* saturated hydraulic conductivities were normally, lognormally, or exponentially distributed, and statistically different, and if the saturated hydraulic conductivities for the various soil layers possessed statistically different means. In addition, directional variograms of the log of the saturated conductivities were generated to estimate correlation lengths. Details of these analysis are provided in Appendix C (M.T.

Goodrich). While visual comparisons between contour plots of observed and predicted water contents and relative tracer concentrations were made, quantitative comparisons were limited to comparisons of the spatial moments of these quantities (see Appendix C, J.B. Kool). Additional quantitative comparisons of predicted and observed water flow and transport will be made during Phase II of INTRAVAL.

5.2.3 Acceptance Criteria

The acceptance criteria for the statistical tests of the Las Cruces Trench Site saturated hydraulic conductivities were based on the Mann-Whitney test at the 90% confidence level, Lilliefors test at the 90% confidence level, and the t-test at the 90% confidence level. See Appendix C (M.T. Goodrich) for more detail. In addition to the statistical tests, relative rankings of predictive water flow and transport models were made for several different conceptual models of soil heterogeneity (see Appendix C, J.B. Kool).

6. CONCLUSIONS

6.1 Conceptual Models

6.1.1 Processes

- Definition of processes are adequate for modeling of individual processes. There currently exists an incomplete understanding of coupled processes.

6.1.2 Characterization

- Parameter Importance: Need to determine which parameter has the greatest impact on flow and transport for a given site and performance criteria.

- Distribution of Parameters and the Estimation of Effective Parameters: Importance of scale and heterogeneities greatly contribute to parameter uncertainty.

- Spatial Variability: Significantly affects flow and transport. Solute concentration appears to be more sensitive to spatial variability than moisture potential.

- Equations of State

6.2 Experimental Methods

6.2.1 Experimental Design

- It is important to identify validation issues and objectives including physical models and processes, conceptual models, hypothesis testing method, and acceptance criteria.

- Detailed characterization is critical to experimental design for model validation.

- Modeling is required to assist in experimental design. The design determines which data are to be collected, including characterization and experimental data.

- Detailed site characterization is performed in parallel with experimental design modeling.

- The experiment is performed independently and compared to model forecasts. Model validation is performed independently from the experiment.

- It is important to recommend and identify needs for additional work.

6.2.2 Experimental Findings

- The neutron probe technique provides adequate measures of changes in matrix moisture content distribution but is not necessarily adequate for absolute moisture content without calibration in specific media. Also, the neutron probe averages water content over a large volume.

- Discrepancies are observed between *in situ* saturated hydraulic conductivity and laboratory measured values.

- Mass balance errors and inconsistencies in model results occur due to a lack of agreement on a definition for residual water content and the difficulty in its measurement.

- Presently there is a lack of data on pore scale hysteresis and understanding of its relative importance to spatial variability.

- Field and laboratory methods for the determination of rock thermal conductivity are presently adequate due to their spatial uniformity and relative insensitivity to water content variability.

- Limitations exists in concentration profile data without coincident moisture content data.

- Certain fracture geometric properties (e.g., orientation and density) are relatively easy to measure, other parameters (e.g., areal extent, connectivity) are more difficult to measure methods and techniques to determine unsaturated, fracture hydraulic properties (e.g., fracture transmissivity and conductance as a function of matric suction) are under development.

6.2.3 Experimental Difficulties

- The measurement of matric suction using thermocouple psychrometers under field conditions is limited to greater than ten bars suction. Measurement of matric suction using a tensiometer under field conditions is limited to very wet conditions (less than 0.6 bars suction). The two methods are subject to greater errors than moisture content techniques due to instrument-media contact and the representative volume measured. That is, the neutron probe averages water content over a larger volume than either the thermocouple psychrometer or the tensiometer.

- The determination of unsaturated hydraulic conductivity in the laboratory is very difficult, especially for low water contents and matric suctions greater than one bar.

- Techniques to measure unsaturated hydraulic conductivities *in situ* for low water contents and high matric suctions (e.g., arid environments) are presently not well established. There are substantial difficulties in collecting unsaturated hydraulic conductivity relationships which would be amenable to geostatistical interpretation.

- It is very difficult to obtain fluid samples in dry soils using present techniques (e.g., suction candles and lysimeters) to determine solute concentrations. The difficulty in obtaining contaminant samples as moisture content drops is due to decreasing wetted contact with the sampling surface.

- There are substantial difficulties associated with collecting transient concentration profiles over a 3-D grid for porous matrix or over a 2-D grid for fractures due to spatial variability and preferential flow paths.

- Field and laboratory air permeability tests can be used as an indirect method to determine hydraulic properties such as matric suction and hydraulic conductivity

- While there are laboratory derived dispersion coefficients or dispersivity values being used to model field scale problems, it has not been resolved how to extrapolate laboratory values to field scales and conditions which include variable water content.

- There are no field methods to directly measure dispersivity. There is also some doubt as to whether such measurements would be meaningful.

6.3 Numerical Solution Techniques

- Traditional numerical solution techniques were inadequate to simulate sharp wetting fronts because of numerical oscillations, convergence and associated mass balance errors.

- Alternative formulation of Richard's equation using water content or mixed water content/pressure based formulations as well as improvements in solution schemes have greatly reduced computer CPU requirements and algorithmic errors. Detailed three-dimensional simtulations are only becoming feasible as the result of recent activities.

- Fracture-matrix discretization using boundary integral method allows reduction in the number of nodes and dimensionality to couple 2-D fractures with 3-D matrix. The method is currently restricted to homogeneous material properties and steady-state conditions.

- In general, most unsaturated codes only provide the ability to specify constant flux or head boundary condition and do not implement a "true" Neumann boundary condition which allows the specification of a head gradient. A few codes, such as CNWRA's BIGFLO code have this capability.

- Computer codes to simulate non-isothermal solute transport experiments have limited availability.

6.4 Validation Conclusions

- Define what will be the validation criteria/model performance measures prior to performing experiments and modeling.

- Separate data set for validation should be available.

- Validation/performance assessment criteria should be quantitative to permit either acceptance or rejection of a model.

- The selected criteria should be relevant to the performance assessment of ~~actual waste sites~~, e.g., time of travel to specified point(s), cumulative fluxes across system boundary, etc.

- The type of general "plume matching" that has been used in modeling so far should be avoided in lieu of matching specific criteria.

- Development of predictive models require close and continuous interaction between modelers and experimentalist from the development of experimental design plan phase through model analysis and acceptance phase. This interaction requires numerous laboratory and field experiments and modeling exercises until the processes are adequately modeled (i.e., meet acceptance criteria).

7. PHASE II RECOMMENDATIONS

everybody prints output

7.1 Conceptual Models

- Develop conceptual models and design experiments to test coupled processes.

- Examine sensitivity methods and experiments for assessing relative importance of parameters.

- Develop conceptual models, scaling laws, and experiments incorporating the effects of spatial variability and heterogeneity in unsaturated flow and transport processes.

- Develop and test models for water flow and transport in spatially variable soils.

- Explore alternative models that describe fracture-matrix interactions.

7.2 Experimental Methods

General

- Develop characterization, sampling, monitoring schemes that quantify complexity of site and meets modeling demands and identification of effective parameters in a parsimonious manner.

- Develop *in situ* instrumentation for measuring solute concentrations, unsaturated hydraulic conductivities, matric suctions and water contents in fractures. Experimentalists need the ability to determine parameters *in situ* in response to boundary conditions and induced stresses.

- Determine hydraulic and transport properties *in situ* for 2-phase flow and transport systems for various matric suctions and water contents.

Suggested Additions to the Las Cruces Data Acquisition

- Determine extent of anisotropy in hydraulic conductivity by taking horizontal as well as vertical soil cores.

- Take coincident (space and time) water content and concentration data in 3-D.

- Measure necessary transport parameters (e.g., dispersivity) directly, for instance, using columns of varying length to determine influence of travel distance, if any.

- Obtain unsaturated soil properties at the site.

7.3 Numerical Solution Techniques

- Develop numerical tools for modelling field scale system while accounting for effects of small scale heterogeneities.

- Investigate alternative numerical models of unsaturated flow and solute transport for strongly nonlinear cases, with coupled fracture-matrix interaction, and applications for various scales.

- Develop coupled-process, numerical models that can account for interactive stress, pressure, temperature, and concentration conditions for hydrothermochemomechanical systems.

7.4 Validation Issues

- Investigate whether effective parameter approximation is valid and can be validated.

- Investigate methods for determining appropriate acceptance criteria for use in validating models.

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OCTOBER 10, 1990 DRAFT

INTRAVAL PHASE 1 FINAL REPORT

G-TUNNEL TEST CASE

1.1 Test Case Summaries

1.1.1 G-Tunnel

Test Case 12, is a subset of activities that support the site investigation study being carried out by the U.S. Department of Energy's (DOE's) Office of Civilian Radioactive Waste Management (OCRWM). The DOE is responsible for managing the site characterization activities for a proposed high-level nuclear waste repository at Yucca Mountain Site in the State of Nevada. Prior to site characterization a series of prototype tests are being performed to develop the necessary methodologies and gain experience in conducting the experiments and analyzing the data. A number of the prototype tests have been performed at the G-Tunnel Underground Facility (GTUF) located at the Nevada Test Site approximately 140 km northwest of Las Vegas and 48 km northeast of Yucca Mountain. GTUF is located in the unsaturated zone 750 m below the surface of Rainier Mesa and 550 m above the static water level.

The activities comprising Test Case 12 pertain to the dry v.s. wet drilling study that was performed in the GTUF (Flint et. al., 1988). Test Case 12 will hereafter be referred to as the G-Tunnel Experiment. The G-Tunnel Experiment investigated three related issues:

- the effect drilling fluids would have on the intrinsic hydrologic conditions of unsaturated tuffaceous core specimen and the rock surrounding the borehole
- the spatial variability of the hydrologic conditions at the field scale (i.e. 10 m)
- the representativeness of core specimen data of field scale processes and conditions.

To address these questions, two pairs of horizontal boreholes 10 m in length were drilled in unsaturated welded and nonwelded tuffaceous rock. One of the boreholes in each pair was drilled using water for circulation, the other air. The boreholes were continuously cored and provided 6.1 cm diameter specimens for measuring the small-scale hydrological properities of the rock and for performing imbibition experiments. The hydrologic conditions in the rock surrounding the boreholes were monitored by installing instrument sets in zones along the length of the boreholes delimited by inflatable packers. After the conditions reached equilibrium, the dry-drilled boreholes were used to conduct field-scale imbibition experiments.

The laboratory imbibition studies were performed with 3.2 and 6.1 cm diameter core specimens. The two sizes of core exhibited similar ranges of sorptivity. Both sets of data successfully predict the behavior of the field-scale imbibition experiment but only if the geometry of the (field) system is considered. The tuff rock mass intersected by the boreholes is heterogeneous over the small scale of the core samples. In addition, several fractures

intersect the boreholes. Without this additional information on the structure of the system the small-scale laboratory data is insufficient for duplicating the moisture content in the field.

The imbibition experiments are being modeled using a number of conceptual models. The laboratory and field data are used as input for the models. The results of the field imbibition study were divided into two data sets; the first used to for model calibration and the second for comparison with the model predictions.

[ADD SUMMARY OF EXPERIMENTAL RESULTS]

1.2 Validation Objectives

1.2.1 G-Tunnel

The objective of the G-Tunnel Experiment is to have a better understanding of the effects the drilling of boreholes will have during site characterization on the intrinsic properties of the surrounding rock mass. The experiment is concerned with three major issues:

- the effect drilling fluids would have on the intrinsic hydrologic conditions of unsaturated tuffaceous core specimen and the rock surrounding the borehole
- the spatial variability of the hydrologic conditions at the field scale (i.e. 10 m)
- the representativeness of core specimen data of field scale processes and conditions.

These issues are important for several reasons. Much of the data collected during reconnaissance studies and later during the detailed evaluation of a site rely on boreholes to remotely access the rock mass from the surface or underground openings. The representativeness of such data is questionable due to the changes the drilling of a borehole may have on the intrinsic or in situ conditions of an unsaturated rock mass. The introduction of drilling fluid into the rock will make interpretation of certain types of testing difficult at best and increase the uncertainty of the data. These same processes will determine how an unsaturated rock mass will respond to large-scale perturbations such as changes in pluvial conditions. For example, the infiltration of surface water and the distance it travels along fractures or faults will depend on the rate it is imbibed into the matrix.

Numerical models of hydrologic processes in an unsaturated rock mass are being used to in the OCRWM program to simulate the ambient hydrologic conditions in tuffaceous rock and the impact certain site characterization activities may have. The models are capable of simulating the simultaneous storage and flow of liquid water, water vapor, pore gas, and heat.

Laboratory tests with core specimens from the dry and wet drilled boreholes have been performed to provide much of the input data required in the models. When combined with information collected in larger-scale field tests, the data provide insight into the spatial

variability of the hydrologic properties and state conditions in the G-Tunnel tuffs and the representativeness of small-scale data for field-scale simulations. Numerical analyses are being used in an attempt to better understand the role geologic structure (heterogeneity, discontinuities, etc.,) plays in determining the response of unsaturated systems to various hydrologic conditions.

2.1 Geometric Models

2.1.1 G-Tunnel

General Geology

Rainier Mesa is composed of a thick sequence of Tertiary pyroclastic rocks (Gibbons et al, 1963) ranging from vitric ash-fall to devitrified ash-flow tuffs. The lowest pyroclastic unit in the vicinity of the G-Tunnel portal was deposited on a paleotopographic surface developed in upper Precambrian and lower Paleozoic sedimentary rocks. Subsequent deposition resulted in the smoothing or flattening of the Tertiary landscape that was being developed, as indicated by a progressive decrease in the dips of these units when moving up through the stratigraphic section (Thordarson, 1965). The deposition of the overlying Grouse Canyon ash flow and the emplacement of a thick bedded tuff sequence completed the process of leveling the Tertiary landscape.

figure

The volcanic glass in the lower 335 meters of the sequence of tuffs has been diagenetically altered to zeolites and clays by the interaction with ground water. GTUF intersect the upper 30 meters of this interval and contains boreholes USg.12 DD-1 (dry-drilled) and U12g.12 WD-1 (wet-drilled). The unit is overlain by the Grouse Canyon Member of the Belted Range Tuff, an approximately 14 meters thick unit consisting of: a basal vitrophyre; a lower rubble zone; a middle moderately to densely welded, devitrified unit; an upper rubble zone; and, an upper partially to moderately welded, devitrified unit (Connolly, et al., 1983). The Grouse Canyon Member contains boreholes U12g DD-2 (dry) and U12g WD-2 (wet).

The Grouse Canyon Member is overlain by the nonwelded Paintbrush Tuffs, a sequence of bedded, ash-fall tuffs up to 305 meters thick. With the exception of the lower 30 meters which are locally zeolitized, these units are vitric.

The water table beneath Rainier Mesa is approximately 1300 meters above sea level, at an average depth of 550 meters below the drifts of the G-Tunnel complex. Recharge occurs on the upland surface of Rainier Mesa where precipitation infiltrates into the fractured caprock. A portion of this water percolates downward either by fracture flow or a combination of matrix and fracture flow to a depth where it can no longer be removed by evapotranspiration. If unimpeded, this water may continue to migrate downward under the influence of gravity to the regional water table. Where the downward movement of water is interrupted, perched-water zones may form (Thordarson, 1965). Perched water has been observed in the GTUF in fractures and at lithologic contacts.

Boreholes U12g.12 DD-1 and U12g.12 WD-1 intersect a series of tuffaceous beds with an

apparent dip of 5 - 7 degrees from horizontal. The bed alternate between zeolitized and silicified ash-fall tuffs. The apparent dip of the units resulted in lithologic contacts that intersect the top of the boreholes, angle through the boreholes, and then exit the bottom of the boreholes.

The second pair of boreholes, U12g DD-2 and U12g WD-2 were drilled to investigate the effects of conventional drilling (wet) on fractured, densely welded tuffs. The boreholes were cored into the middle of the moderately to densely welded unit in the Grouse Canyon Member. A "rubble pocket" was encountered in U12g DD-2 consisting of welded lithic fragments in a clayey matrix. A number of argillized pumice fragments were intersected in both of the boreholes.

Core logs and borehole video survey tape recordings were used to compile fracture data from the boreholes. A total of 45 fractures were logged in the U12g.12 boreholes. All but one of the fractures occurred in silicified or mixed silicified-zeolitized areas. The strikes of the majority of the fractures were approximately parallel to the drift and a nearby fault. The 19 fractures in U12g.WD-1 and 21 of the 26 fractures in U12g.12 DD-1 had strike directions between N. 50° W. and N. 65° W and dipped 90-90 degrees to the northeast. The remaining fractures in U12g.12 DD-1 had strikes of N.40° E. and N. 55° E. In general, the fractures were located in the more indurated and brittle silicified units.

The two boreholes cored into the moderately to densely welded tuffs intersected numerous fractures. A total of 46 fractures were intersected in borehole U12g DD-2 and 40 in U12g WD-2.

Dips were generally steep (80 to 90 degrees) and to the northeast with strikes between N. 20° E. and N. 45° E. for a majority of the fractures. The higher fracture frequency in the welded tuff is consistent with observations throughout the GTUF and other tuffaceous units. Water loss during drilling of U12g WD-2 suggests that some of the fractures were open and may be persistent.

2.2 Process Models

2.2.1 G-Tunnel

It is initially assumed that the rock matrix constitutes a porous medium in which the flux of both liquid water and pore gas may be calculated using Richards Equation (1931). Combining Richards' Equation with the equation of continuity to account for transient as well as steady-state flow process gives the general flow equation in one dimension:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(\theta)\frac{\partial \psi_m}{\partial z} + K(\theta)\frac{\partial \psi_z}{\partial z}\right]$$

where θ is volumetric water content, t is time, z is distance, $K(\theta)$ is hydraulic conductivity as a function of θ, ψ is the potential gradient (subscripts m and z are matric and gravitational

potentials, respectively).

Two additional relationships are necessary to model the movement of water in unsaturated rock. The first describes the water content-water potential relation ($\theta(\psi)$) during sorption and desorption and the second describes the dependence of the hydraulic conductivity on water content $K(\theta)$. Although the initial conditions of θ and ψ_m can be estimated from core samples, the calculated flux applies only if conditions are constant (steady state). Since it is expected that the perturbation of drilling alters steady state conditions (if they exist at all), transient air and water flow will occur until equilibration is established it is necessary to obtain characteristic curves for both $\theta(\psi)$ and $K(\theta)$.

A number of models have been proposed to describe functional relationships of $\theta(\psi)$ and $K(\theta)$ (eg. Van Genuchten (1980), Mualem (1976), Brooks and Corey (1964), and Burdine (1953)). These models are currently being evaluated to determine their applicability to welded and nonwelded tuffaceous rock.

3.1 Measured Parameters

3.1.1 G-Tunnel

A number of laboratory and field experiments were conducted to obtain the following information:

- the physical characteristics of nonwelded and welded tuffs
- the impact of the drilling method on the *in situ* hydrologic and thermal conditions in tuffs
- rate of equilibration for the hydrologic conditions after drilling
- the sorptivity (Philip's, 1957) of welded and nonwelded tuffs over a range of scales

Table 3.1.x lists parameters that were measured as part of the G-Tunnel Experiment. More detailed information is provided in the appendix for a number of the parameters. Additional information will also be made available on a request basis.

Table 3.1.x: Information measured in the G-Tunnel Experiment.

METHOD	INFORMATION
Drilling of Core	Water loss to formation
	Air loss to formation
	Rock temperature

METHOD	INFORMATION
Borehole Logs	Neutron log
	Television log
	Fracture log
	Lithology log
Laboratory Core	Gravimetric water content
	Volumetric water content
	Bulk density
	Porosity
	Grain density
	Water potential
	Imbibition as func(time)
	Sorptivity as func(saturation)
	Composite $\phi(\Psi)$
Field Tests	Imbibition
	Air temperature vs time
	Barometric pressure vs time
	Water potential vs time

Additional measurements of saturated and unsaturated hydraulic conductivity, air permeability and water retention are currently being conducted on representative core samples. Saturated measurements are being done on both welded and nonwelded tuff samples. Methods for measuring unsaturated conductivity are under development.

The hydrologic properties of the fractures are inferred from the empirical fracture data including fracture aperture, density, orientation, and the quantity of drilling fluid lost during drilling. The fractured, welded tuff is being modeled by representing the fractures and the rock-matrix as separate hydrologic systems. Because the modeling of fluid movement in complex fracture systems remains poorly developed, the fracture system is treated as an

equivalent porous medium with a high saturated hydraulic conductivity and small storage coefficient. The hydrologic properties for the fracture system are estimated by determining the best fit of the parameters to describe observed the observed fluid loss during drilling.

3.2 Experimental Setup

3.2.1 G-Tunnel

The G-Tunnel Experiment was comprised of two activities. The first was the drilling of two pairs of parallel boreholes in welded and nonwelded units. One of the holes in each pair was drilled with water as the drilling fluid and the other with air. Fluid loss and rock temperature were monitored during drilling and neutron probe logs were run to estimate the water content along the length of the boreholes. Fracture data were collected from core and televiewer inspections. All of the boreholes were logged for fractures and water content and then instrumented to monitor water potential, air temperature, and pressure to monitor equilibration of conditions. The core samples were sealed and packaged for later laboratory measurements of water content, water potential and physical and hydrologic properties.

After the hydrologic conditions in the rock surround the boreholes reached equilibrium, imbibition experiments were performed in the dry-drilled boreholes. An inflatable packer was installed at the collar of the borehole and water was introduced through tubing fitted in the packer. The borehole was filled with water and a constant head of 3-5 cm was maintained during the test.

The flow rate into the heavily fractured borehole in the welded tuff exceeded the capacity of the reservoir system. The transmissivity of the fractures suggest they are pervasive and possibly connected to other open fractures. The imbibition experiment was successful in the borehole in nonwelded tuff where there are fewer fractures having low conductivity.

Imbibition experiments were also conducted in the laboratory using samples from the recovered core. A constant head Mariotte system was used in the experiments with water supplied to the base of the sample through a funnel fitted with a fritted glass plate (Figure 1). Imbibition was measured by monitoring the water loss in the Mariotte bottle via an analytical balance. The system was placed inside a glove box and exposed surfaces sealed to minimize evaporation and maintain stable conditions.

Imbibition tests were performed with sixteen nonwelded and five welded core samples having a diameter of 6.1 cm. Ten of the samples (five welded, five nonwelded) were used to examine what impact the initial water content had on the test results. Moisture content conditions of 25%, 50%, 75%, in situ, and oven and air dry were used. The tests were repeated with smaller diameter samples, 3.2 cm in diameter, undercored from the 6.1 cm samples.

3.3 Available Experimental Results

3.3.1 G-Tunnel

The laboratory and field imbibition data were compared to evaluate the influence of the scale on the experimental results. The sorptivity term of the Philip's infiltrations equation (1957b) was used for comparison:

$$I = S \cdot t^{1/2} \cdot At$$

where I is the infiltration into the rock, S is the sorptivity and t is time. Sorptivity is defined as the measure of water uptake by a porous media without gravitational effects. It was assumed that the second term in the right side of the equation can be ignored if the very early portion of the experimental data is used (Talsma, 1969).

Bouwer (1978) concluded that the sorptivity of a material depends on its structure and water content. Based on this assumption, the laboratory scale measurements of sorptivity, porosity, matric potential, etc., provide a means to evaluate the heterogeneity of the rock over small distances. The sorptivity of the rock mass in the larger-scale field experiment provides a means of assessing the representativeness of the small-scale data.

Table 3.1.x lists the data that were collected as part of the G-Tunnel Experiment. The data set is available on 5.25" diskettes in ASCII format. Saturated and unsaturated hydraulic conductivity, air permeability and water characteristic data are still being collected. These data will be added to the data set during periodic updating of the files.

4.1 Inverse Modeling

4.1.1 G-Tunnel

Standard nonlinear numerical techniques are being used to fit a variety of empirical equations such as those proposed by Van Genuchten (1980), Mualem (1976), Brooks and Corey (1964), and Burdine (1953). A nonlinear least squares method are used to fit the equation to the measured data. Initial results suggest that any of the water characteristic curves provide reasonable representations of the data. The hydraulic conductivity curves are less satisfactory. None of the proposed correlations between unsaturated conductivity and water characteristic curve are capable of reproducing the experimental observations. Alternative empirical equations are being considered.

Two possible explanations for the lack of fit are: 1) the water characteristic curve data or unsaturated hydraulic conductivity data are in error or; 2) the standard formulation of the $\theta(\psi)$ and $K(\theta)$ equations are inappropriate for tuffs under investigation. The equations are being evaluated by comparing measured values of imbibition with modeled values using the TOUGH code (Pruess, 1987). TOUGH requires estimates of $\theta(\psi)$, $K(\theta)$ and saturated hydraulic conductivity (K_{sat}). Sensitivity analyses will be performed to determine the importance of the relationships in modeling imbibition.

4.2 Predictive Modeling

4.2.1 G-Tunnel

Once all appropriate data is collected and models selected or derived, the TOUGH code will be used to perform all of the hydrologic modeling tasks. TOUGH was selected since it is capable of treating the storage and flow of liquid water, water vapor, gas, and heat in three-dimensional systems of arbitrary geometry. The details of code implementation for this experiment will depend on drilling fluid flux measurements, on the system geometry as inferred from the borehole locations in the GTUF and the borehole logging operations, and on the locations of the instrument stations within the boreholes.

TOUGH will be used to predict the results of the borehole imbibition experiment as well as the results of wet and dry drilling experiments. Water loss into the formation from drilling should be similar to the imbibition experiment, in both the welded and nonwelded tuff units. The fracture geometry and aperture are probably the most critical information for the welded unit whereas matrix properties are most critical for the nonwelded unit.

The hydrologic property data for the rock matrix and estimates of the fracture properties will be used for modeling the field experiments. Analyses will be performed both for the steady-state and transient effects observed in the wet-cored boreholes.

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THE INFLUENCE OF SCALE ON CALCULATED SORPTIVITY VALUES FROM IMBIBITION EXPERIMENTS ON WELDED AND NONWELDED TUFF

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ABSTRACT

Imbibition experiments were conducted on welded and nonwelded volcanic tuffs to determine the influence of sample size on the calculation of Philip's sorptivity parameter at four different scales. Rock cores, 3.2 and 6.1 cm in diameter by an average of 5 cm long, were used in two laboratory scale experiments. A horizontal borehole, 10 cm in diameter by 10 m long, was used for the two field scale experiments. Imbibition into the entire borehole was the largest scale experiment and neutron log data collected before and after the imbibition experiment yielded the intermediate scale data. The two sizes of core exhibited virtually the same sorptivity and either could be used to predict the results of the borehole scale experiment as long as the number of samples was large enough to represent the spatial heterogeneity. Core samples could be used to predict the neutron log data only if the unique system geometry was known and accounted for *a priori*. The neutron log data could be used to predict the results at the borehole scale but could not be used to predict the results of the core samples due to the spatial heterogeneity and the larger sampling volume.

1. Introduction

Yucca Mountain, Nevada, USA, is currently being investigated as a potential site for the nations's first high-level nuclear waste repository [1]. Standard hydrologic methods may not be applicable since Yucca Mountain is composed of a series of partially-saturated and fractured vitric to devitrified ash-flow and ash-fall tuffs [2]. Therefore, before full site characterization begins a series of prototype tests will need to be conducted to develop the necessary methodologies and models required to characterize the physical and hydrologic properties of these tuffs. One prototype test being conducted is designed to determine the influence of drilling fluids (air and water) on *in situ* conditions and core samples obtained during drilling [3]. The prototype drilling activity is being conducted in an analog site located in the G-tunnel Underground Facility (GTUF), which is in the Rainier Mesa area of the Nevada Test Site, 145 km northwest of Las Vegas, Nevada (48 km NE of Yucca Mountain). GTUF is a mined research facility that penetrates welded and nonwelded tuffs, similar to those at Yucca Mountain.

One major issue in site characterization that needs to be addressed is the applicability of core measurements to field scale processes, particularly water flow. Core analysis will be a major source of information on the hydrologic characteristics of Yucca Mountain [4]. As part of the prototype activity, an analysis of spatial variability and scale effects (sample volume) is being conducted. Imbibition was selected as the test to be conducted at both core and field scales and used to evaluate how representative each sample was of the hydrologic flow characteristics.

For short term experiments imbibition data can easily be converted to sorptivity which is defined as the measure of the uptake of water by a porous media without gravitational effects [5]. This uses Philip's infiltration equation ($I=St^{0.5}+At$), where I is infiltration (imbibition), S is sorptivity, t is time [6], and A is related to the full analysis of the infiltration relation developed over long time periods [7]. This method is based on the assumption that for the early portion of infiltration, the second term of the right-hand side of the two-parameter equation can be neglected [8]. Sorptivity ($S=I/t^{0.5}$) varies with media structure and water content [9] and is linearly related to saturation [10]. Therefore, sorptivity at a particular saturation (e.g. *in situ*) can easily be compared at different scales. This, along with comparisons of physical properties and state variables, can help to evaluate the physical and hydrologic variability existing in the field.

2. Materials and Methods

Laboratory analyses on two different diameters of rock core were used to represent the laboratory scale processes. Core samples are 6.1 cm in diameter, which is the size that will be collected at Yucca Mountain, and 3.2 cm diameter core which is the standard size used by most commercial laboratories testing core for the oil and gas industry. Two experiments were conducted in the GTUF boreholes to represent the field scale processes. The field experiments were conducted in two dry-drilled horizontal boreholes (10 m in length). One hole was in slightly fractured, nonwelded tuff, with five alternating layers of zeolitized and silicified materials in dipping beds. The other hole was drilled in highly fractured densely welded tuff. Both boreholes were continuously cored and provided good quality 6.1 cm diameter core samples.

a. Laboratory measurements

(i) Imbibition Experiments

Five nonwelded (3 zeolitized and 2 silicified) and 5 welded core samples were selected to determine the influence of the sample volume on sorptivity. Once imbibition measurements were made and porosity measured on the large core samples, the samples were undercored to 3.2 cm diameter and the same experiments and measurements were repeated. Imbibition measurements were conducted on each core at approximately 75, 50, and 25 percent saturation and at *in situ*, air dry, and oven dry water contents. Cores were brought to specific water contents by vacuum saturating and evaporating to the required weight, then left enclosed in an air tight container and allowed to equilibrate for at least 4 days. (One-dimensional simulations using a Richard's equation based flow code [11] were run which indicated that redistribution would be complete for all cores within 4 days.) An additional 12 nonwelded samples (6.1 cm diameter) were selected and used in the analysis of the field scale processes (5 were zeolitized and 7 were silicified). Imbibition experiments done on these core were at *in situ* saturations to enable direct comparison with measured and estimated borehole sorptivity.

A constant head Mariotte system was used to measure imbibition. The system was composed of a Mariotte reservoir connected to a buchner funnel fitted with a fritted glass disk (Fig. 1a). The core sample was placed on filter paper on the fritted glass disk and the Mariotte reservoir was located on a computer-controlled top loading balance. It was assumed that water loss from the Mariotte reservoir was imbibed into the sample. The entire system was placed inside an acrylic glove box to keep it free of drafts and to maintain temperature stability. Parafilm was placed over the top of the funnel to minimize evaporation from the core or the fritted glass disk.

Imbibition versus time was plotted for each core at each saturation. The early part of the data was linearized by transforming time to the square root of time and plotting against the volume of water imbibed through the cross sectional area of each core. Sorptivity is the slope of the linear portion of the plot.

(ii) Physical and hydrologic analyses

Core samples were analyzed for bulk density, particle density, porosity, *in situ* volumetric water content and relative saturation. Bulk density was measured using Archimedes' principle. Particle density was measured using water pycnometry [12]. Porosity was calculated as 1-(bulk density/particle density). Volumetric water content and relative saturation were calculated from the measured gravimetric water content and above measured parameters.

b. Field measurements

(i) Imbibition experiments

The boreholes were fitted with a packer which inflated to seal the opening of the borehole while allowing water to move through the packer (Fig. 1b). A valve through

the packer was connected to a large Mariotte bottle (160 L). A pressure transducer at the top of the Mariotte bottle was calibrated to allow for the determination of the volume of water entering the borehole. The transducer was connected to a datalogger which collected readings at 30 second intervals and was verified by occasional readings of the site tube installed on the outside of the Mariotte bottle. The bubbler valve at the bottom of the Mariotte bottle maintained a constant head 3-5 cm above the opening of the borehole.

Initially the boreholes were rapidly filled with water by opening the air entry valve at the top of the Mariotte bottle. Before the borehole was completely filled the Mariotte bubbler system was started to maintain a constant head. The borehole then filled up at a rate somewhat less than what the Mariotte system was delivering, as water was imbibing into the borehole as it filled. Water flow into the welded tuff exceeded the supply rate of the Mariotte bottle due to the high amount of fracture flow. Therefore, the only field scale imbibition estimates made in the welded tuff were from neutron logs.

Imbibition into the borehole was assumed to be 1-dimensional and linear through the surface area of a cylinder to simplify modeling, although it is recognized as 3-dimensional and radial. Since the imbibition into the rock matrix was at a slow rate and the penetration distance was small, the initial 1-dimensional linear flow assumption was assumed to be adequate for the comparison of different scales.

(ii) Neutron Logging

Boreholes were logged at 0.1 meter intervals for determination of volumetric water content before and after the field scale imbibition experiments using a neutron moisture meter (Model 503, Campbell Pacific Nuclear, Martinez, CA.). (The neutron moisture meter was calibrated using the core collected during the wet and dry drilling experiment.) The radius of influence (volume of detection) of the moisture meter was calculated to be 0.25 m using a procedure similar to that used by Klenke and Flint [13].

c. Analytical analysis of sorptivity

Four methods were used to calculate sorptivity at the borehole scale, two using laboratory measurements on the two different sizes of core and two using field measurements in the borehole, from the neutron moisture meter and the Mariotte system.

(i) Calculations from core

Estimates of borehole sorptivity from laboratory core measurements were made using 2 methods. Weighted averages based on surface area were calculated for each of 5 zones in the borehole using laboratory core data with estimated *in situ* sorptivities. Another method utilizing the core data was that of defining the relationship between sorptivity, porosity and relative saturation to estimate the sorptivity of all of the core collected (n=95). A regression equation was developed using porosity and relative saturation for all measurements from large and small core to predict sorptivity. This equation was then used with borehole porosities and saturations measured on the remaining core from approximately each 0.1 m depth to predict borehole sorptivity.

(ii) Calculations from neutron logs

The difference in water content calculated from the neutron moisture meter logs at each increment was assumed to be the amount of water imbibed by the formation during the experiment. Sorptivity was calculated by knowing the total amount of time that water was imbibing, the surface area for imbibition and by assuming that all of the water imbibed by the formation was within the 0.25 m radius of influence of the neutron moisture meter probe.

(iii) Calculations using Mariotte system

The final method used the data from the direct measurements of water entering the borehole using the Mariotte system. Once the borehole was full, a sorptivity was calculated from a linear regression developed using water supplied to the borehole and the square root of time. The time the borehole was completely full was verified by an iterative technique using a surface area corresponding to the height of the water in the borehole at each time step during filling, and assuming imbibition into that surface area at the rate corresponding to an initial estimate of sorptivity. The new sorptivity was put back into the calculation until convergence was achieved. The calculation of sorptivity averaged in any loss of water to fractures causing an overestimation of sorptivity since the surface area for imbibition would have been underestimated.

(iv) Sensitivity of sorptivity to fractures

The presence of conductive fractures complicates the calculation of borehole sorptivity because of the uncertainty of the surface area for flow and of the length and aperture of the fractures. An analysis of the importance of the fractures was done by increasing the value of surface area for the imbibition calculation. The additional area was estimated by assuming, 1) the fractures could be simulated as parallel plates, and 2) the fractures originate in the silicified zone and terminate some distance into the zeolitized zone. The second assumption is supported by fracture mapping utilizing television logs and core analysis. It was assumed that fractures contributing additional surface area were of an aperture large enough to allow for imbibition from approximately a free water surface.

d. Spatial analysis using variography

Another technique to estimate the adequacy of a sample to describe the rock properties some distance away is the use of geostatistics. Experimental variograms were calculated for bulk density, porosity, relative saturation and sorptivity. The range of the experimental variogram is the distance at which a sample is representative of the surrounding rock properties. This type of analysis is good for addressing the question of the number of core samples required to describe larger scale properties.

3. Results and Discussion

a. Laboratory measurements

(i) Imbibition

Sorptivities for the large core samples were calculated from imbibition measured at a variety of water contents to determine the relationship between sorptivity and saturation (Fig. 2). Although visually distinct, one of the silicified core behaved very similar to that of the fully zeolitized rock in terms of sorptivity, while the other silicified core exhibited sorptivities similar to that of the welded core. This disparity is due to the diffuse hydrologic nature of the silicified-zeolitized boundary. The sorptivity values determined on oven dry samples for most of the core samples were slightly less than the air dry values which were located between 0.10 and 0.15 relative saturation. Although the effect is present to a small degree in the welded tuff it is most readily apparent in the nonwelded tuff (Fig. 2). The stronger effect in the nonwelded tuff may be due to alteration of zeolites and swelling clays during oven drying.

Individual linear regressions between relative saturation and sorptivity were calculated for both the large and small core samples. The regression equations were used to predict sorptivity at 50% saturation for each core to provide a common reference to compare the two core sizes. Porosity and sorptivity means at 50% saturation are presented in Table I. There was no significant difference (alpha=0.05) between large and small core although it should be noted that a decrease or increase in sorptivity was accompanied by a similar decrease or increase in porosity. When the large core samples were undercored there were inclusions or exclusions of higher porosity pumice fragments in the smaller core. The concentration of the pumice fragment in the small core may have lead to the increase in sorptivity whereas the exclusion of the pumice fragment could easily lead to a decrease in sorptivity. Once it was determined that there was no difference in sorptivity between cores of different sizes, remaining analyses to compare core with borehole sorptivity estimates were done with large core samples (n=12) from the nonwelded borehole.

(ii) Physical and hydrologic properties

The remaining physical measurements were done on all core samples collected approximately every 0.1 m from the nonwelded borehole. These data were used to evaluate the spatial variability in physical and hydrologic properties. Figure 3 shows volumetric water content with depth determined from core samples and measurements using the neutron moisture meter before and after the borehole imbibition experiment. Along the bottom of the figure is the fracture and lithology log for the borehole. The core data represents the water content at a point, whereas the neutron log represents the average water content some distance into the formation. Note that the different lithologic zones are tilted to a degree that when the neutron probe is in one zone it may be measuring the water content in the zones above and below rather than the zone from which the core were taken. This disparity is seen in silicified zones where the neutron probe is sensing the water in the wetter zeolitized zone, and in the middle zeolitized

zone were the neutron probe is sensing the drier silicified zones. The same disparity shows up in the neutron data where the difference in logs before and after the experiment indicates the change in water content due to the imbibition of water into the rock surrounding the borehole. It appears that the silicified zones take up considerable water but it is actually an increase in the water content of the surrounding zeolitic zone. The most probable path was through the fractures in the silicified zone.

b. Field measurements

(i) Imbibition

The data collected during the borehole imbibition experiment are presented in Figure 4. There are 5 important points in time (noted in Fig. 4) that were used to evaluate the imbibition data. Initially the air valve at the top of the Mariotte bottle was open and water was allowed to flow freely into the borehole. At time 1 the air valve was closed and at time 2 the bubbler started and a constant 5 cm head was maintained for the remainder of the experiment. At time 3 one borehole volume of water was delivered but the borehole was not completely full at that time since some water had been imbibed. The borehole was full at time 4 and remained full for the remainder of the experiment. Imbibition appears to be continuing at a constant rate (using the square root of time) until time 5, about 9 hours after the experiment started, when imbibition started to noticeably decline. A regression analysis was done with the data between time 4 and time 5 to calculate a borehole sorptivity of 0.295 $cm/hr^{0.5}$.

As the welded borehole drained faster than the Mariotte bottle was able to supply water, there was no sorptivity estimated using the Mariotte data. The Mariotte bottle air valve was opened and the system operated as a falling head infiltrometer. This data was still not adequate to calculate borehole sorptivity due to the large unknown fracture contribution to flow. Neutron logs were, however, used to estimate a lower limit of sorptivity (0.019 $cm/t^{0.5}$) since some water was imbibed into the formation. Sorptivity of the original 5 large welded core samples was calculated for *in situ* saturations and a mean sorptivity of 0.015 $cm/t^{0.5}$ was estimated for the borehole. The large fracture network and subsequent increase in surface area for imbibition led to the higher estimate of sorptivity for the neutron data (Table II).

(ii) Neutron logs

Figure 5a shows estimates of borehole sorptivity for the nonwelded unit using the neutron logs before and after the field imbibition experiment, along with the mean estimate. Also shown are the mean estimates from the core samples and the Mariotte system. The major difference between the sorptivity values from the core data and the neutron estimates is again the disparity of the measurement between point samples (core) and large volume sampling (neutron logs). The apparent increase in sorptivity in the silicified zone is likely due to fractures supplying water to the zeolitized zone above and below. The reduced estimate of sorptivity in the middle zeolitized zone is likely due to the bed being thin and bounded by low sorptivity silicified zones. One uncertainty in the neutron log is in the assumption used for the radius of influence of the neutron

moisture meter. Changing the estimate of the radius of influence will move the neutron plot up or down. Some estimates of the actual radius can be made by examining the upper and lower limits. The value used in the calculations is 0.254 m (slightly higher than the 0.25 m cited by Klenke and Flint [13]) which is a maximum estimate as it numerically accounts for 100% of the water delivered by the Mariotte system. A minimum value would be 0.223 m which would calculate a sorptivity matching the core mean. The true radius of influence should be somewhat higher than the lower limit since the core measurements do not properly incorporate the fractures. Although the plot can move up or down under these assumptions, the relative comparison between zones is still valuable in assessing the relative importance of fractures in transporting water.

The sorptivity calculated from the Mariotte system measurement is the highest because of the contribution of fractures which provides an increased surface area. A 55% increase in surface area for imbibition would produce an estimate of sorptivity that matches that of the core mean, suggesting that, as a maximum, fractures contributed to about 35% of the total surface area. Since the fractures penetrate a low sorptivity rock (the silicified zone) and terminate in a high sorptivity zone (the zeolitized zone) the calculation of actual contribution cannot be made.

The mean values between the three methods match quite well despite the assumptions made. The Mariotte and neutron methods are expected to be somewhat higher than the matrix sorptivity measured on the core. This is due to the fractures and their connection to the higher sorptivity rock surrounding the fracture zones in the borehole.

c. Analytical analysis of scale

Fig. 5b shows the comparisons of borehole sorptivity estimates over the length of the borehole using two core methods. The values of sorptivity measured on each core at *in situ* saturations are shown. The measured core data was used to model sorptivity of the borehole at every 0.1 m. A regression equation was developed which used sorptivity data at different core saturations for the 5 large core and subsequent small cores along with measured porosity for each core. This was then applied to the borehole by predicting sorptivity using physical measurements of all core samples taken from the borehole. The equation includes porosity (P) and relative saturation (SAT), plus an interaction term between porosity and saturation (P•SAT), and yields a coefficient of determination of 0.882 (Fig. 5b). The sorptivities predicted with the regression equation are quite similar to those determined for the cores. It is possible that a separate relationship should be determined for each lithologic unit if more data were available. This analytical analysis is attempting to show high degree of inherent variability in the matrix at the borehole scale without regard to fractures.

d. Variography and spatial variability

Experimental variograms were calculated (Figures 6a and b) by using a fixed 0.1 m pair spacing and variable pair number with no pair number less than 30. The experimental variograms for bulk density, sorptivity, porosity and saturation provided some insight into the structure of the spatial variability. The undulation or "hole effect" in the variogram is the result of the alternating zeolitic and silicified beds penetrated by the

borehole. This effect for porosity is more subtle because it is less sensitive to lithology differences than the other three parameters. The beds alternate at approximately 2 m distance as does the experimental variogram.

A Gaussian model with a nugget was fit to each experimental variogram. A Gaussian model fit better than a spherical model due to small scale continuity that showed up at the sample spacing of 0.1 m but not at larger spacings. The nugget values for porosity and bulk density are relatively small because their physical characteristics are independent of any other variable and should show a greater continuity at the sampling scale. Sorptivity and saturation both depend on porosity but introduce additional variables thus increasing the inherent variability displayed in their higher nugget values. Sorptivity has the highest, as characteristics influencing flow, such as tortuosity, clays and zeolites influence the measurement.

The range of each model variogram was 1.12 m. Even though visually the beds repeat at 2 m the contacts are fairly diffuse when judged using hydrologic properties. The range of 1.12 m indicates that a sample may not be representative of the rock more than a meter away and a minimum of 5 samples would be required to use the model variogram to any advantage to estimate properties at all unmeasured locations. No geostatistical analyses have been done on the welded core at this time.

4. Summary and conclusions

Estimates of sorptivity, a hydrologic parameter that is relatively quick and inexpensive to determine, show no scale effects between the core sample size attained from the borehole (6.1 cm) and that used by most commercial laboratories (3.2 cm). Sorptivity estimates for the nonwelded core samples were an order of magnitude higher than the welded core as expected due to the much lower porosities (0.14 cm^3/cm^3 compared to 0.30 cm^3/cm^3) (Table II). Scale differences in sorptivity estimates were present in the field scale experiment when compared to core measurements. The neutron log estimates and Mariotte measurements were both higher than the mean of the large core sorptivities, all at *in situ* relative saturations. This can be attributed to the presence of fracture networks which provided an increased surface area for imbibition in the nonwelded borehole. The Mariotte value was higher because it was calculated independent of fracture flow, using the surface area of the borehole cylinder rather than a larger estimate incorporating fractures. In addition, if the imbibing surface area is correctly accounted for, the total water imbibed into the borehole could be correctly calculated using the core sorptivity values. If, on the other hand, the correctly estimated increase in surface area is used in the calculations of borehole sorptivity, the field experiment would predict the average values of the core. Variography indicated that attempts to define the hydrologic and physical character of the nonwelded tuffs in this location require at least one sample every meter. A proper account of the scale at which sorptivity is measured must account for the system geometry and the flow mechanisms present in the system. Once the mechanisms are understood, smaller scale measurements can successfully predict larger scale processes.

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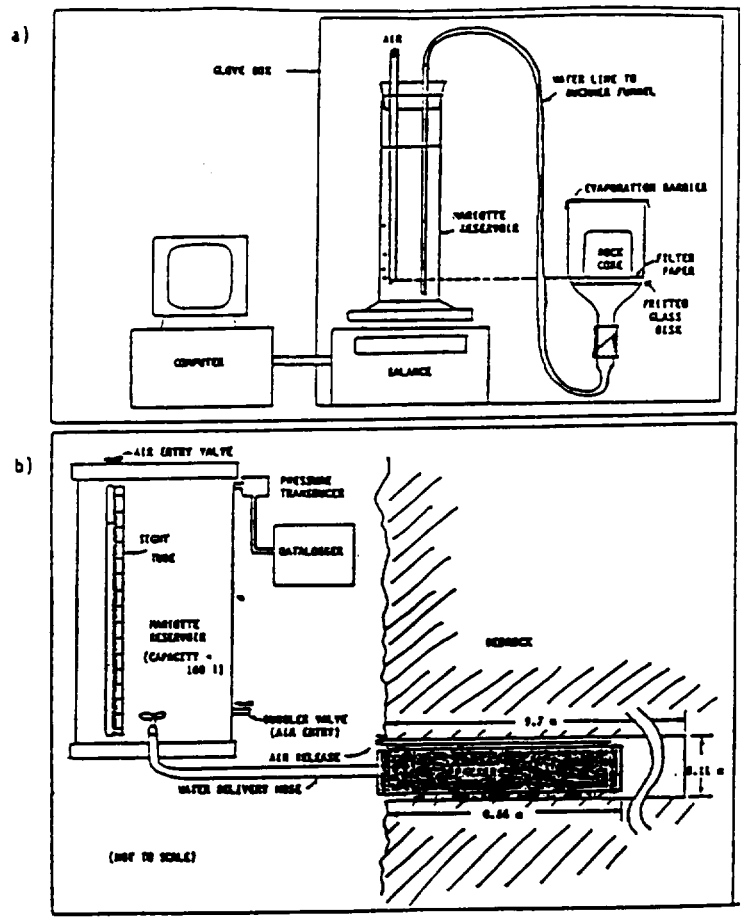

Figure 1. a) Mariotte system for laboratory imbibition measurements.
b) Mariotte and borehole system for field imbibition measurements.

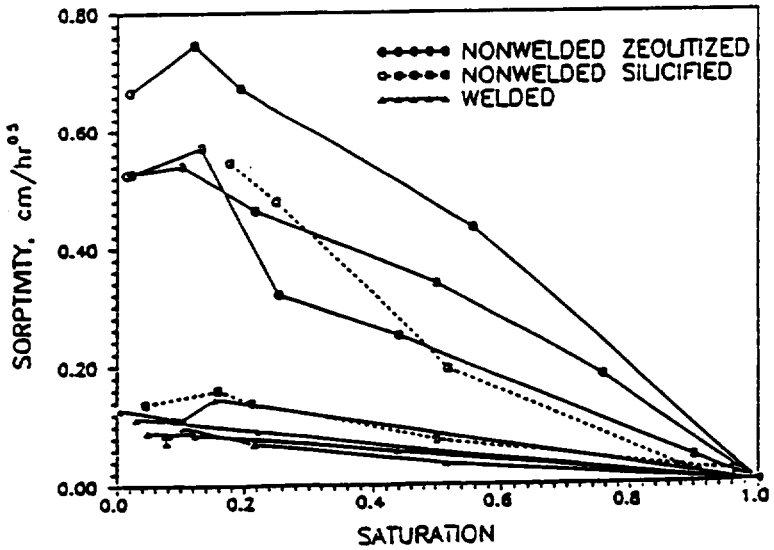

Figure 2. Sorptivity for nonwelded and welded large core at various relative saturations.

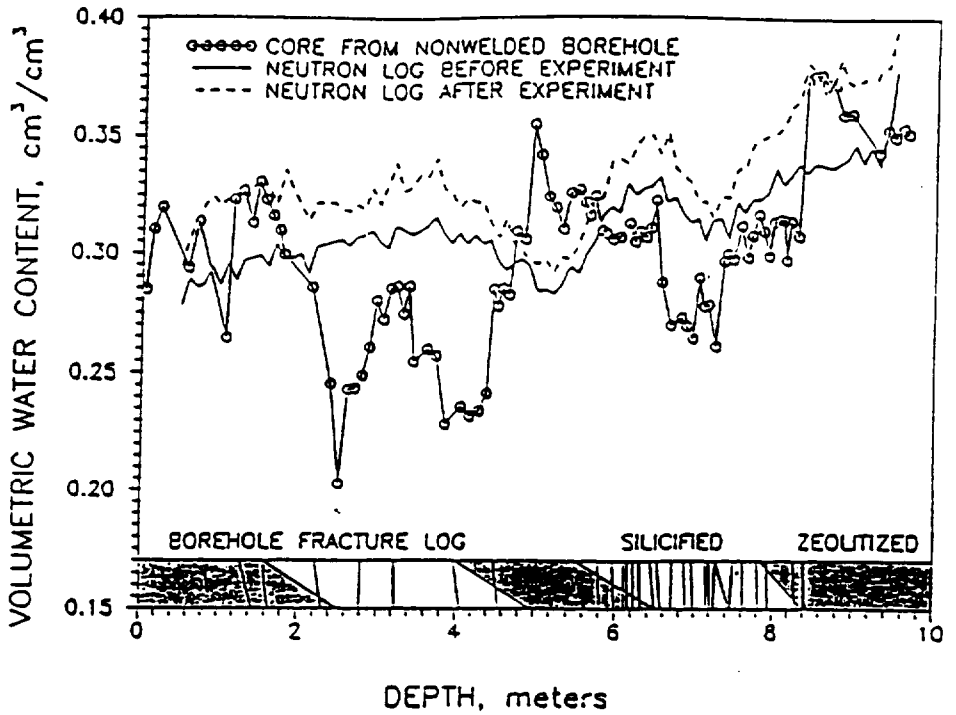

Figure 3. Volumetric water content of core and neutron log (before and after imbibition) both at 0.1 m spacing and fracture logs of nonwelded borehole.

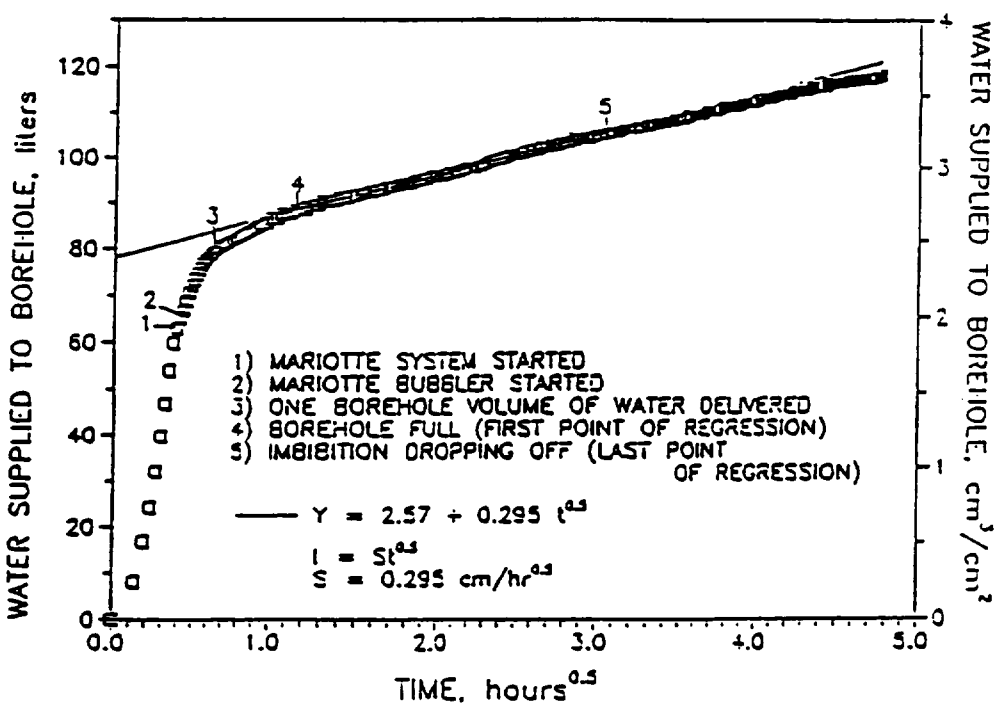

Figure 4. Imbibition as water supplied to borehole from Mariotte system in borehole versus time$^{0.5}$. Regression equation calculates sorptivity.

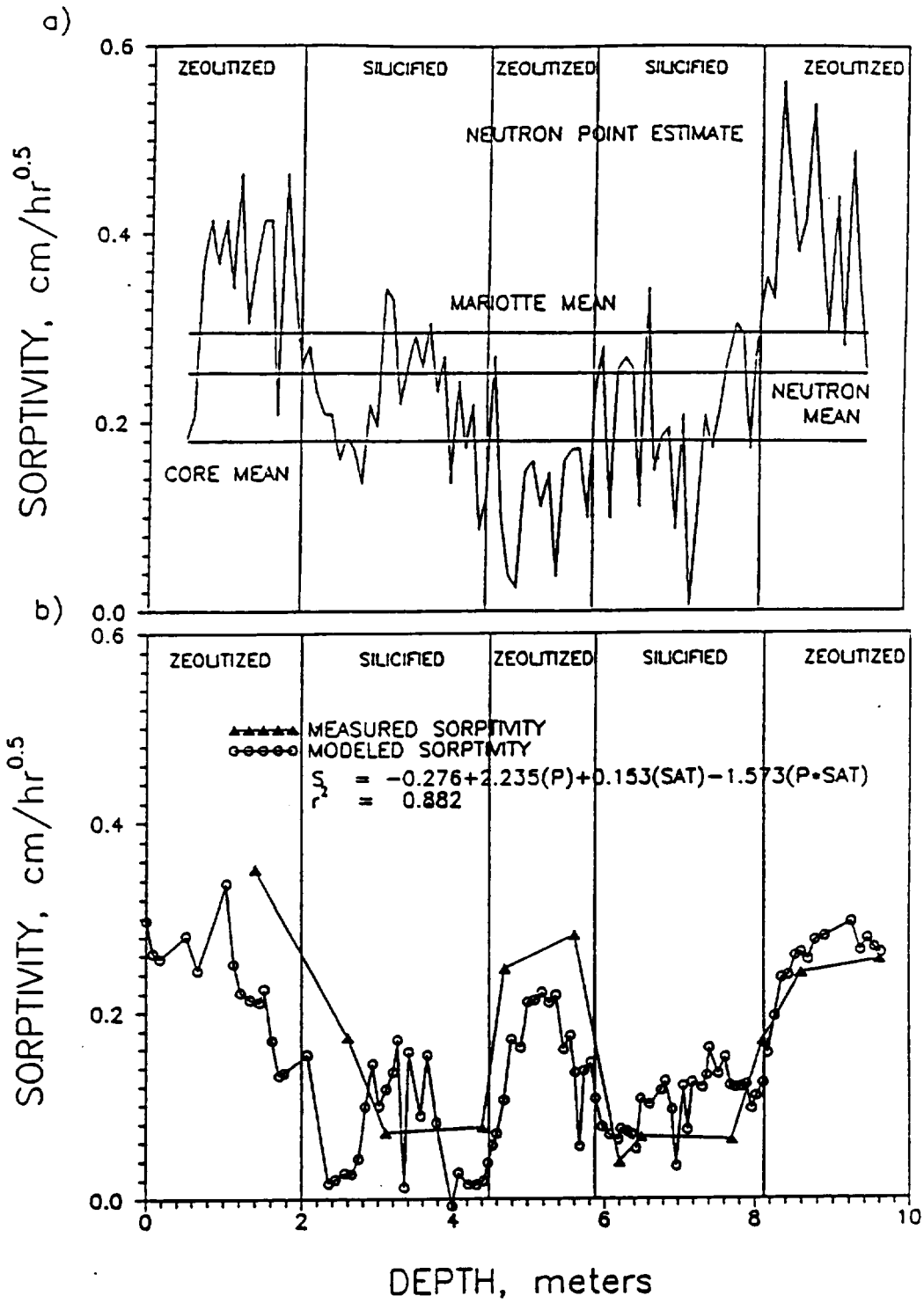

Figure 5. a) Borehole sorptivity measured on 12 core samples and modeled using all borehole core samples.
b) Borehole sorptivity estimated using neutron logs. Included are mean sorptivities from neutron logs, core samples and Mariotte estimates.

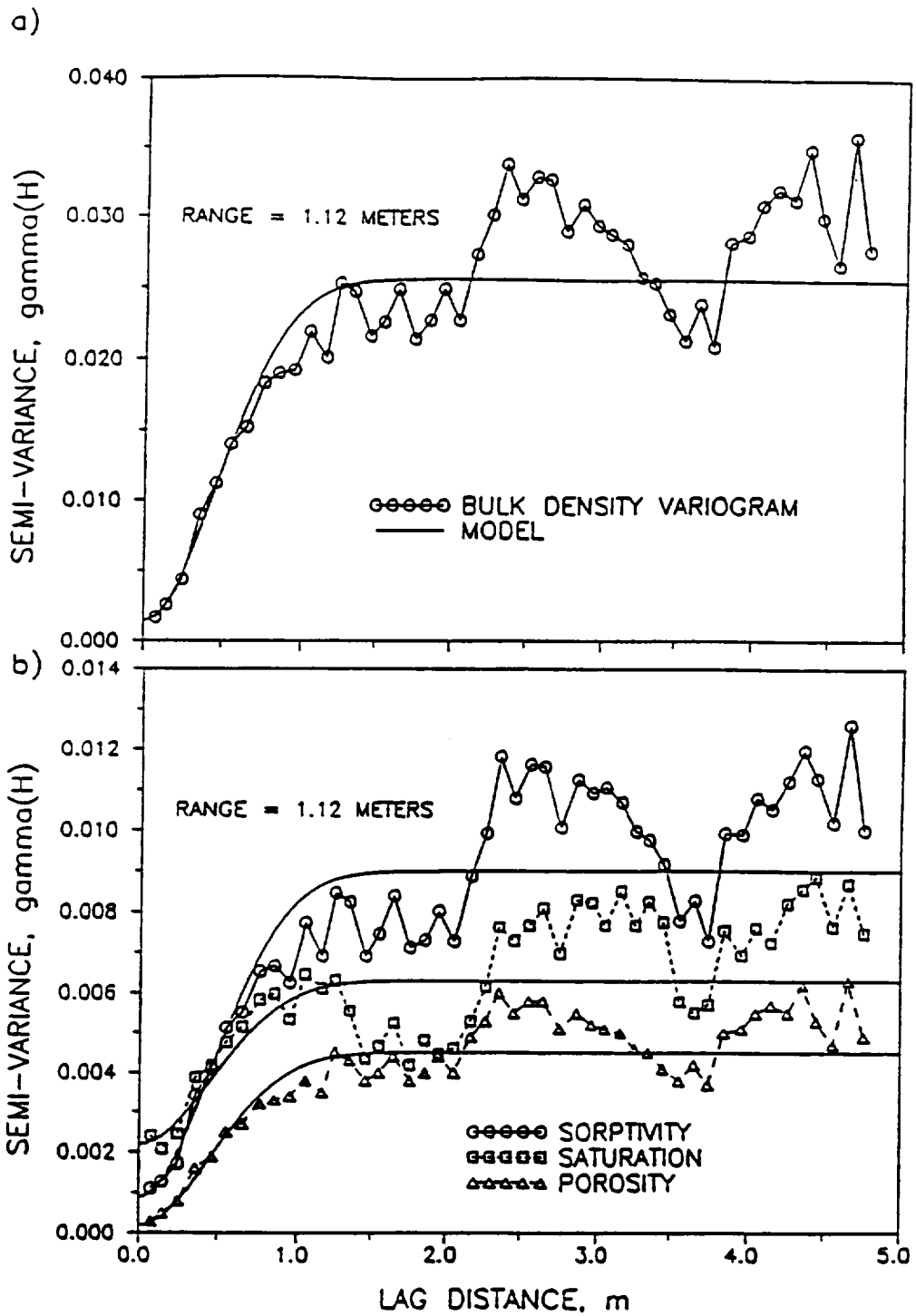

Figure 6. a) Variogram of bulk density and fitted model in nonwelded borehole.
b) Variograms of sorptivity, relative saturation and porosity with fitted models in nonwelded borehole.

Table I. Mean porosity and mean sorptivity at 50% saturation for 10 large and 10 small core.[1]

Core		---- *Large* ---- Sorp	Porosity	---- *Small* ---- Sorp	Porosity
Welded	Mean	0.056[2]	0.151	0.054[2]	0.130
	Std dev	0.009	0.025	0.007	0.034
Nonwelded					
Silicified	Mean	0.190[2]	0.286	0.136[2]	0.263
	Std dev	0.104	0.059	0.052	0.031
Zeolitized	Mean	0.339[2]	0.459	0.362[2]	0.465
	Std dev	0.082	0.031	0.044	0.023

[1]Sorptivity calculated at 50% saturation using regression equations from Table 1.

[2]A paired t test showed no difference between mean values of sorptivity of large and small core at $\alpha = 0.05$.

Table II. Summary of estimated sorptivities from core measurements and borehole estimates at *in situ* relative saturation.

		Nonwelded	Welded
Core comparisons	Large core mean (n=5)	0.099	0.015
	Small core mean (n=5)	0.097	0.015
Borehole estimates	Large core mean (n=12,5)	0.190	0.015
	Neutron log (n=90,90)	0.250	0.019
	Mariotte measurements	0.295	-

Appendix - INTRAVAL Review Comments

by:

L. Lehman for the State of Nevada, USA

INTRODUCTION

The U.S. Nuclear Waste Policy Act of 1982 (Sections 101 and 116) establishes the role of States in the development and siting of a High-Level Nuclear Waste (HLW) Repository within the United States. The Act provides grants be made available to States for the following purposes:

(i) to review activities taken with respect to the Yucca Mountain site for purposes of determining any potential economic, social, public health and safety, and environmental impacts of such repository on such State or affected unit of local government and its residents;

(ii) to develop a request for impact assistance;

(iii) to engage in any monitoring, testing, or evaluation activities with respect to site characterization programs with regard to such site;

(iv) to provide information to its residents regarding any activities of such State, the Secretary of Energy, or the U.S. Nuclear Regulatory Commission with respect to such site; and

(v) to request information from, and make comments and recommendations to, the Secretary regarding any activities with respect to such site.

It was within this review role that the State of Nevada requested permission to observe the activities of INTRAVAL. This is because decisions made within INTRAVAL may directly effect evaluation activities with respect to site characterization or overall repository performance in the US program. The State of Nevada has officially and repeatedly expressed concern over the scientific approaches taken to date by the U.S. Department of Energy (DOE), therefore our review of INTRAVAL will of necessity be from the "critical review perspective". We hope this review will serve to improve the overall quality and scientific merit of the validation research conducted by INTRAVAL and the approach eventually selected by the U.S. DOE.

The State of Nevada believes that the DOE approach will be strongly influenced by the recommendations of INTRAVAL. We therefore greatly appreciate the opportunity for participation and for the opportunity to provide review comments.

Funding for the State of Nevada's technical review has been severely cut back in recent years. Consequently, this has allowed only very limited participation within INTRAVAL. This participation is essentially limited to meeting attendance. It is the desire of the State to be able to independently run the test cases and have "hands on" experience with the test cases, however, funding levels provided to date have not been sufficient to allow this activity. The State, therefore, must focus its analysis and comments only on INTRAVAL test cases most relevant to the Yucca Mountain Site.

Current repository plans call for location of the repository within the unsaturated zone. The test cases dealing with unsaturated zone flow and transport are specifically Test Cases 10, 11 and 12. Our comments will address these Test Cases individually. In addition to the Test Cases, two general validation strategies have been developed within INTRAVAL for comment. The following section provides our comments on these strategies.

COMMENTS ON VALIDATION STRATEGIES

Within the past year, two validation strategies have been proposed for comment within INTRAVAL; one by the U.S. DOE and one by Sandia National Laboratories under funding by the U.S. DOE. The impetus for strategy development is mainly coming from the needs of the U.S. performance assessment program, although such a strategy should be a product of INTRAVAL, if one can be agreed upon. The two approaches, while similar in some aspects, represent different philosophies regarding what constitutes validation. It is clear that during the early phases of INTRAVAL no consensus exists as to what constitutes an acceptable validation. Obviously, it is different things to different people. Given the various roles and objectives of the participants i.e., regulators, researchers, modelers, experimenters and repository developers, the definition of validation will be difficult to pin down and will naturally evolve with experience and time.

U.S. Department Of Energy (DOE) Strategy

The DOE's objective in developing a validation strategy is to provide a systematic approach for establishing the evidence that a performance assessment model has been properly derived from defensible premises and provides a good representation of the system being modeled. There are 3 major components to this approach:

- Record of the derivation of the model (The assumptions on which it is based and the evidence that supports the assumptions.)

- Experiments which support assumptions
- Formal Technical Review

The DOE emphasis is on careful documentation of what has been done. The responsibility for the documentation falls on the modeler. The decision that some model has been validated is made by a formal Technical Review Committee.

The State of Nevada has concerns with this approach in its present form. Basically, as with any quality assurance measure, crossing the "t's" and dotting the "i's" falls short of assuring the science is correct. The assumptions can be listed and debated and some limited experiments can be conducted to provide evidence which supports some of the assumptions. The problem lies in the complexity of the processes involved, their scale, spatial distribution and their complex couplings. While the approach seems logical on the surface, implementation which is convincing to the scientific community has not adequately been addressed.

The DOE approach as currently outlined does not stress the validation of processes or relevant characteristics of processes such as spatial variability. It is preferable to validate that the processes being modeled are understood, are accurately represented by the models and are to some degree predictable, rather than validation by documentation, of computer or conceptual model assumptions and inputs.

Another shortfall of this approach is the limited peer review. By this we mean the limited numbers of select reviewers. Historically, the broad spectrum of open review has not been undertaken by DOE. Typically such review panels are comprised of only DOE or DOE supported personnel. The State, on the other hand, would encourage a more open review process; one which encourages the broadest participation possible and one which encourages affected party participation. Members of the review groups must be knowledgeable of the relevant disciplines by rock type and preferably within the regional setting.

Sandia National Laboratory (SNLA) Validation Strategy

The SNLA philosophy of validation is that validation constitutes "acceptable uncertainty". The focus is on assessing site safety - not merely on investigating scientifically interesting phenomenon. In this approach the computer codes become less important than the underlying model (conceptual or mathematical) used to describe the process of concern. This is because procedures are well established to verify the mathematical performance of computer codes.

The strategy consists of 10 basic steps as follows:

1) Define model purpose.

2) Conceptual model development.

3) Define performance measures and acceptance criteria.

4) Design validation experiment.

5) Measure "independent" parameters and uncertainty.

6) Simulate the experiment with uncertainty.

7) Perform the experiment.

8) Assess adequacy of the model structure.

9) Assess adequacy of the input data.

10) Repeat the experiment over the possible range of conditions expected at the repository only.

SNLA makes a distinction between process models and model geometries. This approach may make sense if one considers the question of spatial variability, however it has been pointed out that this separation may not be appropriate for some types of small scale data or pore scale processes.

Perhaps the most important insight provided by this work is the need to define appropriate performance measures. This is extremely critical since the choice of performance measure will dictate the validity of a model. In many cases, depending on the measures chosen, a model may be determined valid for some and invalid for others. SNLA points out this is where DOE will rely on expert opinion to sort out the "valid" results. The State foresees problems with this reliance on experts and urges INTRAVAL and other participants to focus considerable effort, early on in this process, to defining appropriate performance measures.

We agree that site safety must be the driving force for prioritization of work resources and it soon becomes apparent that with respect to Yucca Mountain, natural processes will be controlling. Here unsaturated fracture flow and transport processes will rank very high in uncertainty. So basic research into these processes is required to reduce uncertainty to acceptable levels, i.e., to validate these processes.

According to SNLA, INTRAVAL to date has approached the problem of validation in a backwards fashion. SNLA believes that INTRAVAL has done their experiments first and are now looking for the purpose. The State is in agreement, but is sympathetic to the INTRAVAL attempts. After all, one must start somewhere and hindsight is always 20/20.

While the SNLA approach has short comings, it does put higher emphasis on processes which are important to safety. The strategy should be exercised over a

range of performance measures and subjected to intense review by the scientific community. In this fashion the approach can be more appropriately defined.

COMMENTS ON TEST CASES

Test cases 10, 11 and 12 deal with unsaturated flow processes. Our current understanding of these processes stems from basic soil physics research which typically is conducted to depths of a few meters. In the U.S. high-level waste disposal program, we are concerned with these processes at depths of up to 750 meters. Unfortunately, there is a dearth of relevant data at these depths and the U.S. DOE program has produced and published almost no hydraulic data over the past 10 years on the unsaturated zone for the Yucca Mountain region. This adds to the difficulties in validation, i.e. a data set must first exist on which to validate conceptual processes.

The U.S. NRC, on the other hand, through their research efforts at Apache Leap and Las Cruces Trench is responsible for producing most of the unsaturated zone data available to date in the US program. These data sets are made available to INTRAVAL participants. While these data are of tremendous value, they cannot compensate for the lack of data at Yucca Mountain in the DOE validation process. We remain convinced that validation is, of necessity, a site specific problem.

These unsaturated zone experiments have all had to be performed more than once, with the exception of the USGS G-Tunnel Experiment. (This experiment should have been repeated, however the U.S. DOE decided to close G-Tunnel in order to save program dollars.) These experiments were redone, each time with a better understanding of data requirements and likely glitches. While nothing is wrong with this approach (repeatability is in fact preferable), it points out that high quality results are generally not obtained on the first run of an experiment. This is especially true of prototype testing needed to characterize unsaturated fracture flow and transport processes. Basically, we have come a long way, but we have even further to go before we can make the statement that unsaturated flow process models have been validated.

Test Case 10 - Las Cruces Trench

This test case is geared more to near-surface processes commonly associated with low-level waste disposal. However, it is of general interest to the State of Nevada. A number of researchers are modeling the experiments performed at this site using a variety of mathematical techniques which range from very simple to extremely complex.

This experiment is worthwhile and has provided a number of valuable insights. First, complexities due to different radionuclide or chemical retardation values is apparent and underscores the need to develop meaningful performance measures. Secondly, the accuracy required for these predictions should be evaluated. These experiments

are extremely well instrumented at very small spacings. The luxury of this much instrumentation will likely not be possible at a proposed low-level disposal site. This is because of cost and time factors related to the siting programs initiated under the Low Level Nuclear Waste Act.

Many of the simple methods have given generally comparable results to the more complex methods, though none of the modeling can be said to be perfectly representative for all performance measures. One must now ask when these results are adequate for licensing a facility. While it is of scientific interest to exactly match lateral spreading and exact concentrations with depth, the accuracy requirements depend on the problem and the timeframe of interest. Much of the required accuracy will be determined by facility design and buffer zone requirements.

Test Case 11 - Apache Leap Tuff

Test case 11 is composed of several individual experiments which are being carried out at the University of Arizona under U.S. NRC funding. These experiments cover differing scales, including laboratory, block and field scale work. Opportunities exist to examine effects of scaling. Continuation of this work, as well as additional field work is proposed for Phase II of INTRAVAL.

1) Laboratory Tuff Core Heating Experiment. The purpose of this experiment is to evaluate the magnitude and distribution of fluids and solutes along a partially saturated tuff core. The experiment utilizes a heat source to induce flow and transport processes in a closed system.

This experiment has done a lot to further our understanding of migration of solutes under thermal conditions expected in the nearfield of a HLW repository. However, since the cores used were mostly unfractured (perhaps some microfractures were present) and the system itself is closed, the experiment should continue to be duplicated to assess effects of fracturing. A Phase II heater experiment has been proposed for the field scale. This experiment should help to clarify these fracture effects under open conditions. Validation work has proceeded well and the experiment's replicability has been established.

2) Block Scale Fractured Rock Experiment. The objective of this experiment is to characterize fluid flow and solute transport in variably saturated fractured tuff rocks. To investigate this behavior, a series of experiments has been designed to characterize the hydraulic properties of the matrix and fractures under a range of matric suctions. The principal question is whether or not the convection-dispersion equation (Richard's equation) is valid for unsaturated tuff.

This experiment has been fraught with problems since its inception, which serves to limit its value as a validation exercise during the first phase of INTRAVAL. These problems include such incidents as students bumping into the block and changing the

aperture. The University of Arizona is continually improving upon the
ental conditions and trying to overcome these problems.

the most significant problem to date has been the assignment of realistic
y conditions to models used to simulate this experiment. For instance, the
the block were not sealed, allowing vapor migration out of the block, yet
oundary conditions have been set as "no-flow". Further initial conditions
t been properly defined and fracture apertures and matrix properties for the
block utilized in the experiment have not been measured.

ommend these block experiments be repeated with hydraulic properties from
cks being used, measured. Further models utilized for simulation need to have
appropriate boundary conditions and input parameters.

Helsinki workshop, SNLA personnel reporting on this test case announced
he fracture was reported to be producing water even though the matrix was not
ted. This result has cast doubt on the commonly held modeling assumption
low would not occur in the fracture unless the matrix was saturated. Models
employ this assumption need to be closely examined now and if not valid must
moved from use in the U.S. DOE validation program. This experimental work
inue into Phase II and, perhaps at a later date, some validation may be

Apache Leap Field Imbibition/Redistribution Experiment. The purpose of this
riment is to evaluate the magnitude and distribution of fluid flow in unsaturated
tured tuff. This experiment, conducted at the Apache Leap field site consisted of
ding a borehole with water and monitoring water movement away from the
hole. It was expected that during the injection phase, flow would be dominated
fracture properties and during the redistribution phase, dominated by matrix
perties. The experiment was to be modeled using equivalent porous media
tinuum models instead of the discrete fracture approach. This approach assumes
t an anisotropic tensor can be used to represent the fractured nature of the rock.

fortunately this experiment was not successful and is being proposed to be
licated for Phase II. The reasons for their failure was the large distance between
monitoring wells and the flooded borehole. In the repeat experiment the
nitoring holes will be placed at 1 meter rather than 5 meters from the flooded
e. It will also be of interest to observe if any fractures are encountered which
vide direct borehole communication.

Field Heating Experiment. The purpose of this experiment is to evaluate the
gnitude and distribution of induced fluid flow around a heat source in unsaturated
ctured tuff. Since this experiment is in its planning stage, it is promising from
alidation aspect. It will provide an opportunity to utilize our knowledge of
ation gained in the first Phase of INTRAVAL. Open discussion of the
erimental set-up at INTRAVAL is encouraged.

Test Case 12 - USGS G-Tunnel Experiment

This USGS experiment was initially designed to examine effects of wet vs. dry drilling techniques on the surrounding fractured tuff rock mass. For what it was designed to do, it was informative. As a validation experiment it leaves much to be desired. It is our opinion that as a validation experiment, it was ambitious and never well posed. This is because it was not initially designed to be a validation experiment, but was backfit. Frequent changes in processes professed to be validated, occurred throughout the experiment. Additionally, lack of supervision of drilling crews lead to unanticipated layout changes and experimental conditions. (Boreholes were intersected and a dry-drilled hole was flooded.)

Since this experiment cannot be replicated due to G-Tunnel closure, it will not proceed into Phase II of INTRAVAL. Therefore, not much discussion is provided herein; except to say that the State of Nevada cannot consider Test Case 12 as a validation of unsaturated flow and transport occurring at Yucca Mountain.

CONCLUSIONS/RECOMMENDATIONS

The first Phase of INTRAVAL has made some progress toward defining what validation means, but has not yet reached a consensus within the group on an exact definition. Many participants, through the analysis of test cases are beginning to understand what validation is not (i.e., calibration) though what it is, is more elusive.

INTRAVAL did not start out with a firm game plan to develop a definition or methodology to prove that a given computer application is valid. This planning is now beginning to develop and should continue in the Phase II efforts. Therefore, at this time, the State of Nevada does not consider any of the test case work on unsaturated fractured tuff to be shown "valid", or in any way representative of flow at the Yucca Mountain Site. Several valuable lessons can be learned by the experiences to date, which should be recognized and incorporated into the HLW siting programs.

First, process model validation must take a priority over simple documentation of code assumptions and inputs. Uncertainties of modeling unsaturated fracture flow at great depths will be dominant in the US program and therefore basic research into our understanding of the processes must occur prior to validation. Further, without a meaningful amount of hydraulic data to analyze, little progress can be made with respect to validating Yucca Mountain flow system models.

Secondly, the time frames required to conduct meaningful prototype experiments and analyze resultant data have been shown to be large. Repeatability is crucial. The timeframes required for these analyses must be longer than is currently planned in the US program.

Thirdly, the State of Nevada would like to see INTRAVAL unsaturated zone Test Cases devote more time to fracture properties when validation of flow in unsaturated fractured media is attempted.

We recommend that the Apache Leap Block experiments be repeated to correct previous shortcomings such as: measurements of fracture aperture and matrix properties on the block being utilized, more accurate assignment of boundary and initial conditions, and examination of fracture matrix equilibrium assumptions which allow fracture flow only after matrix saturation.

Additionally, INTRAVAL work has shown that flexibility in design and conduct of experiments is required. QA measures serving to effectively restrict this flexibility should be revised so as not to inhibit experimental flexibility.

Lastly, due to the importance of developing meaningful performance measures. It is recommended that INTRAVAL focus considerable effort on this issue. A peer review of the total range of performance measures should be undertaken. Also, a sensitivity analyses should be performed to identify factors which contribute to uncertainty. This analysis should include such things as our ability to quantity the physical processes operational at proposed sites. If after these steps reliance on expert opinion is still required, experts must come from the broader scientific community and must not have been selected because of loyalty to one involved party.

THE INTERNATIONAL INTRAVAL PROJECT

TO STUDY VALIDATION OF GEOSPHERE
TRANSPORT MODELS FOR PERFORMANCE ASSESSMENT
OF NUCLEAR WASTE DISPOSAL

BACKGROUND AND RESULTS

1990

The Coordinating Group of the INTRAVAL Project
Swedish Nuclear Power Inspectorate (SKI)

NUCLEAR ENERGY AGENCY
ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT

NEA SKI

ant to article 1 of the Convention signed in Paris on 14th December 1960, and which came into force on 30th September 1961, the Organisation for Economic Co-operation and Development (OECD) shall promote policies designed:

- to achieve the highest sustainable economic growth and employment and a rising standard of living in Member countries, while maintaining financial stability, and thus to contribute to the development of the world economy;
- to contribute to sound economic expansion in Member as well as non-member countries in the process of economic development; and
- to contribute to the expansion of world trade on a multilateral, non-discriminatory basis in accordance with international obligations.

The original Member countries of the OECD are Austria, Belgium, Canada, Denmark, France, the Federal Republic of Germany, Greece, Iceland, Ireland, Italy, Luxembourg, the Netherlands, Norway, Portugal, Spain, Sweden, Switzerland, Turkey, the United Kingdom and the United States. The following countries became Members subsequently through accession at the dates indicated hereafter: Japan (28th April 1964), Finland (28th January 1969), Australia (7th June 1971) and New Zealand (29th May 1973).

The Socialist Federal Republic of Yugoslavia takes part in some of the work of the OECD (agreement of 28th October 1961).

The OECD Nuclear Energy Agency (NEA) was established on 1st February 1958 under the name of the OEEC European Nuclear Energy Agency. It received its present designation on 20th April 1972, when Japan became its first non-European full Member. NEA membership today consists of all European Member countries of OECD as well as Australia, Canada, Japan and the United States. The Commission of the European Communities takes part in the work of the Agency.

The primary objective of NEA is to promote co-operation among the governments of its participating countries in furthering the development of nuclear power as a safe, environmentally acceptable and economic energy source.

This is achieved by:

- *encouraging harmonisation of national regulatory policies and practices, with particular reference to the safety of nuclear installations, protection of man against ionising radiation and preservation of the environment, radioactive waste management, and nuclear third party liability and insurance;*
- *assessing the contribution of nuclear power to the overall energy supply by keeping under review the technical and economic aspects of nuclear power growth and forecasting demand and supply for the different phases of the nuclear fuel cycle;*
- *developing exchanges of scientific and technical information particularly through participation in common services;*
- *setting up international research and development programmes and joint undertakings.*

In these and related tasks, NEA works in close collaboration with the International Atomic Energy Agency in Vienna, with which it has concluded a Co-operation Agreement, as well as with other international organisations in the nuclear field.

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INTRAVAL

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FOREWORD

Currently, radioactive waste management programmes in OECD countries cover a wide range of activities aiming at the gradual implementation of disposal concepts for various types of waste. This concerns, in particular the institutional and regulatory framework as well as research and development activities. In some countries, site selection and characterisation programmes for high-level waste disposal are at a relatively advanced stage. Several countries already have repositories for low-level waste in operation. Among these activities, safety issues are a common concern, and, therefore enjoy a high priority in international co-operative programmes.

INTRAVAL is an international project concerned with the use of mathematical models for predicting the potential transport of radioactive substances in the geosphere. Such models are used to help assess the long-term safety of radioactive waste disposal systems. The INTRAVAL project was established to evaluate the validity of these models. Results from a number of selected laboratory and field experiments as well as studies of occurence of radioactive susbstances in nature (natural analogues) are compared in a systematic way with model predictions. Discrepancies between observations and predictions are discussed and analysed.

Twenty-two organisations from twelve OECD countries participate in INTRAVAL. The Swedish Nuclear Power Inspectorate (SKI) is the managing participant and the OECD/Nuclear Energy Agency, Her Majesty's Inspectorate of Pollution (HMIP/DOE), United Kingdom, and Kemakta Consultant Co., participate in the Project Secretariat. This report was prepared to provide interested parties beyond the group of directly involved specialists with a general background to the INTRAVAL project and a summary of the objectives and achievements achievements of INTRAVAL.

The **OECD Nuclear Energy Agency (NEA)** devotes considerable effort to the further development of methodologies to assess the performance of radioactive waste disposal systems and to increase confidence in their application and results. The NEA provides an international forum for the exchange of information and experience among national experts of its twenty-three Member Countries and conducts joint studies of issues important for safety assessment. It sponsors international research and development activities, including on various tools used in these safety assessments. The NEA co-ordinates activities of its Member Countries involving in-situ research, site investigations and the demonstration of underground disposal concepts. NEA also maintains working links at the international level between performance assessment projects, field projects and underground laboratories.

The **Swedish Nuclear Power Inspectorate (SKI)** is a regulatory body in Sweden for nuclear installations, including waste handling facilities and repositories. As such, the SKI has the responsibility to review applications to build nuclear installations and to recommend decisions on approval to the Government. The SKI also gives operating permits and sets requirements on operation according to the Nuclear Activities Act. In the area of nuclear waste disposal, and in particular final disposal of high-level waste and spent nuclear fuel, the SKI has a research programme focussed on performance assessment as a regulatory tool. Active participation in international co-operation is an important part of this programme. Since 1981, the SKI has initiated three international projects INTRACOIN, HYDROCOIN and INTRAVAL with emphasis on verification and validation of geosphere performance assessment models.

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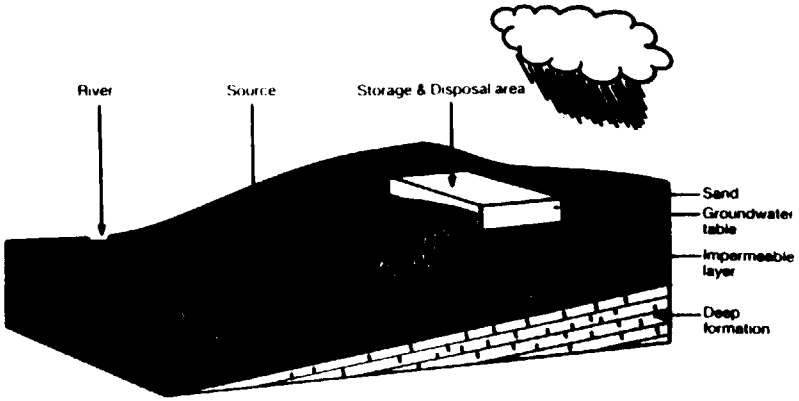
I

THE DISPOSAL OF RADIOACTIVE WASTE

Generation of electricity by nuclear reactors gives rise to radioactive waste which must be disposed of in a safe way. Some wastes contain only a low concentration of radioactive elements that decay quickly. Other wastes are highly radioactive and contain long-lived radioactive elements. Before storage or disposal, the wastes are immobilised and encapsulated. Low-level waste with short-lived elements can be safely treated and disposed of in a rather simple way. Shallow ground burial is a method which is used for the disposal of these types of wastes. Shallow underground disposal, for instance in rock caverns, is also practised.

The most advanced treatment and disposal techniques are needed for long-lived high-level waste. For this case the greatest part of the effort is directed towards development of safe methods of disposal in stable geological formations deep underground.

Many types of geological formations show favourable characteristics for long-term isolation of radioactive wastes: salt, clays, shales, basalts, tuffs and crystalline rocks such as granite. The choice for a particular country depends to a large extent on the availability of formations in that country. All countries with a nuclear power programme are involved in studies to find suitable geological formations for disposal of their wastes. Much of the Research and Development work is accomplished through international co-operative projects. Timetables for site-selection and implementation of the disposal systems vary between countries. Repositories for low- and medium-level wastes are already in operation or being constructed in many countries. The first repositories for the disposal of high-level wastes may be operational at the beginning of the next century. Meanwhile, further research, site-selection studies and evaluation of disposal concepts and proposed sites are being carried out.



Credit: ANDRA

Credit: NAGRA.

Figures 1 and 2. Examples of concepts for the shallow disposal of low-level waste an deep disposal of high-level waste. In both cases, knowledge of groundwater movement modelling of potential transport of radioactive substances in the geosphere will be require evaluate safety.

SAFETY ASSESSMENT AND THE USE OF PREDICTIVE MODELLING

The fundamental function of a disposal system is to isolate and retain radioactive materials so they will cause no harm to man or his environment, either now or in the future. This raises the problem of predicting the behaviour of the system over long time periods. It is not necessary to predict future behaviour in every detail. What is needed is to understand enough to

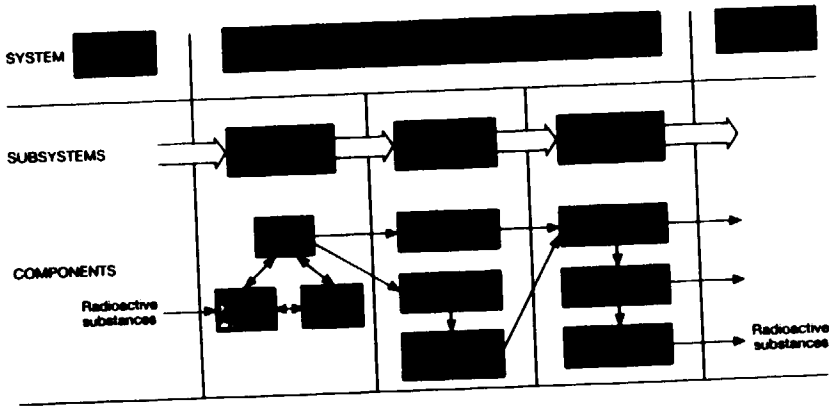


Figure 3. To understand the long-term safety of a waste isolation system a detailed assessment is needed of the performance of all its components and their interactions.

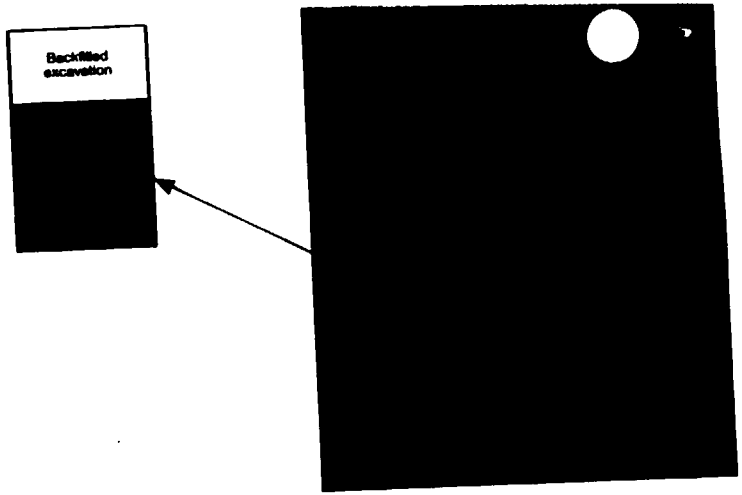


Figure 4. Schematic of natural and engineered barriers in a nuclear waste disposal system.

be assured that no harmful releases will occur. To gain this level of understanding and to describe it to responsible authorities and the public is one of the major tasks in any nuclear waste disposal programme.

The basis for an analysis of the safety is a good scientific understanding of all parts of the system. This encompasses for instance:

- The physical/chemical properties of the waste materials and canisters (the source);

- The chemical interactions and transport phenomena within or close to the repository (the near-field);

- The chemical interactions and transport phenomena in the geological formation surrounding the repository (the far-field);

- The effects of dispersion and/or reconcentration of possible releases to the biosphere.

Research is performed in all these areas through experiments and observations in laboratories or in the field. The large amount of data obtained from experiments and field tests are collected in a systematic way and stored in **data bases**. **Mathematical models** are developed to describe important processes that might occur.

A safety assessment evaluates the future effects of the repository on the environment by using the most appropriate available information and understanding.

Thus, **safety assessments** require effective use of predictive modelling methods and a wide range of information that describes the disposal system and its possible evolution. Safety assessments normally form an integral part of repository development programmes at an early stage. Prior to licensing a particular site and repository design, safety assessments are performed periodically to determine if further information needs to be collected. Safety assessments also form a crucial part of the licensing documentation for disposal systems.

Modelling is used extensively in safety assessments in many different ways. Models are used at different levels of detail and complexity to describe and understand:

- individual processes (for instance dissolution of radioactive elements in groundwater or retardation by sorption on mineral phases of the rock);

- subsystem performance (for instance the migration of radionuclides in the geosphere resulting from the overall effect of water flow, dispersion, diffusion, sorption, radioactive decay, etc.); and finally,

- performance of the overall system (for instance by integrating waste package, near-field, geosphere and biosphere modelling).

The first step is to develop a conceptual model. A conceptual model represents one's understanding of the features and processes of interest. It is an abstraction of reality which need only include those relationships necessary to describe the system for the intended model application. Conceptual models are developed by expert judgement on the basis of well-known principles of physics and chemistry and existing knowledge of behaviour of the type of system under consideration. The relationships of a conceptual model are expressed quantitatively through mathematical equations. A calculational model is based on the mathematical equations and is implemented through a computer code to enable efficient calculation capability. Simplifications are almost always introduced in going from the real world to conceptual models, to mathematical (calculational) models, to implementation in a computer code.

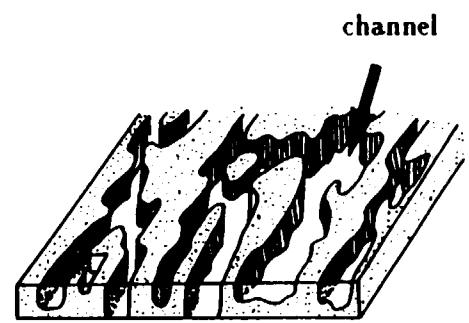


Figure 5. Illustration of a concepti model structure for the availab space for flow of groundwater ir fracture of rock (channelling flow)

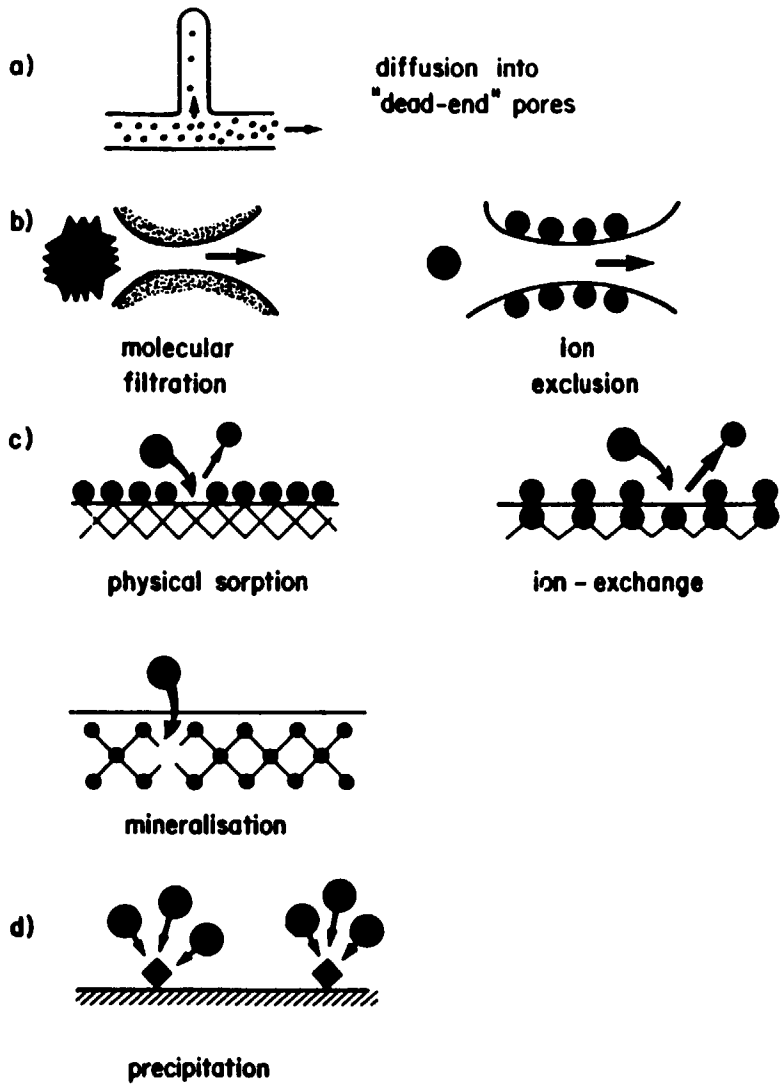


Figure 6. Diagrams of physical/chemical processes that can act as potential retardation mechanisms for the migration of radionuclides.

PROCESSES MODELLED IN THE GEOSPHERE

$$\frac{\partial C_i}{\partial t} = -V\frac{\partial C_i}{\partial x} + D_L\frac{\partial^2 C_i}{\partial x^2} - \lambda_i C_i + \lambda_{i-1}C_{i-1} + D_e a \left.\frac{\partial C_i}{\partial z}\right|_{z=0} - \frac{\partial S_i}{\partial t}$$

a b c d1 d2 e f

a) The rate of change of the concentration of radionuclide i in the flowing liquid phase is dependent on the following processes:

b) **Advection**, which is governed by the Darcy velocity V; x is the distance from the near field-geosphere interface.

c) **Dispersion-Diffusion**, is governed by the dispersion coefficient D_L which is dependent on the interstitial water velocity. If the water velocity is 0, only diffusion of the radionuclides take place.

d1, d2) **Radioactive decay chains** take into account the radioactive decay of the nuclide i, and the formation of nuclide i from radioactive decay of the parent nuclide i-1. These terms are governed by the two decay constants λ_i and λ_{i-1}.

e) **Matrix diffusion**, is governed by the effective diffusivity, D_e, in the stagnant water in microfissures and pores in the rock matrix; a is the area of the surface of the rock matrix in contact with the flowing water per volume of flowing water and z is the distance from that surface.

f) **Interaction with solid phase.** This term takes into account sorption and desorption phenomena on the surface of the rock in contact with the flowing water. S_i represents the concentration of radionuclide i on the rock surface.

Example of the mathematical formulation of a model for radionuclide transport in geosphere.

III

EXPERIMENTS AND FIELD STUDIES IN SUPPORT OF RADIOACTIVE WASTE MANAGEMENT PROGRAMMES

A wide range of experiments and field studies have been performed and are being performed to gain further understanding of phenomena that are important for evaluation of the long-term safety of radioactive waste repositories. Experimental data and models are closely linked. Hypotheses and models based on the examination of data can identify which additional observations and measurements are needed to better understand the process or system being studied.

The space and time scales important to repository safety assessments are ordinarily larger than the times and distances that can be investigated with man-made experiments. This makes it difficult to account for all relevant performance assessment aspects by carrying out a few simple laboratory experiments or field studies. Therefore, a well-planned and complementary set of laboratory experiments and field studies will be needed to fully understand transport of radionuclides in the geosphere.

Laboratory experiments enable physico-chemical processes and mechanisms to be understood under well-defined conditions. They can also be used to obtain data for the interpretation of field experiments and of natural analogues. Another advantage of laboratory experiments is that they can be dissembled when they are finished so that more detailed analysis can be performed to further test model assumptions.

CREDIT AEA TECHNOLOGY

7a) Apparatus used for small scale (1-3 cm) experiments with diffusion in wet clay (Test Case 1a)

CREDIT AECL

7b) Installations for laboratory experiments in a crystalline rock block with a single natural fracture (Test Case 9)

Figure 7. Two of the laboratory experiments included in INTRAVAL Phase 1.

Figure 8. Flow and tracer experiments in crystalline rock performed within the International Stripa Project provided the data for INTRAVAL test case 4. The picture shows the installations of plastic sheets to collect water seeping into the drift along some fractures in the rock

Field experiments are nearer to the real situation in terms of scale and complexity than laboratory experiments. They are important for identifying those processes which influence geosphere radionuclide transport. Furthermore, they provide insight into large scale heterogeneities and varieties of boundary conditions. Field migration experiments performed under well-defined conditions appear to be the most appropriate way to study radionuclide transport in the geosphere and they are an essential component in the validation of geosphere transport models.

Natural Analogues are potentially capable of providing important insights into the behaviour of radionuclides over the long time periods that are relevant to repository safety assessments. They can indicate which mechanisms are important over long time periods and they can provide evidence that the models actually describe the migration of radionuclides in real geological systems for relevant time scales. However, many of the present and past conditions at a natural analogue site are likely to be poorly known. Information obtained from natural analogues cannot provide "stand alone" evidence of model validity but taken together with other information from laboratory and field studies, they can be very valuable in establishing confidence in migration models.

Figure 9 The natural analogue studies at an open pit uranium mine at Poços de Caldas, Minas Gerais, Brazil, provided data for test case 7a concerning modelling of redox reactions and movement. The pictures illustrate the clearly visible difference in appearance between reducing rock (gray) and oxidized rock (brown).

IV

THE INTRAVAL PROJECT

Background

Since 1981, conceptual and mathematical models for radionuclide and groundwater transport in the geosphere have been evaluated through the international co-operation projects INTRACOIN, HYDROCOIN and now INTRAVAL.

INTRACOIN, 1981-1984, dealt with code verification, model validation and uncertainty analysis for radionuclide transport models.

HYDROCOIN, 1984-1987, dealt with the verification and validation of codes and models for groundwater movement.

The purpose of the **INTRAVAL** project is to increase the understanding of how various geophysical, geohydrological and geochemical phenomena of importance for the radionuclide transport from a repository to the biosphere can be described by mathematical models developed for this purpose. This is being done by systematically using information from laboratory and field experiments as well as from natural analogue studies as input to mathematical models in an attempt to validate the underlying conceptual models and to study the model validation process.

Seventeen test cases have so far been included in the study. The test cases are based on experimental programmes performed within different national and international projects. Several of the cases are based on international experimental programmes, such as the Stripa Project, the Alligator Rivers Project, and the Poços de Caldas Project. A Pilot Group has been appointed for each of the test cases. The responsibility of the Pilot Group is to compile data and propose formulations of the test cases in such a way that it is possible to simulate the experiments with model calculations.

It is an important policy of the INTRAVAL study to support interaction between modellers and experimentalists in order to gain reassurance that the experimental data are properly understood and that the experiences of the modellers regarding the type of data needed from the experimentalists are accounted for. In order to support this interaction and provide for the development of a strategy for the systematic application of the experiences and knowledge gained from the INTRAVAL test cases, a special committee, the Validation Overview and Integration Committee (VOIC), has been set up within the INTRAVAL study.

The INTRAVAL Phase I study is now approaching completion. The documentation of the test cases is available. The work with the laboratory and field experiments is intensive and modelling results from many Project Teams have been presented and discussed at INTRAVAL Workshops and is now being documented.

Validation Procedure

A key question about the models used in safety assessments is: do the models simulate sufficiently accurately the processes or systems for which they have been developed? The procedure of validation seeks to answer this question. Validation, therefore, is concerned with providing a genuine understanding of nature, that is, of the reality behind models.

> **Validation is a process carried out by comparison of model predictions with independent field observations and experimental measurements. A model cannot be considered validated until sufficient testing has been performed to ensure an acceptable level of predictive accuracy. (Note that the acceptable level of accuracy is judgmental and will vary depending on the specific problem or question to be addressed by the model).**
>
> **(IAEA-TECDOC-447 Radioactive Waste Management Glossary, 2nd edition, 1988)**

There is no such thing as a validated model in the generic sense. However, one can say that "a model is validated with respect to a given process", or that "a model or group of models are validated with respect to a given site". Ranges of applicability should always be included in statements regarding model validation. The decision of whether a model is valid must not be made only by those using the model. In the end the scientific community must decide on the validity of models and whether they are correctly used in a specific application.

The validation of a model for transport of radionuclides involves testi different aspects of the conceptual model in order to answer several iss e.g.:

- Does the model describe and include all relevant processes?
- Is the geometrical structure of the system well described by model?
- Are the underlying assumptions valid for the physico-chemical en ronment (redox conditions, pH, etc.)?
- Can appropriate experiments be adequately simulated using the model?
- Does the model used to describe the experimental situation account for the spatial and temporal scale of the experiment?

The INTRAVAL Validation Overview and Integration Committee (VOIC) has identified three major elements in the validation procedure:

1. **Understanding and Research**. Without proper understanding of the processes and system structures involved, validation cannot be achieved. Thus, a thorough understanding of processes and system structures represents a major element of validation.

2. **Comparisons of Theory and Modelling Calculations with Experiments**. This element is to study how well one is able to quantitatively predict or simulate experimental results. Discrepancies may be due to parameter uncertainties, statistical nature of the system or lack of understanding. Improving our lack of understanding requires further effort in item 1. It is important to be cautious and avoid curve fitting without proper understanding and additional confirmatory results.

3. **Peer Review and Public Scrutiny**. This last element involves publishing the work in the open literature, both to receive the benefits of anonymous technical review and to open the model and its validation to public scrutiny. A study whose results are in the open literature, examined and used by the general scientific community over long periods of time stands a better chance of receiving the appropriate scrutiny and of being correct.

Results of Phase 1

Phase 1 of the INTRAVAL study is comprised of seventeen test cases ranging from laboratory scale experiments through field experiments on several different scales as well as natural analogue studies. The multitude of test cases is explained by the fact that the participants represent twelve different countries planning for waste disposal in different media such as crystalline rock, clay, rock salt and unsaturated tuffaceous rocks. INTRAVAL also addresses a large range of spatial and temporal scales.

Most of the progress in Phase 1 of INTRAVAL has been made in the area of Process Identification. It has been demonstrated that experiments at different scales, flow rates, tracer concentration etc., are needed in order to unambiguously distinguish between the effects of different dispersion phenomena and matrix diffusion. It has also been demonstrated that statistical analysis forms an important part of the Process Identification step of validation. Although work remains to be done for the identification of processes active in specific systems, there are good prospects that Phase 1 of INTRAVAL will significantly increase the confidence in our ability to mathematically describe many of the processes believed to be of importance in radionuclide transport in a wide range of geological media.

The work has resulted in a number of ideas for further experiments or improved designs of already performed experiments. It has been suggested that many of the laboratory experiments be run at different waterflow rates, different concentrations, and over different sample lengths, in order to be able to discriminate between different processes considered in the applied models. Thus, it can be concluded that a significant advantage can be gained if the modellers are given the opportunity to interact with the experimentalists to ensure that the data required by the models will be gathered satisfactorily. The modeller can provide the experimentalist with perspectives on the various type of data needed, e.g. for distinguishing between different phenomena either directly or by analysing different suggested experimental setups.

The detailed results of INTRAVAL Phase 1 are now being documented in technical reports for each test case and in a summary report for Phase 1. These reports are planned for publication during 1991.

INTRAVAL Phase 2

The need for a continuation of INTRAVAL into a second phase (1991-1993) was foreseen at the start of the project. Discussions have now been initiated with the participants regarding the technical content of Phase 2. In Phase 2 there will be more emphasis on validation efforts based on field studies and natural analogues.

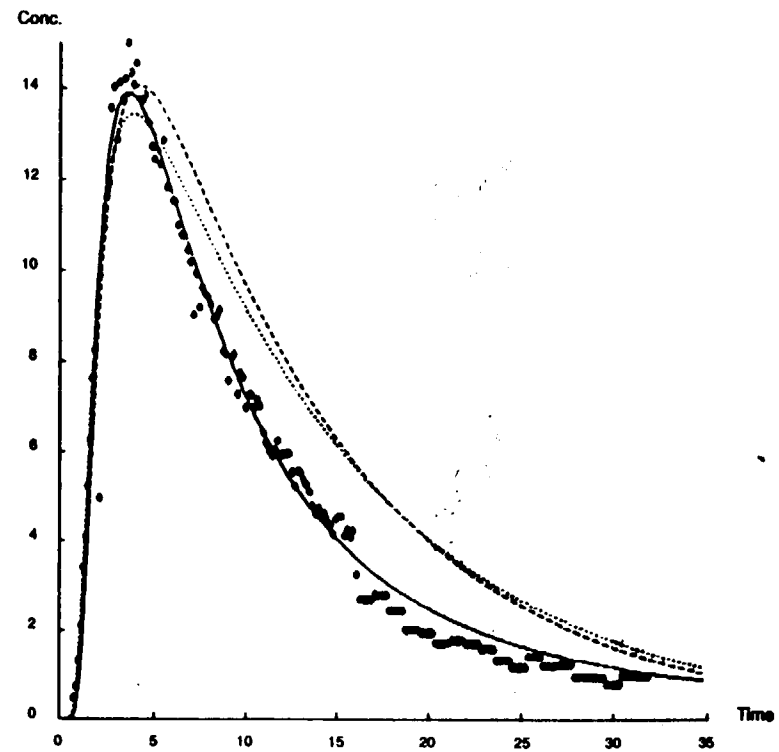


Figure 10. Illustration of Phase 1 results (Test Case 1b). The points are the experimental data. The curves represent model predictions of break-through of a migrating radionuclide, after calibration, for three conceptual models with different assumptions regarding the type of processes for interaction between migrating radionuclides and the rock.

Experience from Phase 1 indicated that the effort needed to analyse a field experiment is much greater than that needed for the analysis of a laboratory experiment. As a result, the number of test cases in Phase 2 will be less than in Phase 1. Only cases where there is a possibility for close interaction between modelling and experimental studies will be included in Phase 2. This will promote a focussed effort on a limited set of field experiments and natural analogue studies with comprehensive data bases able to cover relevant validation issues like scale dependency, heterogeneity, and coupled processes.

Figure 11. Test Case 10 of INTRAVAL Phase 1 is based upon a field experiment with migration of a wetting front in a superficial desert soil performed within a U.S. NRC trench study at Las Cruces, New Mexico, United States. The picture shows the trench before it was covered.

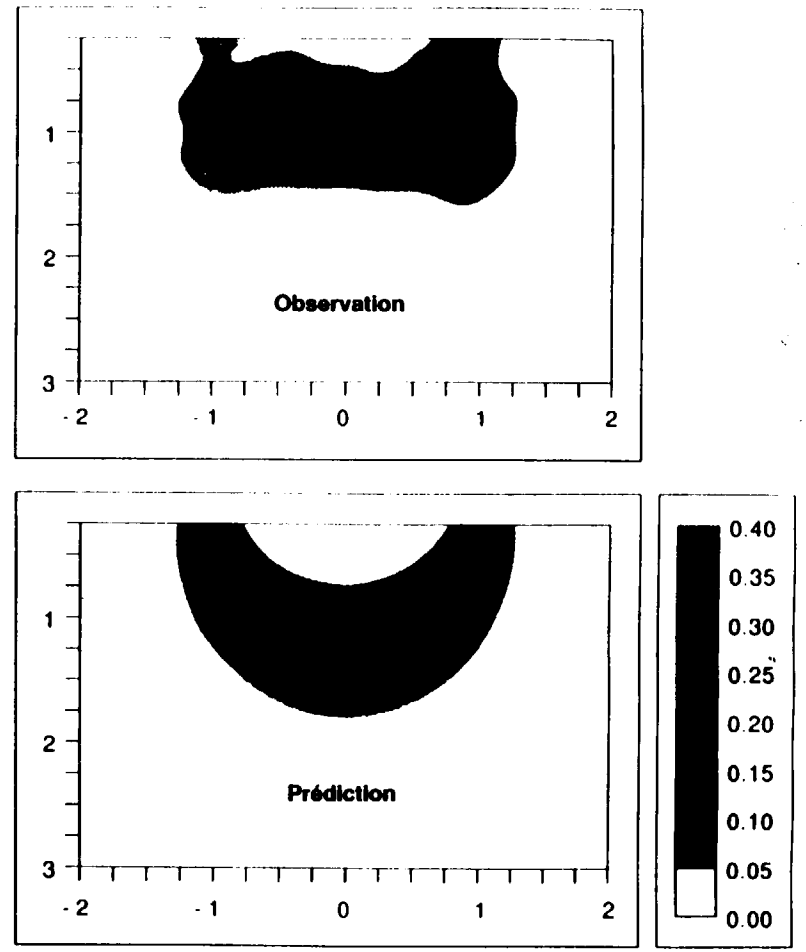
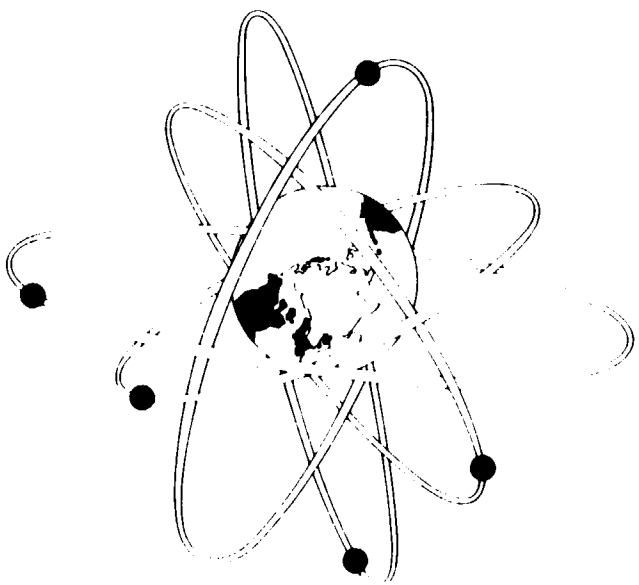


Figure 12. Illustration of Phase 1 results (Test Case 10). Observed and predicted relative bromide concentrations.



V

SUMMARY REMARKS

As demonstrated by the large number of active participants throughout the world, and the great variety of laboratory and field experiments, natural analogue studies, and numerical experiments involved, INTRAVAL has developed into a major international effort studying validation issues associated with geosphere transport models.

It should be remembered that real progress in validation can only be achieved when the work on the individual test cases focusses on specific relevant issues associated with radionuclide transport experiments and simulation studies. Considerable progress has been achieved along these lines. It should also be noted that validation is a learning process. Both experimental work and the modelling of specific data bases help to increase the general knowledge of crucial performance issues. It is also necessary to constantly integrate and evaluate the results in the context of performance assessment, and to develop strategies for further validation work considering the needs of the various disposal programmes.

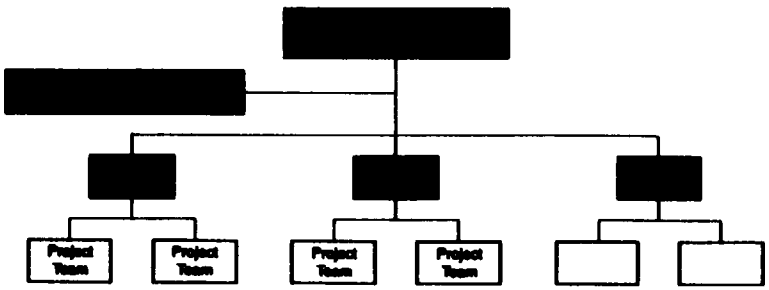
The active involvement of the many national and international co-operative programmes has contributed greatly to INTRAVAL's success. Similarly, the positive and collegial interaction between the experimentalists and modellers, as demonstrated in the numerous formal workshops and special meetings convened by the test case participants, has contributed to INTRAVAL's progress and achievements.

VI

THE INTRAVAL ORGANISATION

The organisation of the INTRAVAL study is regulated by an agreement which has been signed by all participating organisations (Parties). The study is directed by a Co-ordinating Group with one member from each Party. The Swedish Nuclear Inspectorate (SKI) acts as Managing Participant. The Managing Participant sets up a Project Secretariat in co-operation with Her Majesty's Inspectorate of Pollution (HMIP/DoE), U.K. and the Organisation for Economic Co-operation and Development/Nuclear Energy Agency (OECD/NEA). KEMAKTA Consultants Co. is contracted by SKI to act as Principal Investigator within the Project Secretariat.

The Parties organise Project Teams for the actual project work. Each Party covers the costs for its participation in the study and is reponsible for the funding of its Project Team or Teams, including computer cost, travelling expenses, etc.



A Pilot Group has been appointed for each Test Case in order to secure the necessary information transfer from the experimental work to the Project Secretariat and the Project Teams. The Project Secretariat co-ordinates this information transfer.

Workshops are periodically held, usually in conjunction with meetings of the Co-ordinating Group. During the workshops, Test Case definitions and achieved results are discussed as a preparation for decisions in the Co-ordinating Group. A Validation Overview and Integration Committee (VOIC) for the development of a strategy for the systematic application of experience and knowledge gained from the various INTRAVAL test cases has been set up by the Co-ordinating Group.

REFERENCES

Additional information can be found in the following publications:

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- Geological Disposal of Radioactive Waste: In Situ Research and Investigations in OECD Countries. A status report prepared by the NEA Advisory Group on In Situ Research and Investigations for Geological Disposal (ISAG), OECD/NEA, Paris, 1988.
- INTRACOIN Final Report Level 1, Swedish Nuclear Power Inspectorate, February 1984.
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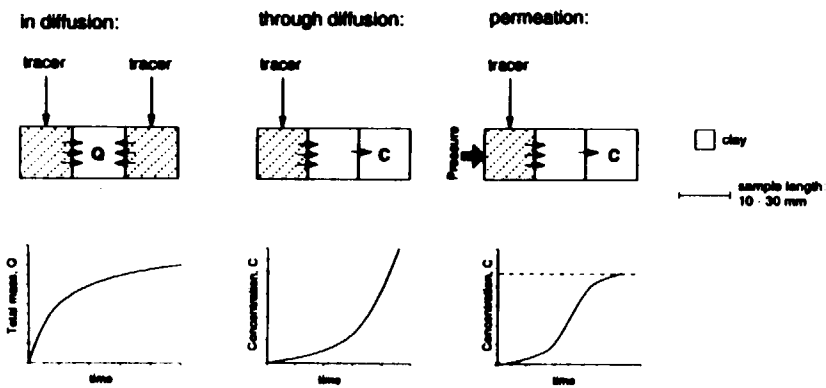
- The International HYDROCOIN Project. Background and Results. brochure published by OECD/NEA, Paris, 1987.
- HYDROCOIN Final Report Level 1 - Code verification. Published by OECD/NEA, Paris, 1987.
- HYDROCOIN Final Report Level 2 - Model validation. Published by OECD/NEA, Paris, 1990.
- INTRAVAL Progress Reports 1-5. Published by Swedish Nuclear Power Inspectorate, 1988, 1989, 1990.
- Safety Assessment of Radioactive Waste Repositories. Proceedings of a joint CEC/IAEA/NEA International Symposium. OECD/NEA, Paris, 1990.

APPENDIX 1

INTRAVAL test cases

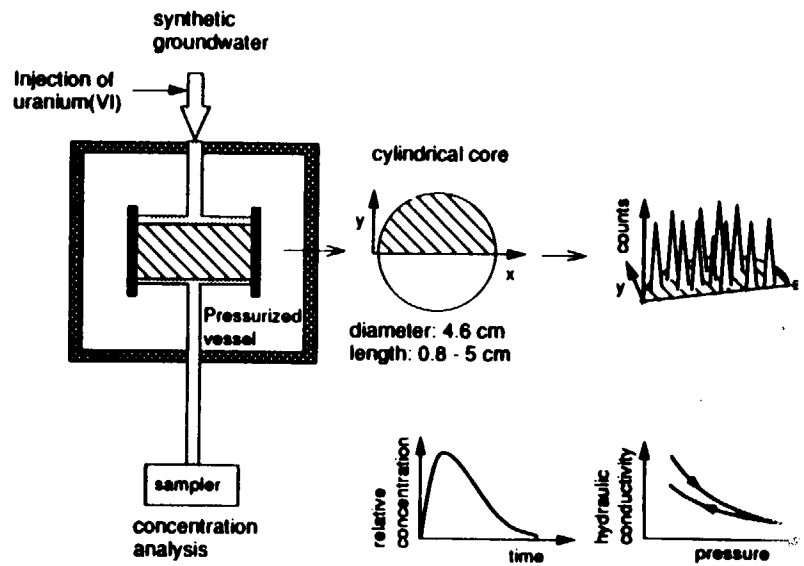
Test Case 1a: Radionuclide migration through clay samples by diffusion and advection based on laboratory experiments performed at Harwell, United Kingdom. The transport of radioactive substances into and through samples of wet clay were studied in laboratory experiments over a few months.

Test case 1a



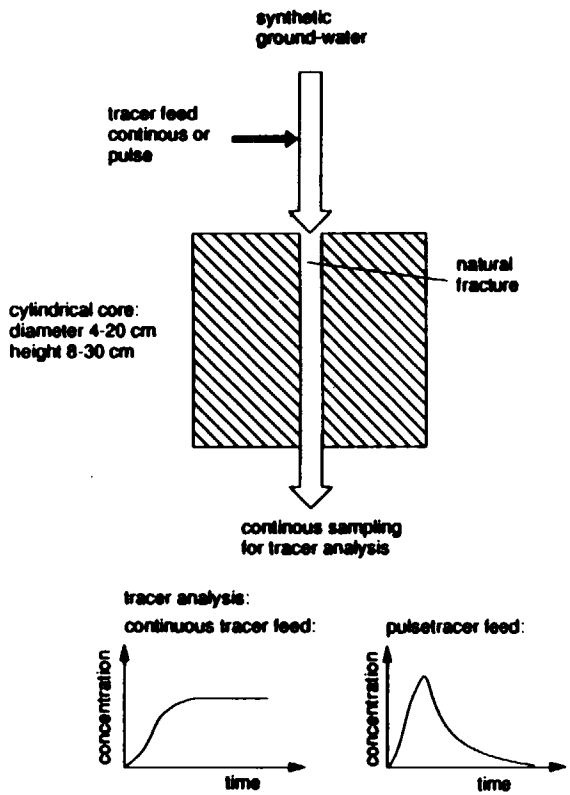
Test Case 1b: Uranium migration in crystalline bore cores based on experiments performed at PSI, Switzerland. Schematic diagram of the pressure infiltration apparatus. When the experiment was ended, the core sample was cut in thin (1 mm) slices which were autoradiographed to yield information on flow paths and sorption sites.

Test case 1b



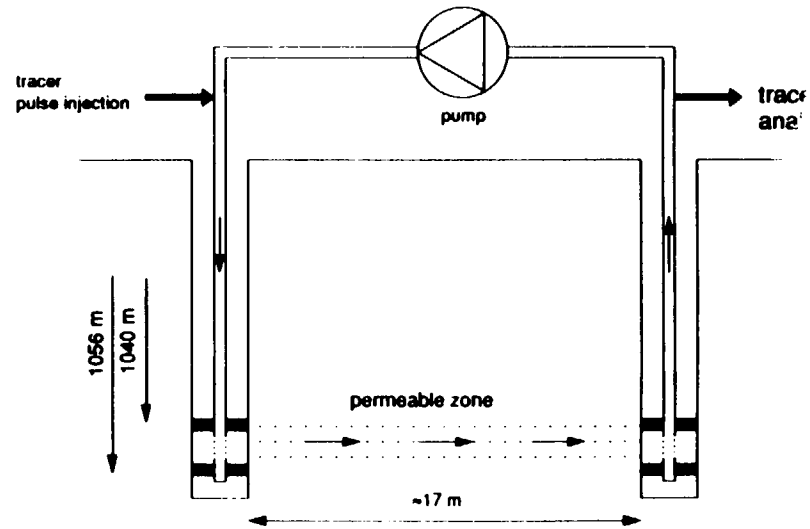
Test Case 2: Radionuclide migration in single natural fissures in granite based on laboratory experiments performed at KTH, Sweden. The experiments address important phenomena such as retardation, matrix diffusion, channelling and fracture properties.

Test case 2



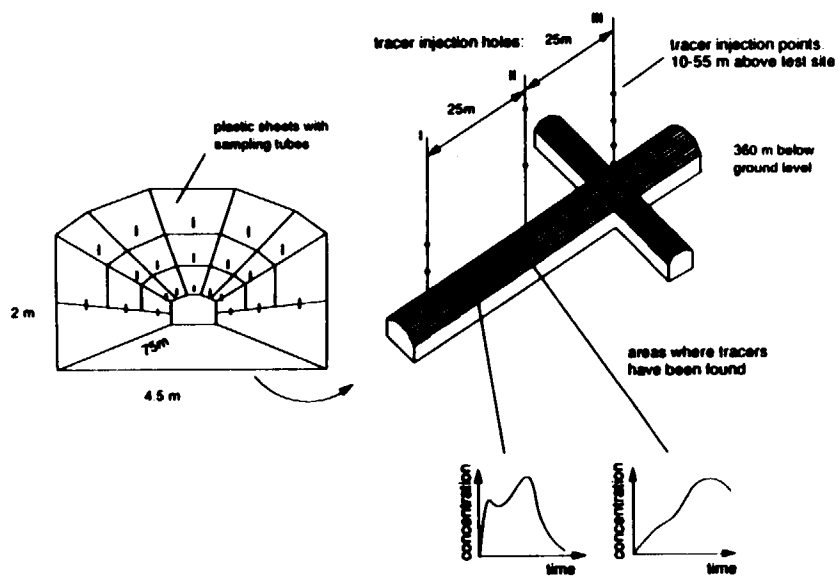
Test Case 3: Tracer tests in a deep basalt flow top performed at th Hanford reservation, Washington, USA.

Test Case 3



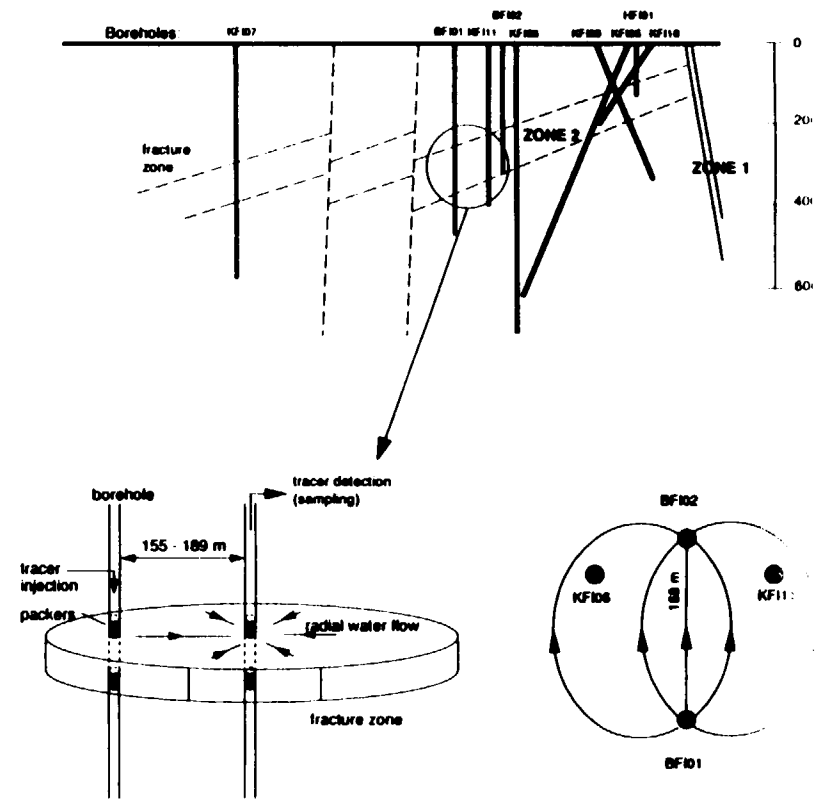
Test Case 4: Flow and tracer experiments in crystalline rock based on the Stripa 3D experiment performed within the International Stripa Project. The main purpose of this experiment was to investigate the spatial distribution of water flow paths in a larger block of rock.

Test Case 4



Test Case 5: Tracer experiments in a fracture zone at the Finnsjön resear area, Sweden. The aim of the test was to investigate the transport prope ties in a highly conductive rock over distances of several hundred meters

Test Case 5

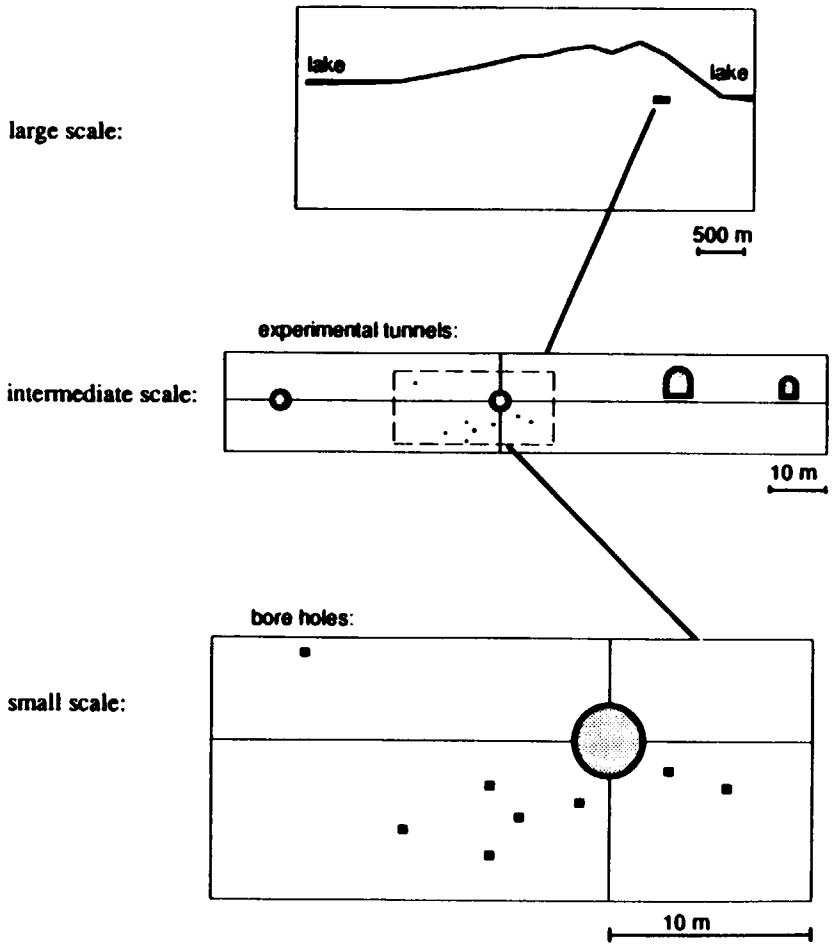


a) Radially converging experiment.

b) Dipole experiment

Test Case 6: Synthetic data base, based on single fracture migration experiments in Grimsel Rock Laboratory in Switzerland. Geography of hypothetical test site for synthetic migration experiments. Geologic and hydrologic boundary conditions are defined for large-, intermediate-, and small-scale studies.

Test Case 6

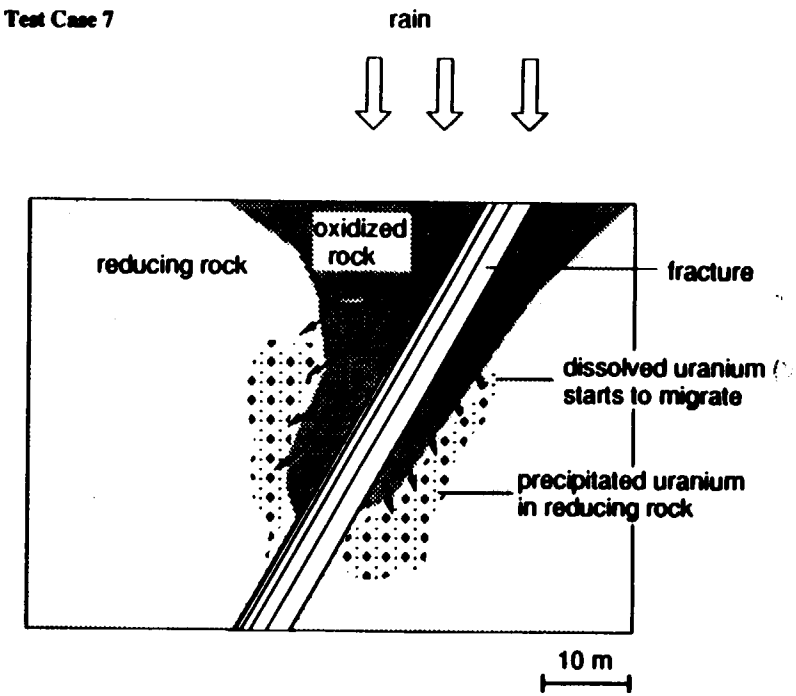


Test Case 7a and 7b: Natural analogue studies at Poços de Caldas, Mi Gerais, Brazil.

7a: Redox front and radionuclide movement in an open pit uranium mi The deeper portions of the rock are strongly reducing while the up portions have become oxidised by oxygen carried by infiltrating rainwa The geochemical processes involved and the locations of the redox front modelled.

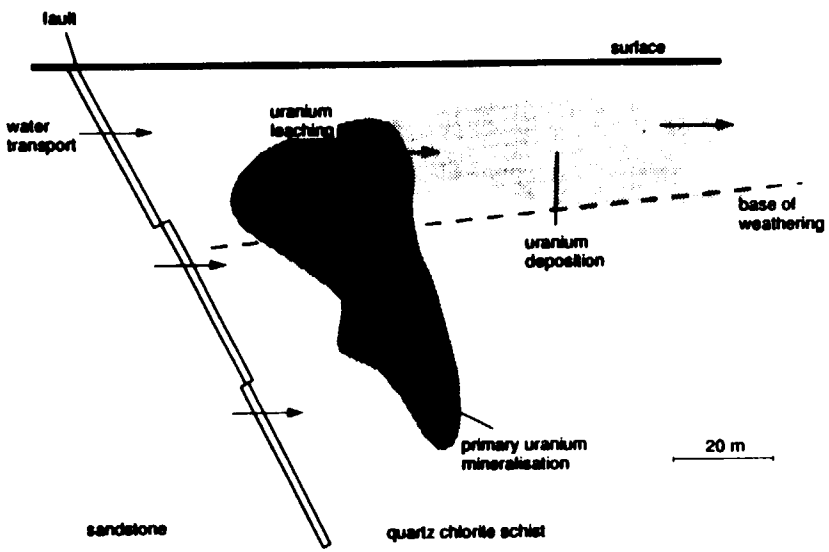
7b: Morro do Ferro colloid migration studies.

Test Case 7



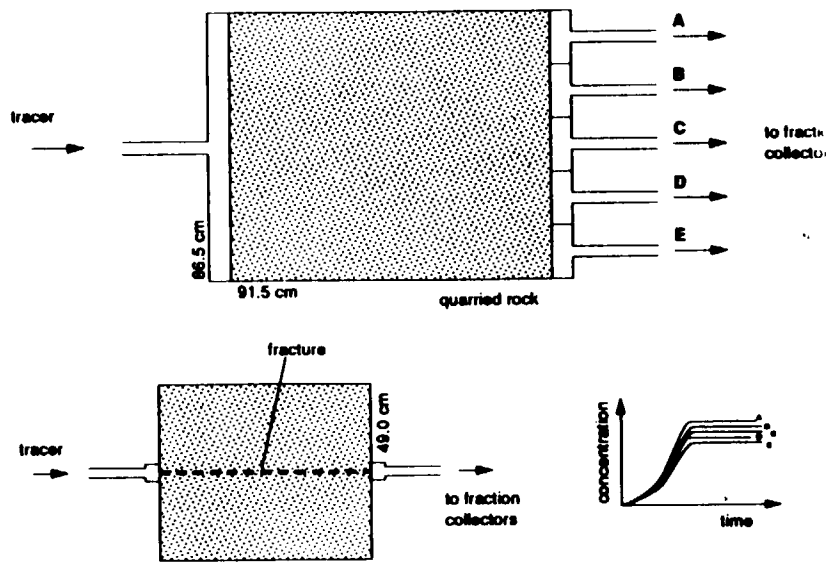
Test Case 8: Natural analogue studies at the Koongarra site in the Alligator Rivers area of the Northern Territory, Australia. The phenomena involved in leaching and transport of uranium and other elements at a natural ore body site are extensively studied within the International Alligator Rivers Project. A test case based on data for migration of uranium in the weathered zone is included in INTRAVAL.

Test Case 8



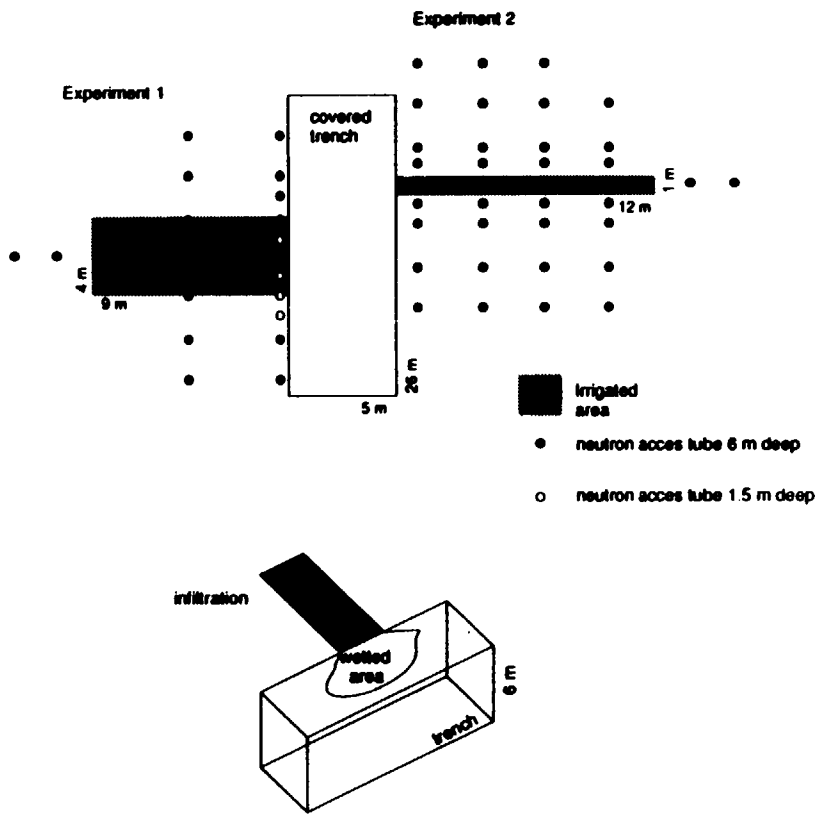
Test Case 9: Radionuclide migration in a block of crystalline rock based on laboratory experiments performed at AECL, Canada. The block contained a single natural fracture and the flow along this fracture was studied.

Test Case 9



Test Case 10: Evaluation of unsaturated flow and transport in porous media using an experiment with migration of a wetting front in a superficial desert soil performed within a U.S.NRC trench study at Las Cruces, New Mexico.

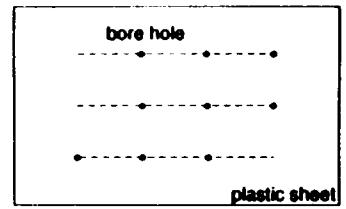
Test Case 10

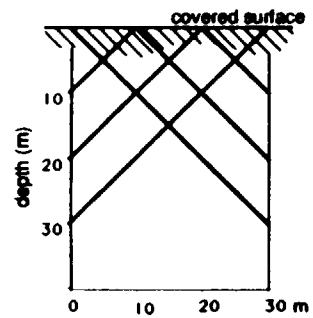


Test Case 11: Evaluation of flow and transport in unsaturated fractur rock using studies at the U.S.NRC Apache Leap Tuff Site near Superi Arizona. The case includes both field and laboratory experiments.

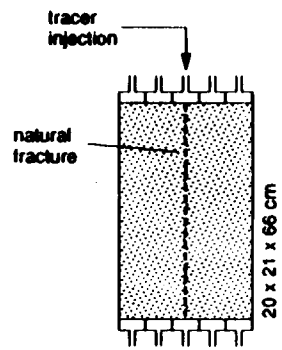
Test Case 11

field experiments:

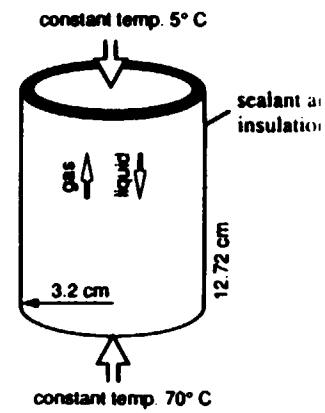




block experiment:

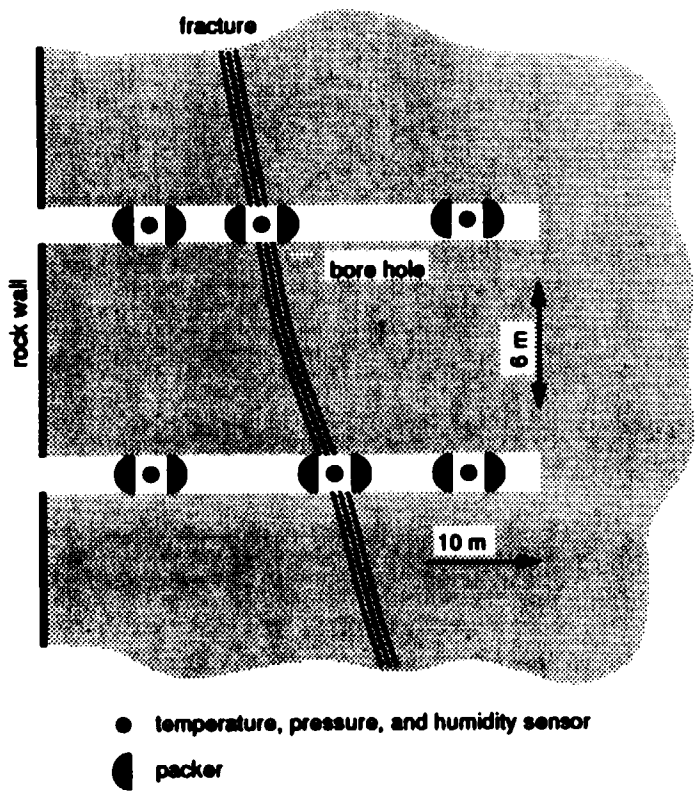


core experiment:



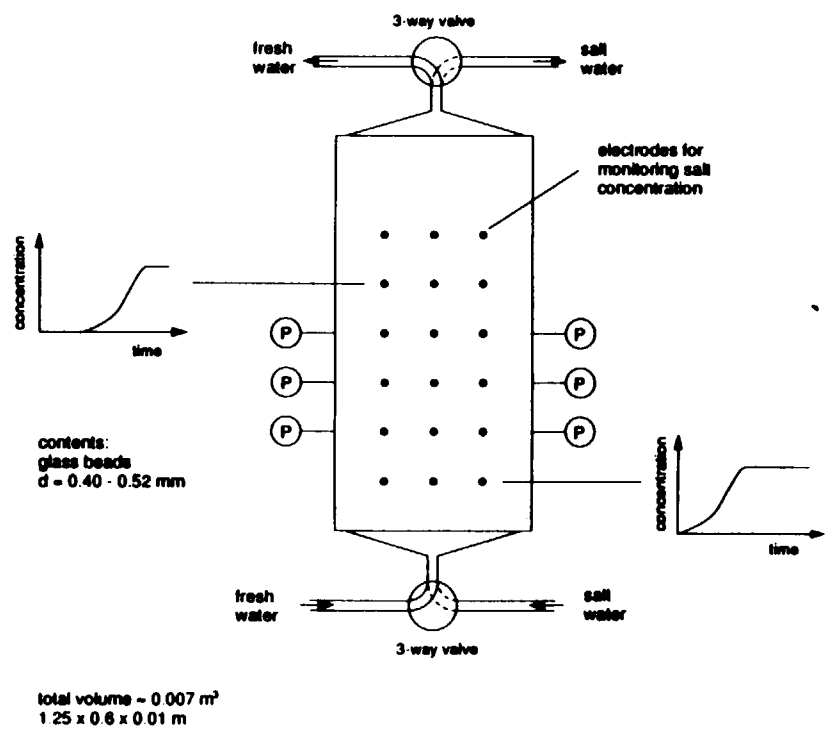
Test Case 12: Experiments with changing near-field hydrologic conditions in partially saturated tuffaceous rocks performed in the G-Tunnel Underground Facility at the Nevada Test Site by the Nevada Nuclear Waste Investigation Project of the U.S.DOE. This test case deals with near-field effects produced by propagating transient disturbances.

Test Case 12



Test Case 13: Experimental study of brine transport in porous m
performed at RIVM, the Netherlands. Information on brine transport p
nomena are important for the assessment of repositories in deep salt form
tions as foreseen in some countries.

Test Case 13

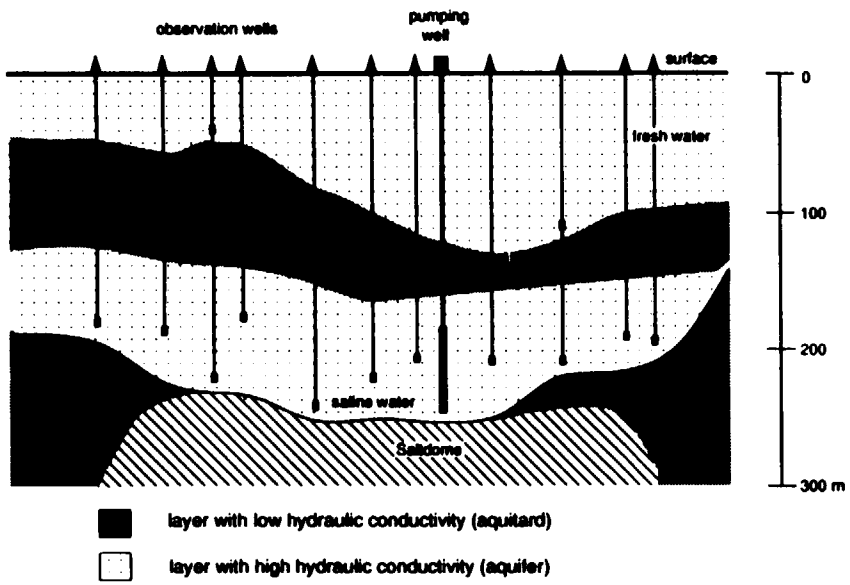


Test Case 14a and 14b: Groundwater flow in the vicinity of the Gorleben Salt Dome, the Federal Republic of Germany.

14a: Pumping test in highly saline groundwater.

14b: Saline groundwater movement in an erosional channel crossing a salt dome.

Test Case 14



LIST OF INTRAVAL PARTICIPANTS

Party		Project Team(s)	
Agence Nationale pour la Gestion des Déchets Radioactifs, France	(ANDRA)	Commissariat à l'Energie Atomique	(DEM
Atomic Energy of Canada, Ltd., Canada	(AECL)	Atomic Energy of Canada Ltd	(AE
Australian Nuclear Science and Technology Organisation, Australia	(ANSTO)	Australian Nuclear Science and Technology Organisation	(ANST
Bundesanstalt für Geowissenschaften und Rohstoffe/ Bundesamt für Strahlenschutz, Federal Republic of Germany	(BGR/BFS)	Bundesanstalt für Geowissenschaften und Rohstoffe	(B
		Bundesamt für Strahlenschutz	(B
Commissariat à l'Energie Atomique/Institut de Protection et de Sûreté Nucléaire, France	(CEA/IPSN)	Ecole Nationale Supérieure des Mines de Paris	(ED
Empresa Nacional de Residuos Radioactivos S.A., Spain	(ENRESA)	Universidad Politéchnica de Cataluna	(U
Gesellschaft für Reaktorsicherheit Federal Republic of Germany	(GRS)	Gesellschaft für Reaktorsicherheit	(G
Gesellschaft für Strahlen- und Umweltforschung, Federal Republic of Germany	(GSF)	Gesellschaft für Strahlenund Umweltforschung	(G
Her Majesty's Inspectorate of Pollution, United Kingdom	(HMIP/DoE)	British Geological Survey	(B
		Atkins Engineering Sciences	(A
Industrial Power Company Ltd, Finland	(TVO)	Technical Research Centre of Finland	(V

Japan Atomic Energy Research Institute, Japan	(JAERI)	Japan Atomic Energy Research Institute	(JAERI)
		Central Research Institute of the Electric Power Industry	(CRIEPI)
		Hazama-gumi	
Nationale Genossenschaft für die Lagerung Radioaktiver Abfälle, Switzerland	(NAGRA)	Paul Scherrer Institute	(PSI)
National Institute of Public Health and Environmental Hygiene, The Netherlands	(RIVM)	National Institute of Public Health and Environmental Hygiene	(RIVM)
National Radiological Protection Board, United Kingdom	(NRPB)	National Radiological Protection Board	(NRPB)
Swiss Federal Nuclear Safety Inspectorate, Switzerland	(HSK)	Swiss Federal Nuclear Safety Inspectorate	(HSK)
Power Reactor and Nuclear Fuel Development Corporation, Japan	(PNC)	Power Reactor and Nuclear Fuel Development Corporation	(PNC)
Swedish Nuclear Fuel and Waste Management Co, Sweden	(SKB)	The Royal Institute of Technology	(SKB/KTH)
Swedish Nuclear Power Inspectorate, Sweden	(SKI)	The Royal Institute of Technology	(SKI/KTH)
U.K. Nirex Ltd., United Kingdom	(NIREX)	Harwell Laboratory	(HARWELL)
		Intera-Exploration Consultants Ltd.	(ECL)
U.S. Department of Energy, United States	(US DOE)	Battelle Pacific Northwest Laboratories	(DOE/PNL)
		Office of Waste Technology Development	(OWTD)
		Nevada Nuclear Waste Storage Investigation Project	(NNWSI)
U.S. Environmental Protection Agency, United States	(USEPA)	U.S. Environmental Protection Agency	(USEPA)

U.S. Nuclear Regulatory Commission, United States	(US NRC)	U.S. Nuclear Regulatory Commission	(US
		Massachusetts Institute of Technology	
		Battelle Pacific Northwest Laboratories	(NR
		Sandia National Laboratories	
		Center for Nuclear Waste Regulatory Analyses	(C
		University of Arizona, Department of Hydrology and Water Resources, and Department of Soil and Water Sciences	(UAZ/H (UAZ/SV
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INTRAVAL - PHASE II PROPOSAL
Apache Leap Tuff Site

I. INTRODUCTION

A. Pilot Group Identification - U.S. Nuclear Regulatory Commission (NRC), Division of Engineering, Office of Nuclear Regulatory Research, Washington, D.C.; NRC Contractor: Department of Hydrology and Water Resources, University of Arizona, Tucson, AZ. Pilot Group Leader: Thomas J. Nicholson (NRC), Daniel D. Evans (UAz).

This project is designed to provide simple and more complex data sets for validation of fluid flow and solute transport models. The Pilot Group is committed to interactions with the Project Teams in the planning and conduct of experiments and the sharing of experimental results. As data sets are generated, they would be forwarded to interested Project Teams for use in their modeling studies. As additional data needs are identified cooperatively by the Pilot Group and Project Teams, changes in the experimental plan will be incorporated, subject to budgetary constraints. If additional experiments are identified as being necessary, the Pilot Group will seek the necessary funding to perform the studies.

B. Experimental Location - Field experiments are conducted at the Apache Leap Tuff Site in tuffaceous rock (dated approximately 19 m.y. B.P.) near Superior, Arizona, located approximately 160 km north of Tucson, and 100 km east of Phoenix. At the experimental site, the tuff formation is approximately 600 m thick and grades from a densely welded unit near its base to a slightly welded tuff which has a total porosity of 17 percent. The unsaturated zone extends to great depth due to topography and to pumping associated with a nearby underground mine. Vertical and horizontal fracture traces are evident on the land surface and can extend for several hundred meters. Laboratory experiments and measurements are conducted using cores obtained during borehole drilling at the field site and using shaped blocks removed from the field site.

C. Original Purpose - To assess field and laboratory characterization techniques and to generate data sets for the calibration and validation of analytic and numeric flow and transport models for unsaturated flow in fractured media.

D. Phase II Objective - The ultimate objective is to predict water flow and solute transport through unsaturated fractured rock under field conditions. Specific objectives leading to the ultimate objective are:

(1) To further assess appropriate technology for characterizing and monitoring water flow and transport through unsaturated fractured rock, including interaction between the rock matrix and the fracture system.

(2) To examine relevant hydraulic, pneumatic, thermal and solute transport processes, singularly and coupled, at laboratory scales (1 to 60 cm) and at field scales (1 to 30 m).
(3) To generate data sets, for simple, uncoupled systems as well as more complex, coupled flow and transport systems, for use in the validation of unsaturated flow and transport models related to the INTRAVAL program.
(4) To assess, cooperatively with other INTRAVAL participants, various experimental and modeling approaches and their limitations in predicting flow and transport through unsaturated fractured rock.

These objectives are related to the assessment of characterization methods based primarily on soil science techniques for determining the hydraulic, pneumatic, thermal, and solute transport properties of rock matrix cores, and the comparison with transport properties determined from in situ experiments. These objectives include the evaluation of the use of moisture characteristic and unsaturated transmissivity and conductance curves for fractures. They are also related to the examination of relevant processes at selected scales.

Relevant processes include hydraulic, pneumatic, thermal, and solute transport components, which will be investigated using experiments conducted over several length scales, on unfractured tuff cores measuring 6 and 10 cm in length, on rock blocks with a single discrete fracture measuring approximately 50 cm in length, and on in situ measurements taken over distances of from 1 to 30 m. Time scales also vary, from the order of minutes for small core samples, through months for discrete fracture block experiments, to years for large-scale field experiments. A summary of the various proposed experiments are described in the Appendix.

Coupled processes are examined using non-isothermal core experiments, as well as field heater experiments under conditions of partial liquid saturation. The determination of the significance of material heterogeneities and multiple discontinuities will be made at the field site. Due to presence of multiple porosities (including various microporosities, fractures, and vugs), hydraulic properties can vary seven orders of magnitude as a function of position as well as water content.

The objectives will incorporate the evaluation of the predictive ability of various alternative modeling strategies (including the equivalent porous medium representation of fractured flow, as opposed to discrete fracture network flow representation within a porous matrix) for their ability to accurately represent fluid flow and solute transport processes in unsaturated fractured rock. NUREG/CR-5097 by Yeh et al. (1988) discusses the various conceptual models being considered along with a review of possible numerical codes for providing simulation results prior to performing the experiments.

E. Validation Aspects - Predictions of solute transport from a high-level waste repository to the accessible environment are uncertain due to the possible exclusion of relevant processes and the inability to correctly identify and estimate material properties which are highly variable. This proposed INTRAVAL study is designed to evaluate the relative significance associated with excluding various processes, and to evaluate scale dependent procedures used to estimate material properties. Extrapolation of laboratory tests conducted over short distance and time scales with simple analytic solutions to field tests conducted over longer distance and time scales using complicated stochastic models will be used to guide validation activities.

The approximation of multiple porosities and multiple dimensional flow using an effective porosity and dimensionality must be validated prior to application of effective parameters for predictive purposes. Performance assessment issues include the influence of high permeability zones of reduced dimensionality (i.e., one-dimensional channels within fractures) on the ability to contain high-level waste, and the importance of non-isothermal conditions on near field hydraulic conditions. From the proposed experiment, useful performance assessment related information can be extracted directly. Modeling of the experimental results is an important validation aspect, and is the principal reason for conducting the tests. Ideally, the tests will be designed using calibrated models, with calibration data sets having been obtained using laboratory and field tests. Once calibrated, the model will be validated by proposing a perturbation of the system not related to calibration experiments for the purpose of evaluating the assumptions inherent in the model.

Specific validation exercises will be conducted with respect to the conceptual models described in the experimental plan, below. The validation exercises include:

(1) Use of an equivalent porous medium model for characterizing the rock matrix properties with respect to hydraulic, pneumatic, thermal and solute transport;
(2) Evaluation of various parametric relationships between material properties and water content, relative saturation and matric potential;
(3) Assessment of the ability to properly parameterize and conceptualize flow through a discrete fracture bounded by a porous matrix;
(4) Identification of relevant processes related to non-isothermal flow through an unfractured porous tuff rock; and
(5) Ability of existing numerical and analytic methods to predict flow and transport through nonisothermal, unsaturated fractured rock.

The validation data sets will not be limited to these exercises alone, and can be expected to yield additional value as other validation exercises are identified.

II. DESCRIPTION OF THE EXPERIMENTAL PLAN

A. Parameters Measured - A multistage experimental plan is used to estimate parameters related to hydraulic, pneumatic, thermal, and solute transport. The effect of variable fluid saturation on the parameters will be evaluated for a wide range of matric suctions, from oven-dry to saturated. Also, the effect of fractures on bulk properties at various scales will be determined. A more complete discussion of the proposed experiments are presented in the Appendix. Table 1 presents the stages, scales and processes to be incorporated.

Table 1: Experimental stages designed to predict fluid flow and solute transport through unsaturated fractured rock. Each stage introduces additional complexity.

Stage	Experimental Scale (m)	Medium	Processes
I	0.05 x 0.06 (hours)	Matrix (core)	- Liquid, Gas, Thermal Flow - Gas Diffusion
II	0.2 x 0.5 (months)	Matrix/Fracture (block)	- Matrix, Fracture Flow - Solute Transport
III	10 x 30 (months)	Matrix/Fracture (in situ)	- Matrix, Fracture Flow - Solute Transport
IV	0.10 x 0.12 (days)	Matrix (core)	- Nonisothermal matrix flow - Coupled liquid, vapor, air, solute, and heat flow
V	10 x 20 m (years)	Matrix/Fracture (in situ)	- Nonisothermal matrix/fracture - Coupled liquid, vapor, air, solute, and heat flow

Specific parameters from rock core segments (Stage I) include:

- Rock physical properties, including porosity, bulk and grain density, total and incremental pore surface area, and pore size distributions.
- Moisture characteristic curves.
- Saturated and variably saturated rock matrix hydraulic, pneumatic, and thermal conductivity and diffusivity curves.

Parameters from fractured blocks (Stage II) include:

- Fracture surface roughness, aperture, characteristic curves.
- Fracture hydraulic and pneumatic transmissivities, and fracture hydraulic conductance as a function of matric suction.
- Solute transport properties of individual fractures.

Parameters estimated from in situ borehole measurements (Stage III) include:

- Fracture system characterization using geophysical methods, core logging, televiewer logs, and pneumatic tests.
- Rock matrix hydraulic, pneumatic and thermal conductivities obtained at three meter intervals from Stage I activities.
- Ambient borehole water contents obtained at three meter intervals.
- Spatial and temporal ambient temperature distributions.

Laboratory core heater measurements (Stage IV) will be used to estimate parameters including coupled liquid, vapor, air, thermal energy, and solute transport coefficients for the rock matrix. Some of these coefficients will be estimated independently before, during, or after the tests on core samples or on core samples obtained from immediately surrounding the test samples.

Field heater tests (Stage V) will be used to determine the effects of fractures on coupled liquid, vapor, air, thermal and solute transport coefficients. The effect of material property heterogeneity on field scales will be examined with respect to the change from estimates based on laboratory core measurements.

B. Spatial and Temporal Scales - Comparisons of matrix and bulk properties can then be compared to infer the influence of heterogeneities, and scale effects. Various temporal scales are employed at the different physical scales, ranging from minutes for core experiments to years for field experiments (Table 1).

C. Experimental Setups - Multistage experiments are being conducted to incrementally increase complexity from simple systems to complicated ones. The focus of the Phase II study concentrates on two related field experiments, one with and the other without imposed temperature gradients and in similar geologic settings (slightly welded unsaturated fractured tuff). The experimental site with an undisturbed thermal regime has been under study for three years. Fifteen boreholes were installed and used for in situ site characterization, while the obtained cores are used for logging the fractures and characterizing the rock matrix. Water and gas injection-recovery tests are currently underway at the site to determine temporal and spatial responses as well as other flow characteristics. The Appendix presents a more complete description of the experimental plans for the various stages.

D. Sampling Strategy - The core and borehole sampling strategy is to repetitively measure material properties at the same depth interval. Additional details regarding the sampling strategies for the various experimental stages are presented in the Appendix.

E. Independence Between Data Sets - Substantial correlation should exist between data sets for the various stages. Evaluation of the correlation is an integral part of data evaluation. By evaluating differ-

ences between field and laboratory results, an improved conceptual model can be obtained. Also, validation of computer models can be performed more effectively if certain parameters can be maintained constant, allowing other variables to be altered. Calibration data sets obtained from controlled experiments will be used as preliminary input data for simulation models. Simulation results will then be compared to experiments conducted using different initial or boundary conditions. The predictive ability of the validation data set will be related to design of the validation experiment, and must be determined prior to conducting the test.

F. Biases Inherent in the Design - Due to the small size of the field site relative to the scale of a repository, variabilities at scales which may be important to the repository will not be examined. Only processes and variations on the order of 30 meters will be evaluated. Regional variations and processes must be characterized by performing repetitions of the local sampling scheme at other sites. Such repetitions are beyond the scope of the present study. Laboratory measurements on unfractured core segments will be biased toward the matrix properties, while field experiments will be biased more toward fracture properties. Reconciling the experiments will require that the laboratory fracture experiments be integrated with the laboratory matrix measurements.

G. Complementary Experiments - Additional experiments in an abandoned road tunnel and mine haulage tunnel will also provide important data in welded tuff. Comparison of parameters between sites should allow models developed at one site to be verified at another. Regional geochemical experiments are being performed which provide supplementary data sets. Natural analog experiments are recommended to extend the time scales of current analyses, but are beyond the scope of the present study. Nonisothermal studies in the G-tunnel at Yucca Mountain (Daily and Ramirez, 1989) also provide complementary data sets for comparison with experiments proposed here.

H. Background Information - The Apache Leap Tuff Site (ALTS), a field site in central Arizona, is being used to gather data and evaluate methods for the purpose of meeting the objective described above. The Apache Leap Tuff Site is located near the extreme western edge of the Pinal Mountains, which rise to over 2100 m in elevation. Lying immediately east of Superior, Arizona is the Apache Leap which forms a 600 m west-facing escarpment that exposes a volcanic zoned ash-flow tuff sheet and an underlying carbonate. The Apache Leap Tuff Site is approximately one km to the east of the escarpment at an approximate elevation of 1200 m. The rocks exposed at the site are the uppermost unit of a sequence of ash-flow tuff sheets. The tuff is a consolidated deposit of volcanic ash, with particle diameters less than 0.4 mm, resulting from a turbulent mixture of gas and pyroclastic materials of high temperature about 19 million years ago. The ash-flow deposits at one time covered an area of approximately 1000 km^2 with a maximum thickness of 600 m but have been eroded in some places to about 150 m in thickness.

Atmospheric precipitation has been recorded near the site, with the long-term average estimated to be approximately 538 mm/year. Most of the precipitation occurs during two periods, from mid-July to late-September, and from mid-November to late-March. Summer storms are characterized by high-intensity, short-duration thunderstorms during periods of high temperature and evapotranspiration demand. Winter storms are of longer duration and lower intensity during cooler periods with much lower evapotranspiration demand.

Regional ground water levels below the site have been substantially modified by dewatering activities at the nearby Magma mine which extends to a depth of 1500 m below the site. The water levels have been drawn down to levels below the tuff unit. Perched water has been observed at several locations near the site, notably in shallow alluvial aquifers along major washes and from seeps near washes. Noticeable increases in inflows to the main haulage tunnel for the Magma mine are observed within days following streamflow in Queen Creek, which is located approximately 100 m above the haulage tunnel. Observations in mine workings at deeper levels demonstrate increased inflows up to several weeks following streamflow events.

Twelve inclined and three vertical boreholes have been installed at the site in five sets of boreholes. Each set consists of three boreholes drilled in a plane. The inclined boreholes are not of the same length, with the lengths of the boreholes being 15, 30 and 45 m. This design results in the bottom of each borehole in a series lying along the same vertical line. Two inclined borehole sets are parallel to each other and the other two inclined sets are oriented 90° and 180° to the first two sets. A plastic cover has been placed over the rock surface to cover an area of approximately 30 x 50 m. The cover is designed to prevent evaporation from the rock to the atmosphere as well as to prevent precipitation from infiltrating into the rock.

III. AVAILABLE EXPERIMENTAL RESULTS

A. Raw Data - Existing processed data are available.

B. Processed Data - Existing processed data are available in Rasmussen et al. (1990).

C. Data Storage - Raw data are currently stored in microcomputer database files. Processed data are available as printed or ASCII files.

IV. PREVIOUS MODELING

Huang and Evans (1985) have published a discrete fracture network computer model. Extensions by Rasmussen et al. (1985), Rasmussen (1986, 1987, 1988) and Rasmussen and Evans (1989) have been performed using data from other sites. Laboratory experiments on heat flow through a rock core have been modeled by T. McCartin (NRC) using TOUGH. T. McCartin has also modeled field scale water injection and redistribution processes using SUTRA and

VAM2D. At the Third INTRAVAL Workshop at Helsinki, D. Codell presented a particle tracking model to evaluate solute transport in non-isothermal unsaturated, unfractured tuff. Flow through a fractured rock block has been modeled by P. Davis and N. Olague at Sandia National Laboratories using VAM2D.

V. CURRENT STATUS AND EXPERIMENTAL SCHEDULE

Data sets related to Stage I activities (i.e., matrix properties) have been completed and are currently available in draft form. Data sets for Stage II activities (i.e., block experiment) are partially completed. Stage III activities (i.e., field injection tests) are also partially completed with additional experiments planned. The planned experiments include single- and cross-hole air flow characteriation, followed by the long-term injection redistribution experiment. Prototype experiments for Stage IV activities (i.e., non-isothermal core experiments) are currently underway. The experimental plan related to Stage V activities will consider a preliminary experiment conducted in the road tunnel, for which some data sets are available.

VI. INFORMATION EXCHANGE

A. <u>Experimentalist Address</u> -

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Todd C. Rasmussen (602) 621-6216
Department of Hydrology and Water Resources
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University of Arizona, Tucson AZ 85721

B. <u>Modelers Address</u> -

A proposed list of modelers for phase II simulation activities related to the Apache Leap Tuff Site Test Case are provided in Table 2. This list will be revised as additional individuals use the data sets for simulation purposes.

Table 2: List of modelers involved with Apache Leap Tuff Site Test Case.

Stage		Simulation Modeling Groups
I	Core	- UAz, NRC, LBL
II	Fractured Block	- UAz, NRC, LBL, SNL, CNWRA, PNL
III	Field Imb./Redist.	- UAz, NRC, LBL
IV	Nonisothermal Core	- UAz, NRC, LBL, MIT
V	Field Heater	- UAz, NRC, LBL, CNWRA

UAz - Dept. of Hydrology & Water Resources, Univ. of Arizona, Tucson, AZ
NRC - U.S. Nuclear Regulatory Commission, Washington, D.C.
LBL - Earth Sciences Div., Lawrence Berkeley Laboratory, Berkeley, CA
SNL - Division 6415, Sandia National Laboratories, Albuquerque, NM
CNWRA - Center for Nuclear Waste Regulatory Analyses, San Antonio, TX
PNL - Pacific Northwest Laboratories, Richland, WA
MIT - Massachusetts Institute of Technology, Boston, MA

VII. POSSIBILITIES FOR COMPLEMENTARY EXPERIMENTS AND DATA COLLECTION

It is expected that as additional knowledge becomes available with regard to processes important to the modeling of variably saturated non-isothermal flow, complementary experiments and data collection will be required. In such circumstances the Pilot Group and its contractor will be available for designing, constructing and conducting the necessary experiments and collecting any and all data of interest to the Project Teams, subject to budgetary constraints.

VIII. EXPECTED OUTPUT FROM PROJECT TEAM

It is anticipated that the modeling groups will provide design basis inputs for the experimental plan. The simulations will be based on available information and initial designs. The Project Teams will be expected to help define the performance measures and comparison criteria, as well as the data sets required for model validation.

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APPENDIX

Apache Leap Tuff Site Experimental Plans

STAGE 1: Laboratory Core Measurements

Purpose:

The objective of this stage is the characterization of fluid flow, including air and water, thermal energy and solute transport in unfractured, variably saturated tuffaceous rocks at laboratory scales. The data from these measurements will be used in the simplest flow models which do not incorporate fractures or coupled processes. Additional complexity is introduced in subsequent stages.

Background:

The rock matrix excluding fractures is highly heterogeneous with substantial porosity and other material properties changing rapidly over short distances. In order to determine the magnitude and correlation structure of the heterogeneities, as well as to determine the effect of variable fluid saturation on material properties, a large number of measurements on cores obtained at various locations are required. The cores examined in this analysis were removed from borehole cores at three meter intervals from nine boreholes. A total of 105 core locations were examined.

Conceptual Model:

The rock is assumed to be a homogeneous porous medium at the scale of the laboratory measurement. Samples are tested at matric suctions of 0, 10, 25, 50, 100, 300 and 500 kPa and oven-dry conditions, whenever feasible. Physical, hydraulic, pneumatic, and thermal transport parameters are estimated using the core segments.

Measurement Techniques:

Hydraulic:

- Saturated hydraulic conductivity is estimated by maintaining a steady gradient, and measuring the flow rate per unit area.

- Characteristic curves are determined in the wet range using pressure extraction vessel maintained at constant pressure. In the dry range, a thermocouple psychrometer is used to measure atmospheric moisture potential surrounding cores maintained at a constant water content.

- Unsaturated hydraulic diffusivity and conductivity are measured using incremental changes in applied pressure in Tempe Pressure cells and measuring cumulative outflow for each pressure step.

Pneumatic:

- Pneumatic permeability is determined using unsaturated samples at two pressure gradients in a permeameter. Moisture potentials of the rock is prescribed by allowing samples to equilibrate in the pressure extraction vessel prior to insertion in permeameter.

Thermal:

- Thermal diffusivity, conductivity and heat capacity are estimated by drilling two small holes are drilled into the core. A heater coil is placed inside a hole drilled in the center of the core, and a thermistor is used to measure the temperature a short distance away. A constant amperage is prescribed through the heater coil for a finite duration. The experiments are repeated at various moisture potentials prescribed using the pressure extraction vessel.

Available Data Sets:

Rock matrix physical and hydraulic properties, including porosity, bulk density, and moisture characteristic curves are available. Also available are the pneumatic and thermal conductivities as a function of water content.

Sampling Strategy:

- Sampling of rock matrix at three meter intervals in nine boreholes.
- Replication of tests on same sample to determine reproducibility.

STAGE 2: Laboratory Fractured Rock Experiment

Purpose:

The objective of this stage is the characterization of fluid flow and solute transport in variably saturated fractures in tuff rocks at laboratory scales. The data is to complement the Stage I experiments which exclude fracture characterization. The scale of Stage II experiments is designed to allow processes to be examined in the laboratory, and the resultant model used to predict phenomena at field scales, which are to be tested in Stage III experiments.

Background:

Fractures and other macropores provide conduits of high conductivity for flow through saturated rock. Because flow velocities through fractures may be orders of magnitude greater than matrix velocities, the confinement capability of fractured rock may be compromised. Fractures in unsaturated rock may not provide these pathways, however, because large cavities are empty except very near saturation. To investigate the behavior of unsaturated fractured rock, a series of experiments have been and are being performed to characterize the hydraulic properties of fractures and the rock matrix for a range of matric suctions.

To perform the analysis, various rock blocks measuring approximately 60 cm high, 20 cm wide and 20 cm deep have been collected which contains a fracture oriented in the longer plane. Three porous plates are used on both upper and lower rock surfaces to impose negative pressure boundary conditions over a range of suctions from 0.1 to 1.5 kPa. On both the upper and lower surfaces, one plate lies immediately over the fracture, while the other two plates lie beside the fracture plate over the matrix only.

Conceptual Model:

- A single discrete fracture bisects a tuff rock along the long axis of blocks measuring approximately (20 x 20 x 50 cm).
- The permeability of the fracture when saturated is much higher than the surrounding matrix, but the relative permeability decreases to near zero at a matric suction between 0 and 1.5 kPa.
- The rock matrix is initially dry, approximately 50 MPa.
- Porous plates are positioned above and below the matrix, with separate plates positioned above and below the fracture.
- At matric suctions greater than 1.5 kPa, the fracture remains unsaturated, while the matrix is saturated.
- At matric suctions greater than 1.5 kPa, flow is vertically downward due to gravity, and also due to capillary forces when a wetting front is present.

- At matric suctions of 0 kPa, fluid flow is through both the matrix and the fracture, with some flow from the matrix into the fracture near the porous plates.

- Solute transport occurs in the fracture and matrix in response to fluid convection, as well as to convection-induced dispersion.

- Solute transport may also result from diffusion.

- Preferential flow within the fracture may cause nonuniform advancement of solutes in channels.

Boundary Conditions:

- Top and bottom surfaces of matrix and fractured maintained at a constant suction.

- Sides of block are enclosed within a chamber held at nearly constant temperature and saturated vapor pressure.

- Alternating concentrations between 0.1 and 0.001 M CaCl solutions are applied to the upper surface as steps and pulses.

Initial Conditions:

- Block is initially dry, with a relative saturation between 10 and 20 percent, corresponding to matric suctions about 50 MPa.

Available Data Sets:

Rock matrix physical and hydraulic properties, including porosity, bulk density, and moisture characteristic curves are available. The unsaturated hydraulic conductivity of the rock matrix is available from measurements of flow rates through the rock matrix for constant matric suctions and a constant vertical gravitational gradient. During these tests, the absence of fracture flow can be confirmed using visual evidence of wetting front advance and by comparing flow rates through the plate over the fracture with flow rates through the porous plates over the matrix.

Time series of matric potentials are monitored in a vertical fracture and in the rock matrix surrounding the fracture in response to a step increase in the matric potential at the inflow surface. Flow rates and fluid potentials in the matrix and fracture at the inflow and outflow surfaces are also monitored before and after the step change in matric potential.

Time series of solute concentrations at interior sampling ports and at the outflow surface resulting from a step change in solute concentration at the inflow surface are being monitored. A steady influent concentration of $CaCl_2$ is used until a steady outflow concentration is observed. Once steady outflow concentrations are obtained, a step change in the influent

$CaCl_2$ concentration is imposed. The complete data requirements for simulation studies include:

- Matrix/Fracture material properties including fracture aperture distribution, fracture surface characteristics, porosity, matrix and fracture permeabilities, and relative fracture permeability.
- Temperature, relative humidity and matric potential of chamber.
- Initial and time-dependent water contents as a function of depth.
- Initial and time-dependent rock matric potentials as a function of depth and distance from fracture.
- Solute concentrations as a function of time, depth, and distance from fracture.

Sampling Strategies:

- Sampling of fractures and matrix at various horizontal and vertical locations.
- Sampling of outflow from lower porous plates.

STAGE 3: Field Imbibition/Redistribution Experiment

Purpose:

The purpose of this stage is to evaluate the magnitude and distribution of fluid flow in unsaturated fractured tuff. Results from Stage I experiments conducted on unfractured rock are combined with Stage II experiments conducted on fracture segments in the laboratory in order to form a prediction model for flow through fractured rock under *in situ* conditions. Results from Phase III activities will be combined with Phase IV experiments in nonisothermal rocks under laboratory conditions for the purpose of designing Phase V experiments in nonisothermal *in situ* conditions. The dimensions of this experiment are larger than the Stage I and Stage II experiments, with the range of investigation ranging from 1 to perhaps 30 meters.

Background:

When a borehole is flooded with water, fractures may allow the rapid movement of water away from the boreholes. Subsequent movement of the fluid from the fractures into the matrix may result in fingers of saturation along planar discontinuities around the injection region. The fingers may not develop if the matrix intake is large due to low fracture transmissivity, a high matrix hydraulic conductivity, or a high initial water content. Also, if the matrix permeability is practically zero, the fingers will not be observable using the neutron probe due to low water contents over the intervals being monitored. Following the injection phase, the matric suction will decrease, causing a decrease in fracture transmissivity and matrix hydraulic conductivity, with the fracture transmissivity decreasing faster than the matrix hydraulic conductivity. While flow during the injection phase may be dominated by the physical and hydraulic properties of fractures, flow during the redistribution phase may be dominated by matrix properties.

The use of equivalent continuum models is to be tested for describing the processes associated with water infiltration into unsaturated fractured rock and the redistribution of infiltrated water over time. Instead of modeling flow through discrete fractures, the equivalent continuum models assume that an anisotropic tensor can be used to represent the fractured medium. Of particular concern are the potential effects of multiple porosity (i.e., matrix and fracture porosities) on fluid movement during the injection and redistribution phases. The dependency of flow regime on matric suction may or may not be accurately represented using equivalent continuum models.

To obtain characterisation data sets for the fractures present at the field site, a series of single- and cross-hole pneumatic tests are performed. The tests provide information regarding fracture hydraulic properties near saturation, and the behavior of coupled fracture-matrix air flow.

Conceptual Model:

- Liquid water will move in response to a gradient of total hydraulic head. The total head is the sum of elevation, pressure, osmotic, thermal, electric, and other heads.

- The magnitude of liquid water flux is dependent on the product of the total hydraulic head gradient and the hydraulic conductivity of the medium.

- In unsaturated rock, the hydraulic conductivity and the water content decreases with increasing matric suction (i.e., the negative of pressure head)

- The fracture 'transmissivity' (i.e., conductivity parallel to the fracture multiplied by the fracture aperture) may decrease to near zero at matric suctions between 0 and 1 kPa.

- The fracture 'conductance' (i.e., conductivity perpendicular to the fracture divided by the fracture aperture) may decrease less rapidly and at larger matric suctions than fracture transmissivity.

Imbibition Phase:

- Outward water flow from a flooded borehole will occur through fractures and through the matrix.

- Near the flooded borehole, fracture flow away from the borehole will be greater than flow through the matrix.

- Away from the borehole, fracture flow may be attenuated by infiltration into fracture walls.

Redistribution Phase:

- Water in fractures will be imbibed into fracture walls.

- Movement of water will be away from the injection borehole through the matrix, with a preference for downward movement.

- If drained fractures inhibit matrix flow, zones of increased saturation within the matrix on one side of a fracture may develop.

Initial Conditions:

- Ambient water contents of approximately 70 to 80 percent of saturations and ambient matric potentials of approximately 50 to 100 kPa.

Boundary Conditions:

- Upper: covered, no flow. Sides: no flow at infinity. Lower: constant total head gradient, or zero pressure head gradient.

Available Data Sets:

Time series of water injection volumes in four boreholes are available. Water was maintained at a constant total head within inclined boreholes for more than three weeks. Injection volumes were measured approximately every 20 hours. Two of the boreholes are 15 m long, while the other two are 30 m long. Final injection rates varied from a low of 1.27 l/hr in a 15 m long borehole, to a high of 34.68 l/hr in a longer borehole.

Rock matrix and fracture hydraulic properties are available at three-meter intervals for 105 locations in nine boreholes, including the four flooded boreholes. The properties were obtained from oriented cores and single hole testing for bulk density, effective porosity, saturated and relative matrix hydraulic conductivity, moisture characteristic curves, fractured rock saturated hydraulic conductivities, fracture density and fracture orientation. Initial water contents of the rock matrix are also available. Single- and cross-hole injection tests are also being performed to characterize fracture permeability near saturation.

To augment the data sets obtained from the existing boreholes, it is planned to conduct another experiment of longer duration and to monitor the experiment with greater spatial detail. Water contents using the neutron probe will be monitored in the boreholes. The injection phase will maintained for an extended period of time, and then monitored for a year or two after the flooding period. Specific design specifications can be modified as a result of simulation experiments using existing data sets.

The complete data requirements for simulation analysis include:

- Rock material properties, including fracture locations, fracture/matrix permeabilities, and characteristic curves.
- Water contents as a function of space and time.
- Rock matric potentials as a function of space and time.
- Evidence of free water in boreholes.

Solutes will be used during the course of the experiment as tracers to indicate travel rates and paths.

Sampling Strategies:

- Intensive sampling of fractures and fracture zones above and around injection intervals at various distances.
- Intensive sampling of matrix around fractures and fracture zones.
- Moderate sampling of matrix away from fractures.

STAGE 4: Laboratory Tuff Core Heating Experiment

Purpose:

The purpose of this stage is to evaluate the magnitude and distribution of induced fluid flow and solute transport along a partially saturated tuff core. The complicated influences of fractures will be removed in this experiment so that coupling between fluid, heat, vapor, and solute flows can be separated. Stage 5 experiments using *in situ* experiments will incorporate results from both isothermal experiments conducted in Stages II and III, as well as nonisothermal matrix flows conducted here. The scale of this experiment is rather small, on the order of 5 to 10 cm.

Background:

The processes affecting the movement of water and entrained solutes near a high-level nuclear waste repository are of interest for predicting the performance of the waste repository. A thermal source in an unsaturated fractured rock can dramatically affect saturation levels, as well as air, vapor, water and solute movement due to the effect of forced convection and the effects of heat on vapor and air density driven free convection. A laboratory experiment is being conducted to provide calibration and validation data sets for thermal, solute, liquid and air transport as a result of a thermal gradient.

The system to be modeled consists of coupled liquid, vapor, solute and thermal transport in nonisothermal, variably saturated rock. The physics of multiple phase fluid flow under conditions of steady heat flux will be tested using laboratory data sets. Also, theories used to predict the migration of a conservative solute in the liquid phase within a closed system will be evaluated for conditions of an equilibrium thermal gradient. Various complexities can be evaluated including: water plus water vapor only; water plus water vapor and air; and water plus water vapor plus air and solutes. Each additional level of complexity incorporates additional parameters.

Conceptual Model - Heating Phase:

- Liquids around a heat source will vaporize in response to an increase in the vapor pressure deficit, forming a zone of desiccation near the heat source.
- The vapor will move to zones away from the heat source due to pressure gradients and diffusion.
- Heat flux away from the source will occur as sensible heat conduction and latent heat transfer in the vapor phase.
- As the temperature decreases away from the heat source, the vapor will condense at some distance from the heat source, forming a zone of liquid water accumulation.

- Liquid water will move from the zone of accumulation due to a potential gradient.

- Solutes will accumulate in the zone of desiccation due to their low vapor pressure.

Heating Phase:

- Once the heat source has been removed, rock temperatures will decrease over time due to redistribution along the core.

- Vaporization of liquid water will decrease and vapor phase transport will diminish, except along the boundary between the zones of desiccation and accumulation where the greatest temperature gradients may be found.

- Liquid phase redistribution will predominate, with the greatest redistribution occurring between the zones of desiccation and accumulation.

- Solutes will move toward the heat source due to liquid phase convection and away from the heat source due to concentration gradients.

Initial Conditions:

- Ambient initial water contents will be varied.

- Initial solute concentration profile.

Boundary Conditions:

- No flow hydraulic and pneumatic boundary conditions on all surfaces.

- Constant temperature over time at either end, with thermal insulation along the sides of the core.

Available Data Sets:

The physical, hydraulic, pneumatic and thermal properties of the rock matrix will be measured on the rock sample or on samples next to the core. The parameters include the bulk density, porosity, saturated and relative hydraulic, pneumatic, and thermal conductivities, moisture dependent heat capacity, and moisture characteristic curves. The bulk density and initial, transient and final water content distributions within the core will be determined at one cm intervals along the core using gamma ray attenuation methods.

The distribution of solutes concentrations, temperatures, and water contents within the core during the heating experiment will be measured at one cm intervals during the course of the experiment.

STAGE 5: Field Heating Experiment

Purpose:

The purpose of this stage is to evaluate the magnitude and distribution of induced fluid flow around a heat source in unsaturated fractured tuff at field scales. Stage III measurements are also conducted at field scales but neglect the effects of a thermal source. Stage IV experiments were conducted incorporating thermal variations, but ignore field scale processes such as fracture flow.

Conceptual Model - Heating Phase:

- Liquids around a heat source will vaporize in response to an increase in the vapor pressure deficit, forming a zone of desiccation.

- The vapor will move to zones away from the heat source due to pressure gradients and diffusion.

- Outward vapor flow will be greater in undrained fractures than in the matrix due to higher pneumatic permeabilities in fractures.

- Heat flux away from the source will occur as sensible heat conduction and latent heat transfer in the vapor phase.

- As the temperature decreases away from the heat source, the vapor will condense within fractures and the matrix at some distance from the heat source, forming a zone of liquid water accumulation.

- Liquid water will move from the zone of accumulation in various directions:
    - Radially inward towards the zone of desiccation due to a potential gradient;
    - Radially outward, also due to a potential gradient; and
    - Downward due to gravitational forces.

- Below the heat source, the upward flow of liquid water towards the zone of desiccation will be small, with accumulated water draining downward through vertical fractures due to gravitational forces.

- Within the horizontal plane of the heat source, net liquid water flow will be downward, away from the heat source, carried away by gravity drainage in vertical fractures.

- Above the heat source, the largest zone of accumulation will be found. Liquid flow will occur back toward the heat source in fractures, and may reach the heat source, depending upon many factors, including the:
    - Strength and horizontal extent of the heating source;
    - Downward rate of percolation from above;
    - Fracture and matrix permeabilities;
    - Initial rock water content;

- Rock thermal conductivity; and
- Magnitude of free convection.

Cooling Phase:

- Once the heat source has been removed, rock temperatures will decrease over time due to conduction and convection outward.

- Vaporization of liquid water will decrease and vapor phase transport will diminish, except along the boundary between the zones of desiccation and accumulation where the greatest temperature gradients may be found.

- Liquid phase redistribution will predominate, with the greatest redistribution occurring between the zones of desiccation and accumulation above the heat source.

- The rate of liquid phase invasion of the zone of desiccation will be greatest from the zone of accumulation above the heat zone.

- Initial drainage through fractures from the zone of accumulation will occur quickly, while redistribution of rock matrix water contents will occur at a slower rate.

Initial Conditions:

- Ambient water contents of approx. 80 percent of saturation and matric potentials of approx. 100 kPa.

Boundary Conditions:

- Thermal, hydraulic, pneumatic (controlled vs. natural).

Data Requirements:

- Matrix/Fracture material properties including permeabilities, characteristic curves, thermal conductivities, vapor diffusivities.

- Temperatures, relative humidities, water contents, matric potentials.

- Evidence of free water in boreholes.

Sampling Strategies:

- Intensive sampling of fractures and fracture zones above and around heating borehole at various distances.

- Intensive sampling of matrix around fractures and fracture zones.

- Moderate sampling of matrix away from fractures, and lateral and below heating borehole.

INTRAVAL Phase II TEST CASE

I. INTRODUCTION

A. Pilot Group Identification

The pilot group is comprised of the U.S. Nuclear Regulatory Commission (USNRC) Waste Management Branch, Washington, DC (Pilot Group Leader); the Center for Nuclear Waste Regulatory Analysis (CNWRA), San Antonio, TX; Massachusetts Institute of Technology (MIT), Cambridge, MA; New Mexico State University (NMSU), Las Cruces, NM; Pacific Northwest Laboratory (PNL), Richland, WA; Sandia National Laboratories (Sandia), Albuquerque, NM; and the University of Arizona (UA), Tucson, AZ. All participants are currently under contract with the USNRC. University of Arizona and New Mexico State University are currently under contract through September 1992 to do experimental work and to provide data acquisition, data analysis, and data support.

B. Experimental Location

The experiment is located at the New Mexico State University College Ranch, 40 km northeast of Las Cruces, NM, USA. Water and tracers are applied in a carefully controlled fashion to the surface of an experimental plot. The motion of water and the transport of various tracers through the vadose zone are monitored.

C. Original Purpose and Phase I Accomplishments

The original purpose of the Las Cruces Trench Site experiments was to test stochastic flow theories by comparing model predictions with observed measured flow and transport parameters. To do this, a set of characterization experiments and two infiltration/redistribution experiments were designed and completed during Phase I of INTRAVAL.

During the characterization experiments, approximately 600 core and 600 disturbed soil samples were taken to the laboratory to determine soil-water retention and saturated hydraulic conductivity. In addition, the saturated hydraulic conductivity was determined in situ through borehole permeameter tests at a similar number of locations.

The purpose of the Plot 1 experiment was to test the feasibility of using tensiometers and solute samplers in very dry soils and to develop and test the data acquisition methods used in later experiments. Water containing tritium was applied at a rate of 1.76 cm/day to an area adjacent to the south side of the trench. Tritium movement and tension were monitored during infiltration and water content was monitored during infiltration and redistribution. Since this data is available in the Las Cruces Data Base, it can be used for model calibration at higher flow rates.

The experience gained in performing the Plot 1 experiment was used to design and run the Plot 2a experiment. During this experiment, water was applied at 0.43 cm/day to an area north of the trench for 75.5 days. Tritium and bromide was applied with the first 11.5 days of water. The movement of tritium and bromide was monitored through approximately 50 solute samplers inserted through the north face of the trench wall during both infiltration and redistribution (Figure 1). The movement of water was monitored through approximately 50 tensiometers inserted through the north face of the trench wall (Figure 1) and through neutron probe readings taken at approximately 1000 locations in four different vertical planes (Figure 2). The data analysis for the Plot 2a experiment is complete and is presently in the Las Cruces Database. This data will be used for model calibration prior to the Phase II validation experiments.

D. Objectives of INTRAVAL Phase II Test Case

The objective of the Phase II test case is to test deterministic and stochastic water flow and transport theories by comparing model results with measured water flow and transport parameters. The emphasis of the testing is on natural soil systems that are heterogeneous but are well characterized hydrologically. Since the characterization and model calibration data has already been obtained, the emphasis will be placed on model testing and validation during Phase II.

1. The scales of the experiments range from several cm (core and disturbed soil samples) to several tens of meters (field experiments). Temporal scales range from several hours to over a year.

2. Spatial scales for the soil heterogeneities range from less than a meter to several meters. Based on approximately 450 in situ and laboratory based measurements, the saturated hydraulic conductivity ranges over three orders of magnitude. The van Genuchten water retention parameters α and n range over three and one order of magnitude respectively. There appear to be no complex discontinuities such as faults or fracture networks.

3. Water flow and transport of several tracers are monitored during infiltration and redistribution experiments to allow the coupling between these two phenomena to be investigated.

4. There has been little change in overall purpose of the experiment in moving from the Phase I to Phase II. Data for site characterization and model calibration was taken during Phase I. The first Phase II experiment, denoted as the Plot 2b experiment, will utilize the same experimental set-up as was used during the Plot 2a experiment. Water will be applied over the same irrigated area with different tracers and at a different application rate. During Phase II, models calibrated with the Phase I data will be used to predict the Plot 2b water flow and solute transport.

E. Validation Aspects

The ultimate goal of this work is to validate (or invalidate) stochastic and deterministic models for water flow and transport in spatially variable soils. To achieve this goal, mathematical and experimental methodologies required to unambiguously address model validation must be developed and tested. The Las Cruces Trench Experiments are designed by modelers and experimentalists to act as a catalyst in the development of validation methodologies and in the testing of water flow and transport models for spatially variable soils. The spatial variability of the important hydraulic parameters of the site has been carefully characterized on a fine scale and the experiments are run under very controlled conditions.

We plan to address model validation on two levels. On the first level, model predictions will simply be compared to field observations graphically and through simple statistical measures of correlation. While this level of model validation is not rigorous, it does allow the results of many models to be compared with relative little effort. Specifically we plan the following:

1. Using simple deterministic models, various scenarios for the Plot 2b experiment will be simulated by NMSU to help optimize the water/tracer application rates and the choice of tracers.

2. The Plot 2b experiment will then be run and the actual water/tracer application rates will be provided to the modelers.

3. Using the actual water/tracer applications, the Plot 2b experiment will be modeled.

4. After modeling is complete, the modelers will provide NMSU with ASCII files of the predicted water contents, tensions, and solute concentrations at the measurement locations in a predetermined format. In addition, the stochastic modelers will provide NMSU with the predicted statistics of their models. NMSU will tabulate simple statistical measures of correlation between model prediction and observation and will include the predictive statistics provided by the stochastic modelers.

5. After receiving the model predictions, the observed water contents, tensions, and solute concentrations, as well as all of the model predictions, will be distributed in ASCII format to the participants (through the Las Cruces Database). This will allow the individual participants to address the issues of model validation in more detail.

6. Presently, we anticipate using the following models:

   Sandia will utilize the VAM2D finite element code developed by Huyakorn et al. (1989). VAM2D can model water flow and transport in a variable sat-

urated anisotropic soil as well as single-species and chained decay transport.

MIT will use stochastic water flow models (Gelhar (1984), Mantoglou and Gelhar (1987a,b,c), Polmann et al. (1988), Yeh et al. (1985a, b, c)) to simulate the long term water movement in the Plot 1 experiment. These models generate effective media approximations to the important hydraulic parameters allowing non-Monte Carlo simulation of water flow in heterogeneous and anisotropic soils. The Plot 2b experiment may also be modeled by MIT later in Phase II if adequate funds become available.

PNL will model transport of both inert and chemically active tracers (if applied) for the Plot 2b experiment. Initially, the transport analysis will be performed using one or more deterministic codes (e.g., TRACR3D, PORFLO3). Multiple realizations will be simulated using Monte Carlo methods to estimate the variation in the solute front due to spatially variable soil properties. Later, if chemically active tracers are used in the transport experiments, a coupled geochemical code (e.g., FASTCHEM) will be used to predict tracer plume movement in the trench soil profile.

CNWRA will utilize the three-dimensional water flow code of Ababou (1988). This code models the nonlinear effects of partially saturated water flow in a randomly heterogeneous and anisotropic soil. The input parameters will be conditioned using the Las Cruces Database. The algorithm has been used to generate three-dimensional high resolution flow simulations, as described in Ababou and Gelhar (1988).

NMSU will use the water content based algorithms of Hills et al. (1989a, 1990) to model water flow and transport using an isotropic uniform and layered soil model.

On the second level of model validation, MIT is presently developing statistically rigorous quantitative validation methodologies (under contract to the USNRC). Researchers at Sandia and NMSU are also investigating issues of model validation. If funds are available, MIT may demonstrate the model validation methodology using simple models for water flow and the Las Cruces Database for the Plot 1 experiment. Due to the extra effort required, it is not anticipated that the previously described models will be rigorously validated using this methodology during Phase II.

II. EXPERIMENTAL DESIGN

A. Parameters Measured - Key measurements include:

1. Saturated hydraulic conductivity (both in situ and laboratory measurements) and $\theta(h)$ data have been determined for approximately 600 locations in a vertical plane immediately adjacent to the test plots.

2. Measurements of θ_r and θ_s and estimates of the van Genuchten water retention parameters α and n have been determined for each of the 600 locations. Specific water capacity, C, can be estimated from the resulting van Genuchten curves.

3. Moisture content or moisture profiles as a function of time is monitored using downwell neutron-probe logging.

4. Tension data obtained from tensiometers placed on a two dimensional grid on the north trench wall are monitored as a function of time.

5. Concentrations of the tracers are sampled through the trench wall on a two dimensional grid as a function of time. Tracer concentration samples will also be taken at other locations from soil samples taken during and after the execution of the Plot 2b experiment. This destructive sampling will allow a three dimensional picture of the tracer concentration profiles to be generated.

B. Spatial and Temporal Scales

Temporal scales include sampling times for infiltration events ranging from hours (during early infiltration) to hundreds of days for later observations. The time interval for both infiltration tests and redistribution tests exceeds 70 days with measurements taken every several days during infiltration and less often during redistribution. Monitoring locations for tensions exceed 50. Monitoring locations for solute (tritium and bromide) also exceeds 50. Over 1000 neutron probe monitoring locations are used to measure water content.

C. Experimental Set Up

A trench 16.5 m long, 4.8 m wide and 6.0 m deep was dug in undisturbed soil. Water containing tritium and bromide tracers was applied at a controlled rate of 0.43 cm/day on the surface of one side of the trench to generate data for model calibration. The movement of water below the soil surface has been monitored with neutron probes and tensiometers. Soil solution samples have been taken to determine the movement of tritium and bromide below the surface of the soil during the Plot 1a calibration experiment. During construction of the trench, the physical properties of the soil at the site were determined in sufficient detail to allow estimation of many of the statistical parameters needed in the stochastic and comparative deterministic models.

An irrigated area measuring 1.2 m by 12 m is located adjacent to the trench. The walls of the trench were excavated vertically and reinforced to prevent cave-in. The trench and adjacent irrigated area have been covered to prevent surface runoff and recharge due to rainfall and to minimize evaporation.

The drip irrigation system consists of 40 irrigation lines placed parallel to the trench

face with each irrigation line containing 4 drippers. The applied water is metered onto the plot to allow for water balance calculations. Water was applied at an rate of 0.43 cm/day during the model calibration experiment and will be applied at a different rate during the model validation experiment.

Laboratory and field uniformity tests of the drip irrigation system prior to the Plot 2a experiment indicated extremely small non uniformities and a random distribution to the non uniformities.

The water content in the soil is determined with neutron probes. Neutron access tubes were installed vertically in three rows parallel to the trench face (Figure 2). The first row is 2.0 m from the trench wall, the second row is 6.0 m from the trench wall, and the third row is 10.0 m from the trench wall. There are presently eleven neutron access tubes per row, spaced 1 m apart. Additional neutron access tubes are installed as the wetting front progresses horizontally. There is a fourth row of neutron access tubes positioned perpendicular to the trench wall and along the center of the irrigated area (Figure 2). These tubes are spaced at either 1 or 2 m intervals. Additional details of the experimental setup are given in Wierenga et al. (1986), in Nicholson et al. (1987), and in Hills et al. (1990).

Tension is monitored through tensiometers installed in a two dimensional grid through the trench wall (Figure 1).

Tritium at a final concentration of 0.1mCi/l and bromide at a final concentration of 0.8 g/l was applied with the water during the first 11.5 days of irrigation for the Plot 2a calibration experiment. Tritium and bromide concentrations were sampled on a regular basis through solute samplers installed in a two dimensional grid through the trench wall (Figure 2).

Deterministic and stochastic models of water flow and solute transport will be used by personnel at USNRC, MIT, NMSU, Sandia, and UA to optimize the Plot 2b model validation experiment. Sampling rates, water application rate, and the type of tracers used for experiment 2b will also be defined by these personnel.

D. Sampling Strategy

Two sampling strategies are used.

Scheme 1: HYDROLOGIC PARAMETER CHARACTERIZATION.

From a total of 9 horizontal transects (25 m in length) and 3 vertical transects (6 m in length), sampled at intervals of 0.5 m in the horizontal direction, measurements of field saturated hydraulic conductivity have been made in situ with an unsaturated-borehole technique (borehole permeameter). Cores taken adjacent to these boreholes have been taken to the laboratory for analysis of a) water retention characteristics, b) particle-size analysis, c) bulk density, and d) soil chemical prop-

erties (e.g., $CaCO_3$ content, soil paste pH and soluble cations and anions). Over 600 measurements of field saturated hydraulic conductivity have been made to date. Similar numbers of water retention curves, particle-size analysis, bulk densities, and chemical properties have been measured in the laboratory from the core samples.

Scheme 2: INFILTRATION AND REDISTRIBUTION TESTING OF WATER AND SOLUTE MOVEMENT

The face of the experimental trench is monitored intensively with solution samples and tensiometers. The solution samplers are tensiometer cups that are connected to a vacuum line (sometimes called suction lysimeters). These units are used to collect small (2-10 ml) quantities of solution as the water infiltrates into the soil profile. Tracer pulses can be analyzed by periodic collection of samples. A 10 day pulse of tritium was used to trace the transport of water in a preliminary infiltration test performed on the south side of the trench face during the Plot 1 experiment. The Plot 1 experimental results indicated that the use of solution samplers is a viable technique for monitoring solute transport in unsaturated soils, particularly when the tensions were less than 150 cm. At higher suctions the water transmission rate is too low to obtain sufficient quantities of sample to monitor. These samplers were also used during the Plot 2a experiment and will be used during the Plot 2b experiment. Tensiometers placed adjacent to suction samplers (Figure 1) are used to monitor tensions (soil suction) and operated reasonably well after the wetting front had passed. These units do not work in the dry soil. Water tensions in dry soil must be inferred by the water retention characteristics taken from the characterization data of Scheme 1. Neutron probes are used to monitor water contents in three planes located parallel to the trench face and in 1 plane located perpendicular to the trench face (Figure 2). The neutron probe monitoring and tensiometer reading is done on the order of hours during initial infiltration, on the order of days as time progresses and infiltration moves water deep into the soil profile, and finally on the order of weeks during the later stages of redistribution. Higher flow rates require higher sampling rates. During and after the completion of the Plot 2b experiment, additional core samples will be taken from strategic locations throughout the experimental area to better define the three dimensional distribution of the tracers. The characterization methodologies developed by MIT will be used to define core sample locations.

E. Independence Between Data Sets

The hydraulic characterization data are taken from an area adjacent to the Plot 1 and 2 infiltration and redistribution experiments. The results from the Plot 1 and 2 experiments were not used to calibrate or redefine the characterization data in any way. The characterization data is thus independent of the Plot 1 and 2 data.

The Plot 1 and Plot 2a data were taken from opposite sides of the trench and at different flow rates and are thus independent.

The neutron probe data, the tensiometer data, and the solute samples taken through the trench wall will be taken from the same locations during the Plot 2a and 2b experiments. However, additional solution samplers will be installed as the solute front moves through the soil profile. The experiments will be at different flow rates using different tracers. Thus, the Plot 2b data will be independent of the Plot 2a data in the sense that different experiments are run but dependent in the sense that the experiments are run at the same location using the same monitoring system.

The additional core samples taken during and after the Plot 2b experiment will be taken from locations not previously sampled. Thus this data will be independent of the solute concentration data obtained through the trench face during the Plot 2a and 2b experiments.

Water flow is monitored using both tensiometers and neutron probes. Since these methods are different, the corresponding data are independent.

F. Biases Inherent in the Design

1. The soil retention characteristics determined in the laboratory may not be a true representation of the water release characteristic in the field. Sampling and measurement techniques have not been developed to the point that the entire (wet to dry) range of the water retention curve can be measured in the field by a single instrument. Hence laboratory measurements are used to supplement field observations. Pressure plate techniques may tend to over estimate water contents at high tensions (1.0 to 1.5 MPa values).

2. Since tensiometers only operate in the wet range, the majority of the data will be in a range where tensions are not too large (< 150 cm H_2O). This will tend to bias the tensiometer readings toward wetter environments than are normally experienced in arid regions. In contrast, neutron probes can measure very small water contents. However, neutron probes are inherently poor at define sharp wetting fronts due to the relatively large effective area of the probe measurement.

3. The unsaturated conductivity functions determined from pore-size models may inadequately describe the actual unsaturated conductivity values in the field. While these data are independent, they should be checked against laboratory measurements of unsaturated conductivity and possibly with instantaneous profile observations using time dependent tension and moisture content profiles from the infiltration and redistribution tests that have been run at the trench site.

G. Complementary Experiments

A suite of experiments have been performed to evaluate stochastic model capabilities. The large lysimeter tests (described in Wierenga et al. (1986), Wierenga and

van Genuchten (1989), and Hills et al. (1989b)) as well as the laboratory column tests were used to estimate transport parameters (i.e., Peclet number, dispersion coefficients, etc.) that are useful to understand field transport in soils of similar physical and chemical characteristics. These experiments consist of infiltration and redistribution tests in uniform soils and layered soils under similar flow conditions as those imposed in the field tests. The lysimeter tests are complete.

A Plot 3 experiment is planned for the near future at a different location on the north side of the trench. The purpose of the Plot 3 experiment is to further test validation methodologies and to validate stochastic and deterministic water flow and transport models on a larger field scale. Information gained during the Plot 2b experiment and suggestions from the INTRAVAL participants will be carefully considered during the Plot 3 experimental design.

H. Background Information

The field site is on a basin slope of Mount Summerford, which is at the north end of the Dona Ana Mountains. The Dona Ana Mountains form a domal uplift complex of the younger rhyolitic and the older andesitic volcanics intruded by monzonite (Gile, Hawley and Crossman (1970)). The sediments on the mid-piedmont have young soils (6500 to 4000 years B.C.) of the Dona Ana and Onite series (coarse-loamy Typic Haplargids). Sediments on the lower-piedmont slopes are older soils (mid-late Pleistocene) dominated by the Berino series (fine-loamy Typic Haplargids). The geologic features, Oeomorphic surfaces, soil series and vegetation types found in the area around the field test area are typical of many areas of southern New Mexico and are similar to arid and semiarid areas of the southwestern United States.

The climate in the region is characterized by an abundance of sunshine, low relative humidity, and an average Class A pan evaporation of 239 cm/yr. Average annual precipitation is 23 cm with 52% of the rainfall occurring between July 1 and September 30. The average monthly maximum air temperature is highest in June at 36 C and lowest in January at 13 C.

III. AVAILABLE EXPERIMENTAL RESULTS

A. Raw Data

Water retention data, density profiles, particle-size analysis data, and saturated hydraulic conductivities measured through both laboratory and in situ techniques during the characterization experiments and water content data, tensiometer data, tritium and bromide concentrations, and water applications rates measured during the Plot 1 and Plot 2a experiments are contained in the Las Cruces Database. The Plot 2b data will also be incorporated into the database using the same format. In addition, morphological mapping of the trench face, drip irrigation distribution tests, and outflow and inflow measurements from large and small column-support tests are on file at NMSU and at UA.

B. Processed Data

These data have been reported in two annual reports (NMSU to NRC 1985, 1986), in Wierenga et al. (1986), in Nicholson et al. (1987), and in Wierenga et al. (1989). These data consist of moisture profiles determined from neutron probe calibration curves; tension profiles from tensiometer data mapped as a function of time; tritium profiles and breakthrough curves (obtained from solute sample analysis); and wetting front observations from the first trench experiment from visual mapping of the wetting front advance with time. In addition, the van Genuchten water retention parameters α and n for each of the 600 core sample locations and the parameters for uniform and layered soil models are included in the Las Cruces Database and discussed in Wierenga et al. (1989).

C. Data Storage

Data are stored in Las Cruces in laboratory notebooks, on IBM (5 1/2" floppy) disks, and on 10 MByte Bernoulli disks. Redundant copies of the digital data are stored in Tucson on 20 MByte Bernoulli disks and in the Las Cruces Database. The Las Cruces Database is installed on a Digital VAX and is backed up regularly by computer center personnel. The database consists of 26 files in ASCII format, is in the public domain, and is accessible at no cost through the international computer networks using FTP. The database is updated on a regular basis. Copies of the database are also available on IBM compatible floppy disks and will be made available in hard copy form (through NUREG reports) in the near future.

IV. PREVIOUS MODELING

The modeling that has been done to date using the field data sets are described in MIT reports (thesis, etc.), in Nicholson et al. (1987) , and in Hills et al. (1989a, 1989b, 1990). There was some additional work using UNSAT2 (Davis and Neuman (1983)), a deterministic code, but this did not prove successful and will not be used in future testing of the field data. The modeling and the experimentation in Phase I of the study have been interactive in that model deficiencies have been identified and corrections/improvements have been made to the stochastic models as these data became available.

V. CURRENT STATUS AND EXPERIMENTAL SCHEDULE

The characterization, Plot 1, and Plot 2a experiments are complete. The Plot 2b experiment will use existing facilities and will start during the early Spring of 1990. The Plot 3 experiment will be planned during the next year and is expected to run through the summer of 1992.

VI. INFORMATION EXCHANGE

Addresses of Key Personnel

Name	Address	Phone No.
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Dr. Glendon Gee	Pacific Northwest Laboratory Box 999 Richland, WA 99352 USA	509-376-8424
Dr. Lynn Gelhar	Dept. of Civil Engr. 48-329 Massachusetts Institute of Technology Cambridge, MA 02139 USA	617-253-7121
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Dr. Dennis McLaughlin	Dept. of Civil Engr. 48-209 Massachusetts Institute of Technology Cambridge, MA 02139 USA	617-253-7176
Thomas Nicholson (Pilot Group Leader)	USNRC, MS NL/S-260 Washington, DC 20555 USA	301-492-3856
Dr. Peter Wierenga	Soil and Water Science University of Arizona Tucson, AZ 85721 USA	505-646-2028

VII. POSSIBILITIES FOR ADDITIONAL COMPLEMENTARY EXPERIMENTS AND DATA COLLECTION

As discussed above, an additional experiment is planned for the near future at a different location on the north side of the trench. The purpose of the Plot 3 experiment is to further test validation methodologies and to validate stochastic and deterministic water flow and transport models on a larger field scale. Information gained during the Plot 2b experiment and suggestions from the INTRAVAL participants will be carefully considered during the Plot 3 experimental design.

Additional site evaluations (infiltration and redistribution tests) using similar techniques have been discussed. Cooperation with other US experimentalists to obtain well-characterized data sets of hydrologic properties for multiple sites is desirable. These data sets are presently not available in the detail needed to test stochastic models adequately.

VIII. EXPECTED OUTPUT FROM PROJECT TEAMS

A. Experimental View

The criteria for validation and the requirements for precision in measurements will be aided by interchange with scientists who are running similar tests. We expect that much of the validation testing may well be aided by improved techniques that may be available and used by other countries but not currently being tested (because of budget constraints, etc.) in the USA. These ideas, discussed and shared, will be valuable for enhancement of the study. New methods of tracer sampling techniques as well as development and testing of transport codes for unsaturated soil systems will aid the experimentalist in designing appropriate tests to evaluate the transport parameters needed in the modeling component of the study.

B. Modeler's View

The modeler's view is quite similar to that of the experimentalist in that the exchange of ideas and modeling techniques with INTRAVAL participants from the USA and other countries will be useful. For example, as stochastic codes become available from other countries, these codes could be used/tested against data available from this project. The geostatistical approaches can be enhanced by discussion with experts from INTERVAL projects that routinely use spectral analysis and other techniques to obtain the statistical parameters needed in the stochastic model(s). The information exchange will be very valuable during all stages of this project.

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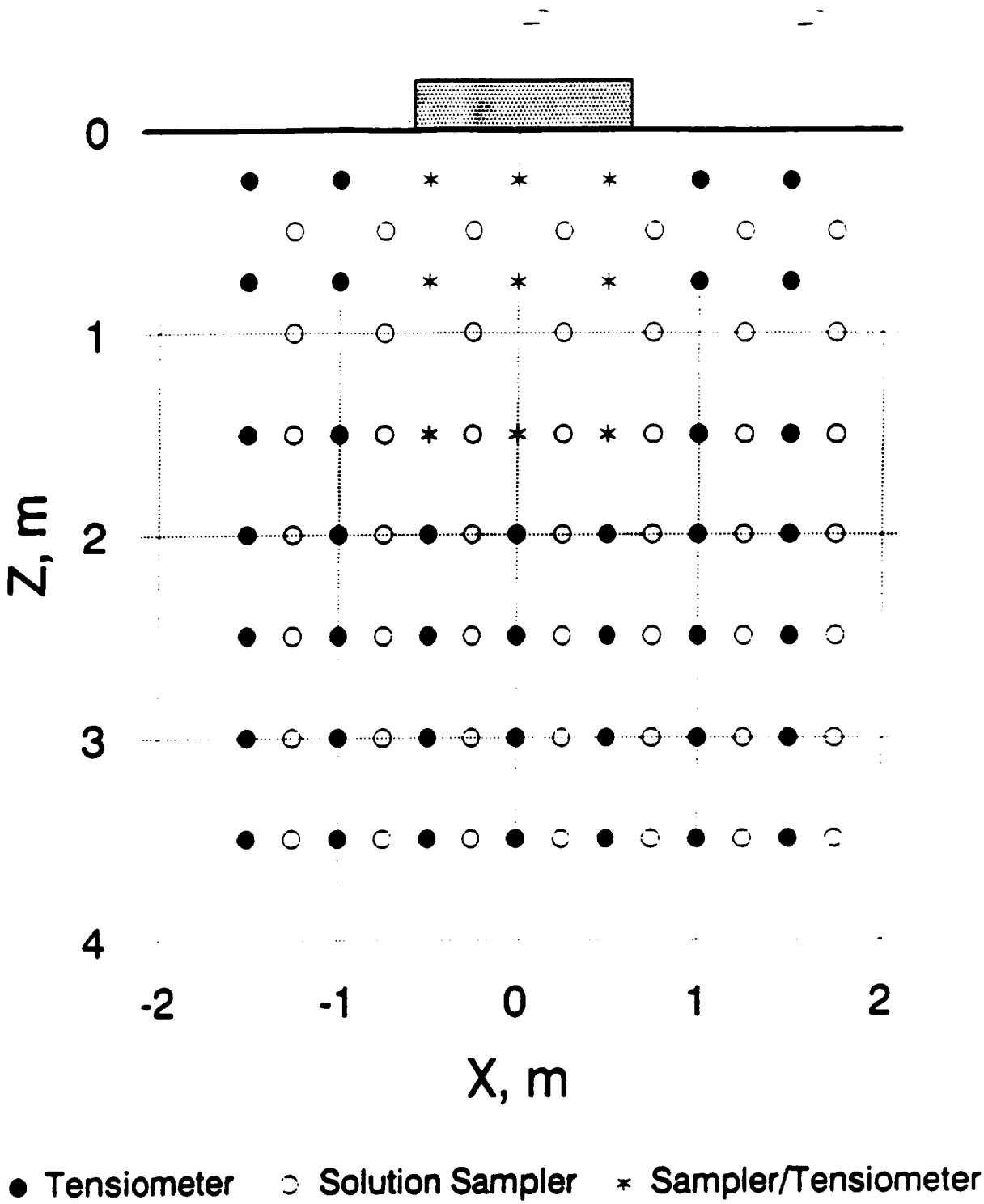

Figure 1: Location of the Tensiometers and Solution Samplers on the Trench Face for the Plot 2a Experiment.

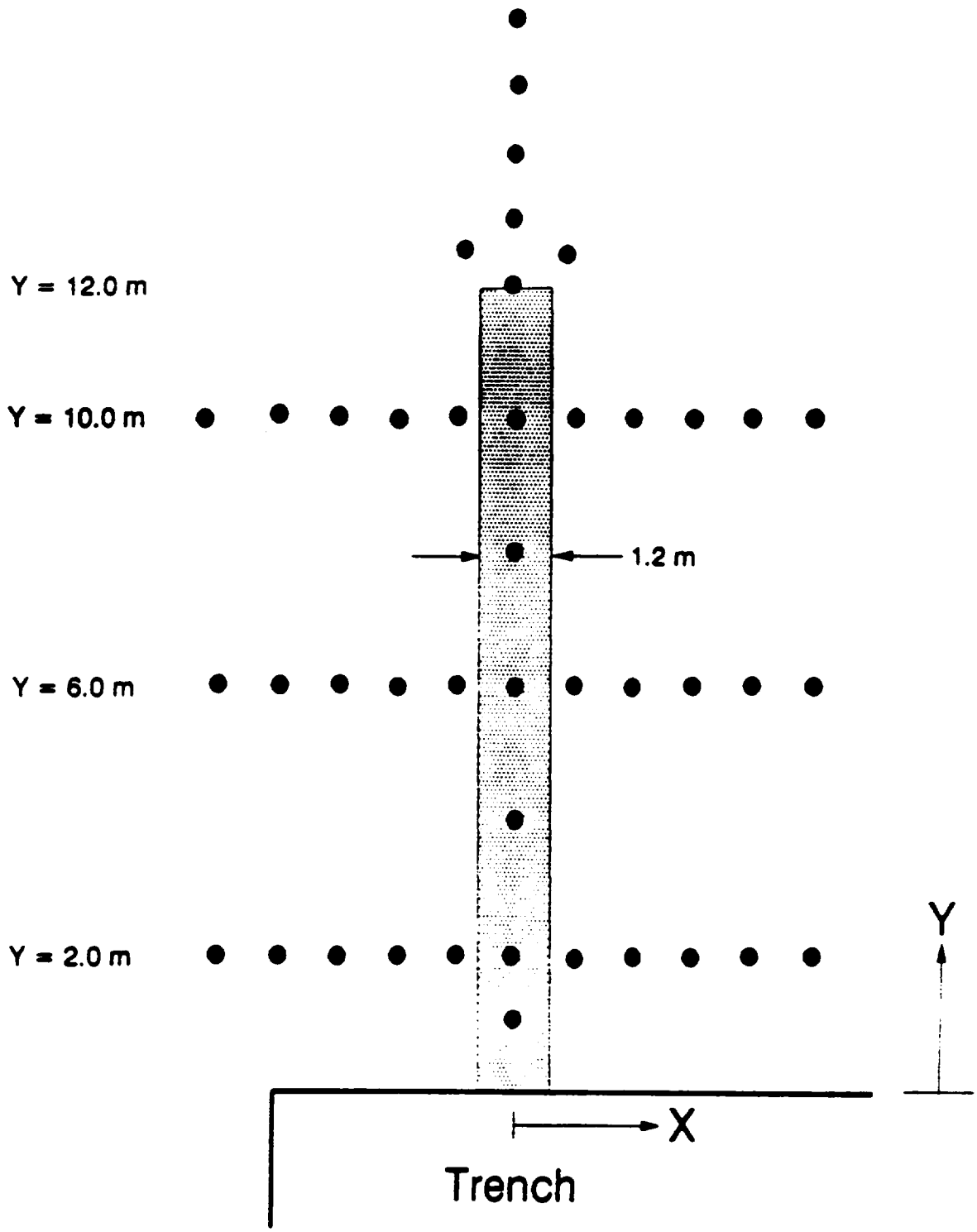

Figure 2: Location of Neutron Probe Access Tubes for the Plot 2a Experiment: Plan View.

Golder Associates Inc.
CONSULTING ENGINEERS

August 2, 1990

Our ref: 903-1106

Office of Geologic Disposal
U.S. Department of Energy
P.O. Box 98518
Las Vegas, NV 89109-8518

ATTENTION: Carl Gertz

RE: INTRAVAL PHASE II PROPOSAL

Dear Mr. Gertz:

Phase 1 of the INTRAVAL Project will end in October of this year. Currently, the experimenters and modeling teams are preparing summary reports to be published over the next year as a series of INTRAVAL Technical Reports. As Phase 1 activities are ending, planning for the second phase of INTRAVAL is underway.

As the OCRWM Coordinating Group Member to INTRAVAL I have been in contact with several of your staff and YMP contractors to coordinate the remaining work for Phase 1 and assess their interest in participating in the Phase 2 activities. A meeting was held in Las Vegas on April 17 of this year. Participating in the meeting were R. Dyer, J. Boak, and R. Levich (YMP), L. Sheppard, P. Kaplan and R. Glass (SNL), D. Hoxie and A. Flint (USGS), D. Chestnut (LLNL), C. Tsang (LBL) and myself. Based on the discussions at this meeting, I have prepared a draft proposal (attachment A) describing a scope of work for YMP in Phase 2 of INTRAVAL.

The proposed tasks are based largely on a number of observations made at the meeting concerning tests that were performed in the G-Tunnel Underground Facility and the programmatic needs of YMP that could be met via participation in Phase 2.

The following comments figured greatly in the content of the proposal:

- A large amount of hydrologic and thermal-hydrologic data exists from the G-Tunnel prototype studies in unsaturated tuff but a significant portion of the data has not been adequately documented. While some of the data will be reported in upcoming reports (e.g., the dry v.s. wet drilling study by the USGS will be documented in an INTRAVAL Phase I Technical Report on Test Case 12) other data are at risk of being lost if they are not processed and archived in the near-

future. An example of the latter is the G-Tunnel heater experiment conducted by LLNL. The principle investigator for this study is purported to have insufficient funding to complete the processing and reporting of the data from this experiment. There is a risk of losing much of the information from this experiment and others if the data are not processed and archived in the near-future. (This concern is based on the periodic changes in staffing and the associated difficulties in recovering and analyzing unprocessed data for which they were responsible.)

- Data from the dry v.s. wet drilling study are being used to develop conceptual process models for flow and transport in unsaturated tuffaceous rock. The completeness of the data set would be much improved with the addition of the LLNL heater test data.

- The robustness of the process models for use in unsaturated tuffs at other sites has not been demonstrated. Additional field experiments are needed to increase our confidence of the applicability of the models to other unsaturated tuffaceous rocks.

- Because the permits necessary for performing field experiments at Yucca Mountain are not being issued by the State of Nevada for the foreseeable future, it is not possible to perform on site studies to confirm the applicability of the conceptual process models. In lieu of this, additional off site experiments are desirable to improve confidence in these models.

Given the above, the participants concluded that Phase 2 of INTRAVAL could play a useful role in furthering the development of thermohydrologic process models for unsaturated tuffs and demonstrating the ability of such models to simulate the performance of large-scale field experiments. Of the currently planned Phase 2 activities, the most relevant is the Apache Leap Heater Experiment sponsored by the Nuclear Regulatory Commission. This experiment will be performed by the University of Arizona (UA) at the Apache Leap tuff site near Superior, Arizona. The experiment is currently being designed and the NRC has expressed a willingness to include OCRWM/YMP in all stages and aspects of the experiment.

The existing site data collected by the UA in earlier phases of the Apache Leap investigation will be used to calibrate the existing p$xcess models. The models will be used to assist the NRC and UA to design the heater experiment and predict the thermohydrological response of the tuff a priori. The OCRWM/YMP involvement in INTRAVAL is seen as an excellent mechanism to consolidate the various sources of property data from the G-tunnel experiments and a unique opportunity for the scientific staff to interact with international experts in flow and transport modeling. This type of exchange will improve DOE's scientific credibility through the international peer review the work will receive.

The next meeting of INTRAVAL will take place October 15-19, 1990 in Cologne, FRG. The Secretariat has requested that all the proposed test cases and working groups be submitted at that time. In order to prepare for this meeting, I would like to meet with you and your

Summary information about the test cases is provided in Tables 1 and 2. The test cases are complimentary in that the advective processes involved are similar. However, the behavior of the soil series at the Las Cruces Trench site is considerably different from that of the tuffaceous rocks at the Apache Leap and G-Tunnel sites. The degree to which the data can be correlated is questionable. On the other hand, the rock types and conditions at the Apache Leap site and the G-Tunnel Underground Facility are similar enough to permit more direct comparison.

The Apache Leap Tuff Site is an escarpment near Superior, Arizona that exposes a 600 m volcanic ash-flow tuff sheet and an underlying carbonate. The tuff formation grades from a densely welded unit near its base to a slightly welded tuff having a total porosity of 17 percent. The regional groundwater level at the site has been modified by dewatering activities at the nearby Magma Mine and is approximately 1500 m below the surface. The annual precipitation is around 50 cm/year. Perched water has been observed at several locations, typically in shallow alluvial aquifers along major washes and seeps near washes. The tuffs contain ubiquitous fractures with an average dip of 65°and a fracture frequency of ~ 0.8 per meter.

The University of Arizona is conducting a series of laboratory and field experiments at Apache Leap for the Nuclear Regulatory Commission. The experiments range in scale from

Table 1. Location, scale and participants associated with the INTRAVAL unsaturated zone test cases.

Test Case	Location	Sponsor	Principal Investigator	Test Scale
Las Cruces Trench	Las Cruces, New Mexico	Nuclear Regulatory Commission	University of New Mexico	>10 m
Apache Leap Core Experiment	University of Arizona		University of Arizona	<20 cm
Apache Leap Block Experiment				~50 cm
Apache Leap Field Experiment	Apache Leap Site, Superior, Arizona			>30 m
G-Tunnel Experiment	G-Tunnel Underground Facility, Nevada Test Site	Department of Energy	U.S. Geological Survey	~6 m

DRAFT PROPOSAL FOR OCRWM/YMP PARTICIPATION IN PHASE 2 OF THE INTRAVAL PROJECT

August 2, 1990
Version 1.0

Proposal Team

The following proposal for Yucca Mountain Project (YMP) participation in Phase 2 of the INTRAVAL Project was developed by the following individuals: C. Voss (Golder Associates Inc.); C. Tsang (Lawrence Berkeley Laboratory); R. Dyer, J. Boak, and R. Levich (Department of Energy/Yucca Mountain Project Office); D. Chestnut (Lawrence Livermore National Laboratory); L. Sheppard, P. Kaplan, R. Glass (Sandia National Laboratory); and D. Hoxie, A. Flint (U.S. Geological Survey).

Background

The INTRAVAL Project was started in 1987 as an international effort among more than 10 countries to perform model validation exercises and develop validation strategies. INTRAVAL is unique in that the project facilitates close interaction between modelers and experimenters in these validation exercises.

Phase 1 of INTRAVAL consisted largely of laboratory and small-scale field experiments where the flow and transport processes were simulated numerically. At the onset of the project, a time period of three years was foreseen for the study while maintaining the possibility of a three year extension to the project if deemed worthwhile. The participants in INTRAVAL maintain that the Phase I effort has led to significant progress in understanding the steps in the model validation process and a number of the physicochemical processes important for the safe disposal of nuclear waste in geologic repositories.

Still, more work is necessary in this area and the INTRAVAL Coordinating Group has recommended that a Phase II effort be initiated in October of 1990 and continue for three years. It is proposed that Phase II be organized and managed similarly to Phase I, building on the findings made during the earlier work. The technical basis for Phase 2 is a set of test cases that were proposed at the last INTRAVAL workshop in Las Vegas. Final decisions on the number and nature of the test cases for Phase 2 will be made at the upcoming INTRAVAL workshop in Cologne. The major emphasis in Phase 2 will be on the use of information from field experiments and natural analogue studies in the validation process, focusing on the need to understand the structure of the systems involved.

While many of the Phase 1 test cases involved flow and transport in saturated environments, three of the test cases addressed multiphase flow under unsaturated conditions:

- Test Case 10 - the Las Cruces Trench Experiment
- Test Case 11 - the Apache Leap Studies
- Test Case 12 - the G-Tunnel Experiment

staff to discuss the proposal in greater detail. I have made arrangements through your secretary to brief you on August 13 at 3:00 PM. If you have a conflict with this time or questions you would like addressed before then, please contact me at (206) 883-0777. Thank you for your assistance in this matter.

Sincerely,

GOLDER ASSOCIATES INC.

Charlie Voss
Senior Engineer

CV/kew

DOE/OCRWM Coordinating Group Member to INTRAVAL

cc: S. Brocoum
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A. Flynt
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D. Chestnut
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D. Shelor
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Table 2. Status and objectives of the INTRAVAL unsaturated zone test cases.

Test Case	Status	Objectives
Las Cruces Trench Experiment	Experiment completed, some modeling ongoing	Validation of parameters and models relevant for radionuclide modeling in soils
Apache Leap Core Experiment	Completed	Study of flow and transport under steady-state temperature gradients
Apache Leap Block Experiment	Experiments ongoing	Study of flow in fractured tuff rock under unsaturated conditions
Apache Leap Field Experiment	Experiments ongoing	Study of flow and transport in unsaturated fractured tuff
G-Tunnel Experiment	Experiment completed, modeling ongoing	Study of the near-field effect of propagating transient heat and moisture disturbances in fractured tuff

core specimens and shaped blocks to twelve inclined boreholes drilled within a 30 x 50 m area at the site.

The G-Tunnel Experiment was performed by the U.S. Geologic Survey and consisted of the coring of pairs of horizontal boreholes into non-welded and welded tuffs using both dry drilling and conventional (wet) methods (this experiment is a derivative of a prototype drilling study funded by DOE). After drilling approximately 10 m from the face of the rib, instrumentation was installed in the boreholes to monitor any crosshole effects caused by the drilling of the adjacent holes and to determine the time required for the conditions to reach equilibrium. The study also included a suite of laboratory experiments to determine the intrinsic hydrologic and thermal properties of the tuffs and their water characteristic curves in order to understand and explain the field observations. A number of empirical and theoretical process models have been developed to simulate the hydrological behavior of the tuffs.

Proposed Scope of Work for Phase 2 of INTRAVAL

The objective of the proposed YMP participation in Phase 2 of INTRAVAL is to test the robustness of the thermohydrologic process models under development. The models will be used to predict the thermohydrologic response of the tuff rock mass to the thermal loads in the planned heater experiment at the Apache Leap site. Participation in Phase 2 of INTRAVAL will benefit OCRWM/YMP in several ways. If the models developed from studies in G-Tunnel can be successfully applied to another tuffaceous rock mass our

confidence that they are valid for modeling the Yucca Mountain Site will be increased. Participation in this effort will also provide the scientific staff the opportunity to gain additional experience in testing and modeling unsaturated tuffs. Finally, the interaction and exchange of ideas between the staff and the international experts in flow and transport modeling will improve DOE's scientific credibility through the peer review their work will receive.

The OCRWM/YMP staff participating in this effort will be part of the Apache Leap Project Team within INTRAVAL. The NRC and the University of Arizona have expressed a willingness to work with OCRWM/YMP staff consistent with the spirit of scientific cooperation within INTRAVAL. The experience YMP staff have in designing, instrumenting, and interpreting data from heater experiments in tuffaceous rocks at the Nevada Test Site will enhance the Apache Leap experiment and avoid many of the technical difficulties associated with this type of experiment. The OCRWM/YMP staff will also have an opportunity to verify that the concepts, instrumentation, and procedures already developed can be successfully applied in other tuffaceous rock types.

The proposed scope of work consists of five tasks. The work will build on findings from the Phase 1 test case by combining the data from other experiments conducted in the G-Tunnel Underground Laboratory, in particular, the heater experiment performed by Lawrence Livermore National Laboratory. The combined data set will be used to develop conceptual models of the thermohydrologic processes in unsaturated tuff environments. The models will be used in the design phase of the Apache Leap heater experiment and to predict the thermohydrologic response as a function of time. A limited amount of laboratory testing will be performed with core from the Apache Leap site to calibrate the conceptual models. The scope of each task is described below.

Task 1: Develop Integrated G-Tunnel Data Set

Two experiments have been performed at the G-Tunnel Underground Laboratory that are relevant to the planned heater test at Apache Leap: the prototype drilling experiment (Test Case 12 in Phase 1 of INTRAVAL) and the electric heater experiment. The objective of this task is to integrate the data from these studies into a single thermohydrologic data set. These data will be used to complete the development of a number of conceptual models to describe the thermohydrological processes in an unsaturated tuffaceous rock. An emphasis will be placed on processing data from the electric heater test conducted by LLNL.

Task 2: Develop Thermohydrologic Conceptual Models

A number of theoretical and empirical conceptual models are being developed within the OCRWM/YMP program to describe the thermal and hydrologic processes in tuffaceous rocks under unsaturated conditions. These models are based in part on the data collected in the G-Tunnel and laboratory experiments. The objective of this task is to assemble the models from SNL, USGS, PNL, etc., and select a subset for modeling the Apache Leap Heater Experiment. It is anticipated that the models will be modified and recalibrated as the integrated data set is made available.

Task 3: Perform Laboratory Measurements to Supplement Apache Leap Data Set

The USGS has developed unique laboratory capabilities for estimating the hydrological properties of tuff. In this task, a limited number of laboratory tests will be performed with core specimens from Apache Leap to calibrate the process models for modeling the heater experiment at the site.

Task 4: Modeling of the Apache Leap Heater Experiment

In this task, the conceptual models developed by OCRWM/YMP will be applied to the Apache Leap heater experiment. The models will be used to assist the NRC and the University of Arizona staff to design the heater experiment and to predict the outcome of the experiment a priori.

Task 5: Integration and Reporting

The work described above will include contributions from experimenters and modelers from many of the OCRWM/YMP contractors. The objective of Task 5 is to coordinate these activities and act as the technical liaison with the NRC and UA involved in the Apache Leap Experiment. This task will also produce annual reports to OCRWM/YMP and INTRAVAL on the annual progress. In addition, three reports will be prepared summarizing: the G-Tunnel thermohydrological data set; (b) the analysis and reduction of G-Tunnel data set; and (c) description of the thermohydrological process models based on these data. The reports will include the G-Tunnel experiments conducted by LLNL and the USGS and model development efforts at SNL, USGS, LLNL, LBL, PNL, etc

Cost and Schedule

The estimated costs and schedule for the Task 1-5 are given in Table 3. The estimates are preliminary and may change depending on budget constraints, manpower limits, etc. The total proposed budget for Phase 2 participation over the three year period is ~ $1.5M. It is suggested that a separate WBS element be assigned for participation in the INTRAVAL Phase 2 project and that a YMP INTRAVAL Task Group be organized to carry out the tasks.

Table 3. Cost and schedule estimates for participating in Phase 2 of INTRAVAL.

Phase 2 Task	Budget ($K)			Schedule	
	FY 91	FY 92	FY 93	Start	Finish
1. Integrate G-Tunnel Data	150			10/90	6/91
2. Develop Conceptual Models	200	200		10/91	9/92
3. Laboratory Measurements	50	150		1/91	9/92
4. Model Apache Leap Exp.	100	300	200	11/92	9/93
5. Integration and Reporting	50	50	75	10/90	9/93
Yearly Totals	**550**	**700**	**275**		

SIXTH INTRAVAL COORDINATING GROUP MEETNG

Cologne, October 19, 1990

TENTATIVE AGENDA

1. Opening of meeting
2. Adoption of the agenda
3. Approval of the minutes of the fifth INTRAVAL Coordinating Group meeting
4. Status report by the Project Secretariat
5. Report from VOIC
6. Decisions on Phase 1 report production and procedure for terminating INTRAVAL Phase-1
7. INTRAVAL Phase-2 participation
8. Status report on INTRAVAL Phase-2
9. Organisation and time schedule for Phase-2
10. Decission on Phase-2 test cases
11. Decisions on the next workshop and Coordinating Group meeting
12. Other matters