



Department of Energy  
Office of Civilian Radioactive Waste Management  
Yucca Mountain Site Characterization Office  
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NOV 20 1998

OVERNIGHT MAIL

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TRANSMITTAL OF KEY DOCUMENTS RELEVANT TO U.S. DEPARTMENT OF ENERGY'S VIABILITY ASSESSMENT: "NEAR-FIELD/ALTERED ZONE COUPLED EFFECTS EXPERT ELICITATION PROJECT," "NEAR-FIELD ALTERED-ZONE MODELS REPORT," "SUBSURFACE HEATING, VENTILATING, AND AIR CONDITIONING," "ENGINEERED MATERIALS CHARACTERIZATION REPORT VOLUME 3," "WASTE FORM CHARACTERISTICS REPORT," AND "THIRD INTERIM REPORT - TOTAL SYSTEM PERFORMANCE ASSESSMENT PEER REVIEW PANEL"

References: (1) Ltr, Brocoum to Greeves, dtd 01/08/98  
(2) Ltr, Brocoum to Greeves, dtd 01/12/98  
(3) Ltr, Brocoum to Greeves, dtd 01/30/98  
(4) Ltr, Brocoum to Bell, dtd 03/06/98  
(5) Ltr, Brocoum to Bell, dtd 04/03/98  
(6) Ltr, Brocoum to Bell, dtd 06/30/98

The Office of Civilian Radioactive Waste Management (OCRWM) will issue the Viability Assessment (VA) in late 1998. The VA will reference supporting technical documents prepared by OCRWM and our contractors. On January 8, 1998, the U.S. Department of Energy (DOE) transmitted a list of these key supporting documents and a schedule for their availability in order to facilitate your review of the VA (Reference 1). We are continuing to provide these supporting documents to you as they are accepted by DOE (References 2-6). Our goal is to ensure the U.S. Nuclear Regulatory Commission (NRC) is aware of these supporting documents to enable you to focus your reviews on key areas prior to DOE's transmittal of the VA to the U.S. Congress. After the Congressional submittal, the NRC and other interested parties will have the opportunity to examine the VA.

DOE will continue to evaluate the science, design, and performance assessment of Yucca Mountain after the VA. We expect to update information from these evaluations after the VA, and will continue to focus our interactions on these evaluations as we approach the License Application.

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PDR WASTE  
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YMP-6

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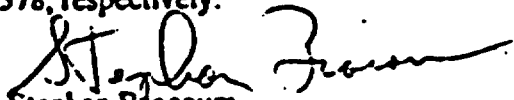
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Michael J. Bell

-2-

NOV 20 1998

Please direct comments on this letter or the enclosures to J. Timothy Sullivan or April V Gil of my staff, at (702) 794-5589 and (702) 794-5578, respectively.

  
Stephan Brocoun  
Acting Assistant Manager, Office of  
Licensing and Regulatory Compliance

OL&RC:AVG-0216

Enclosures:

1. Near-Field Altered-Zone Coupled  
Effects Expert Elicitation Project
2. Near-Field Altered-Zone Models Report
3. Subsurface Heating, Ventilating,  
and Air Conditioning
4. Engineered Materials Characterization  
Report Volume 3
5. Waste Form Characteristics Report
6. Third Interim Report - Total System  
Performance Assessment Peer  
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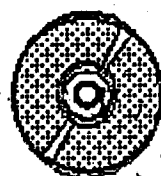
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# ENGINEERED MATERIALS

## CHARACTERIZATION REPORT VOLUME #3 CORROSION DATA AND MODELING

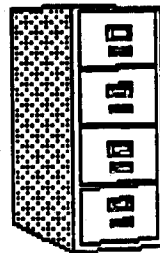


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# WASTE MANAGEMENT SYSTEM

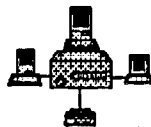
## NEAR -FIELD ALTERED -ZONE MODELS REPORT REVISION 00



ACCESSION#9811250068 LTR. DATED 11/28/98  
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# WASTE MANAGEMENT SYSTEM

## AR-FIELD/ALTERED ZONE COUPLED EFFE EXPERTS ELICITATION PROJECT



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QA: L

**Civilian Radioactive Waste Management System  
Management and Operating Contractor**

**Near-Field/Altered Zone Coupled Effects Expert Elicitation Project**

**May 29, 1998**

**Prepared for:**

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**Under Contract Number  
DE-AC08-91RW00134**

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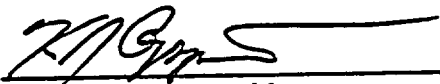
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**Civilian Radioactive Waste Management System  
Management & Operating Contractor**

**Near-Field/Altered Zone Coupled Effects  
Expert Elicitation Project**

**May 29, 1998**

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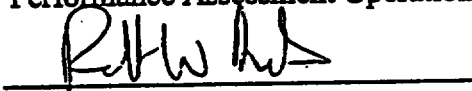
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<b>TABLE OF CONTENTS</b>		<b>Page</b>
<b>1.0</b>	<b>INTRODUCTION.....</b>	<b>1-1</b>
1.1	OBJECTIVES .....	1-1
1.2	RELATIONSHIP OF NFEE PROJECT TO STUDIES FOR YMP .....	1-2
1.3	ORGANIZATION.....	1-4
1.4	PRODUCTS OF STUDY AND STRUCTURE OF REPORT .....	1-5
<b>2.0</b>	<b>PROCESS FOR ELICITING EXPERT JUDGMENTS.....</b>	<b>2-1</b>
2.1	INTRODUCTION.....	2-1
2.1.1	Pertinent Guidance Regarding Expert Judgment.....	2-2
2.2	NFEE METHODOLOGY .....	2-4
2.2.1	Steps in the Methodology .....	2-4
2.2.2	Selection of the Expert Panel.....	2-5
2.2.3	Review of Technical Issues/Expert Interaction .....	2-8
2.2.3.1	Workshop on Significant Issues and Available Data .....	2-8
2.2.3.2	Workshop on Alternative Models and Interpretations.....	2-9
2.2.3.3	Workshop on Preliminary Interpretations .....	2-9
2.2.3.4	Field Trip to Yucca Mountain .....	2-9
2.2.4	Elicitation of Experts .....	2-10
2.2.4.1	Preparation for the Elicitation.....	2-10
2.2.4.2	The Elicitation Interview .....	2-10
2.2.4.3	Documentation and Review.....	2-11
2.2.4.4	Feedback and Sensitivity .....	2-12
2.2.4.5	Aggregation of Expert Assessments.....	2-12
<b>3.0</b>	<b>ASSESSMENT OF KEY ISSUES .....</b>	<b>3-1</b>
3.1	INTRODUCTION.....	3-1
3.2	SUMMARY OF EXPERT INTERPRETATIONS.....	3-3
3.2.1	Overall Processes.....	3-3
3.2.2	TM—Thermal-Mechanical Effects: Induced Stresses.....	3-5
3.2.3	TM—Thermal-Mechanical Effects: Liner Stability .....	3-6
3.2.4	TM—Thermal-Mechanical Effects: Drift Stability .....	3-7
3.2.5	THM—Thermal-Hydrologic-Mechanical Effects .....	3-8
3.2.6	THC—Thermal-Hydrologic-Chemical Effects .....	3-10
3.2.7	Multiply Coupled Effects .....	3-13
3.2.8	Durability of Effects .....	3-14
3.2.9	Recommended Activities to Reduce Uncertainties .....	3-14
<b>4.0</b>	<b>SUMMARY AND CONCLUSIONS .....</b>	<b>4-1</b>

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**TABLE OF CONTENTS****Page**

<b>5.0</b>	<b>REFERENCES .....</b>	<b>5-1</b>
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**TABLES**

Table 1-1	Methodology Development Team Members and Their Principal Responsibilities .....	1-6
Table 1-2	Expert Panel Members .....	1-7
Table 1-3	Technical Specialists Participating in NFEE Workshops .....	1-7
Table 3-1	Issues Addressed by NFEE Expert Panel .....	3-15
Table 3-2	Summary of Key Issues .....	3-17

**APPENDICES**

Appendix A	Biographies of Expert Panel Members
Appendix B	References Distributed to Expert Panel Members
Appendix C	Workshop and Field Trip Summaries
Appendix D	Elicitation Summaries
Appendix E	Quality Assurance

## 1.0 INTRODUCTION

### 1.1 OBJECTIVES

This report presents results of the Near-Field/Altered Zone Coupled Effects Expert Elicitation (NFEE) project for Yucca Mountain, Nevada. This project was sponsored by the U.S. Department of Energy (DOE) and managed by Geomatrix Consultants, Inc. (Geomatrix), for TRW Environmental Safety Systems, Inc. The DOE's Yucca Mountain Site Characterization Project (referred to as the YMP) is intended to evaluate the suitability of the site for construction of a mined geologic repository for the permanent disposal of spent nuclear fuel and high-level radioactive waste. The NFEE project is one of several that involve the elicitation of experts to characterize the knowledge and uncertainties regarding key inputs to the Yucca Mountain Total System Performance Assessment (TSPA). The objective of the current project was to evaluate the temporal and spatial distribution of thermal, hydrologic, mechanical, and chemical effects associated with heating of the host rock due to the emplacement of radioactive wastes. An understanding of these processes is critical to evaluating the performance of the potential high-level nuclear waste repository at Yucca Mountain.

Near-field/altered zone coupled effects will depend on many factors that are uncertain and variable. The temporal and spatial distribution of relative humidity, liquid saturation, liquid flux, and gas flux within the drift caused by the redistribution of moisture prior to waste emplacement and after waste emplacement (due to heat transfer away from the waste packages) must be assessed. The relative humidity, liquid saturation, liquid flux, and gas flux distributions will depend on factors that include (1) the thermal characteristics of the rock, and rock alteration, (2) thermally driven changes to the mechanical attributes of the rock, and (3) thermally driven geochemical changes to the rock mineralogy.

Chemical effects that will occur in response to heating, including mineral dissolution-precipitation during the boiling-condensation process, solid-phase transformations, and

mineral dissolution-precipitation by/from an aqueous phase in response to thermal perturbations, must be assessed. Significant changes in rock hydraulic properties, particularly fracture permeability, due to these chemical effects must also be assessed. Thermally induced changes to the mechanical properties of the rock mass in the near-field must be evaluated, including thermally induced displacements and changes in stress that depend on material properties, the frequency and orientation of existing fractures, and the aperture distribution of those fractures. Given the large number of waste packages and the spatial distribution, it is expected that the thermal/chemical/mechanical/ hydrologic environment will be different for different packages, and this stochastic variability must be incorporated in the analyses.

So that the analyses for the study included a wide range of perspectives, multiple individual judgments were elicited from members of an expert panel. The panel members, who were all experts from outside the Yucca Mountain project but included some experts with some project experience, represented a range of experience and expertise. A deliberate process was followed in facilitating interactions among the experts, in training them to express their uncertainties, and in eliciting their interpretations. The resulting assessments, therefore, provide a reasonable aggregate representation of the knowledge and uncertainties about key issues regarding the near-field/altered zone coupled effects at the Yucca Mountain site.

## **1.2 RELATIONSHIP OF NFEE PROJECT TO STUDIES FOR YMP**

The NFEE project has two principal purposes: (1) to quantify uncertainties associated with certain key issues in the Total System Performance Assessment (TSPA); and (2) to provide a perspective on modeling and data collection activities that may help characterize and reduce uncertainties. The next iteration of the TSPA is being conducted for the Viability Assessment (VA) for Yucca Mountain. The TSPA-VA provides a probabilistic assessment of the performance of the potential repository based on the information developed through site characterization and repository design. The technical components of the TSPA are intended to incorporate a range of knowledge and uncertainties. As such, the expert panel's assessment of key technical issues related to



near-field/altered zone coupled effects—including the expressions of uncertainty in processes and models—will be directly applicable to the TSPA-VA.

In addition, the NFEE study is intended to complement the ongoing modeling, testing, and data collection programs (conducted principally by the national laboratories, including Lawrence Livermore National Laboratory [LLNL], Lawrence Berkeley National Laboratory (LBNL), and Sandia National Laboratory) while contributing to the performance assessment (conducted by the M&O). The NFEE experts were given detailed summaries and presentations of available data, models, and the progress being made in various components of the modeling and testing program. The focus of the NFEE project was on evaluating the uncertainties associated with the various models, parameters, and processes and providing a broad perspective on the models appropriate to characterize near-field/altered zone coupled effects. As such, the NFEE project is a logical step in the design and testing program for the Yucca Mountain project.

The Viability Assessment will rely largely on the next round of performance assessment (TSPA-VA). The TSPA-VA will be an assessment at a particular point in time of the level of knowledge and uncertainties regarding the site characteristics and engineered system that will affect performance of the potential repository system. As such, the performance assessment requires a reasonably complete description of all key processes affecting performance, including near-field/altered zone coupled effects. Further, the TSPA; as a probabilistic analysis, will include appropriate expressions of uncertainties. The quantification of uncertainties at any given time does not imply that issues have been resolved, that additional data should not be gathered, or that the issues will not be revisited during subsequent evaluations (e.g., licensing). A goal of the NFEE project is to support the TSPA-VA by providing an expression of uncertainties regarding key issues. As such, results of the NFEE study are realistic and defensible assessments at this point in the characterization program for Yucca Mountain. In addition to providing inputs to the TSPA-VA, the results of the study can also provide a focus for subsequent data collection aimed at reducing key uncertainties.

### 1.3 ORGANIZATION

NFEE project personnel were organized into four primary groups: the NFEE contractor, the methodology development team (MDT), the expert panel, and the technical specialists. The principal responsibilities of each group are described here; the technical roles of each group are described in detail in Section 2.2 of this report.

**NFEE Contractor:** Under contract with TRW, the NFEE contractor, Geomatrix, was responsible for conducting all aspects of the project and for delivering this report describing the methodology and the results. The NFEE contractor personnel also were members of the MDT.

**Methodology Development Team (MDT):** As a group, the MDT served both to carry out the project and to review its progress. Direct participation included developing a project plan, facilitating workshops, eliciting members of the expert panel, and documenting the methodology and results. The review role included reviewing the progress of the study and recommending mid-course adjustments to ensure that the study met its objectives. The members of the MDT and their responsibilities for the NFEE project are summarized in Table 1-1.

**Expert Panel:** The six widely recognized scientists on the expert panel were responsible for providing and documenting their judgments regarding models, parameters, and uncertainties about near-field/altered zone coupled effects at Yucca Mountain. These subject-matter experts were responsible for developing the interpretations that form the technical substance of the NFEE project. Table 1-2 lists the experts on the panel and their affiliations. Brief biographies for members of the expert panel are provided in Appendix A.

**Technical Specialists:** Numerous technical specialists participated in the project by providing the experts with specialized data, interpretations, or training through workshops. A list of the technical specialists and their affiliations is given in

Table 1-3. In some cases, members of both the MDT and the expert panel also acted as technical specialists.

#### 1.4 PRODUCTS OF STUDY AND STRUCTURE OF REPORT

The NFEE study was conducted in approximately eight months. The project began with developing a plan for the course of the study and identifying the goals to be accomplished and methodologies to be implemented in meeting these goals. Next, the MDT developed and implemented a process for selecting the members of the expert panel, resulting in the selection of six experts. The bulk of the study was centered around three workshops and one field trip. The workshops and field trip were designed to facilitate interaction among the experts, provide all data needed for their assessments, and provide a forum for discussing a range of technical interpretations. Following the third workshop, the interpretations of each expert were elicited in individual interviews and documented in elicitation summaries. After reviewing the elicitation summaries of all members of the expert panel, the experts finalized their assessments.

This report contains the products of the NFEE project outlined above. Section 2 describes in detail the process followed in eliciting the expert interpretations. Appendices B and C provide summaries of the references and reports provided to the experts, and of the three workshops. This information provides written documentation of the technical data discussed by the panel, the formats and content of interpretations presented by outside technical specialists during the study, and the expert panel's preliminary interpretations.

Section 3 of this report presents in detail the final interpretations provided by the expert panel and the results of the study. Both the results for each of the six individual experts and the aggregated results are discussed. Key products of the study are the written elicitation summaries prepared by each expert, which are provided in Appendix D. The experts expended considerable effort to ensure that their summaries provide a reasonably

complete record of the thought process they followed in arriving at their interpretations. Information related to quality assurance is provided in Appendix E.

**TABLE 1-1  
METHODOLOGY DEVELOPMENT TEAM MEMBERS AND THEIR  
PRINCIPAL RESPONSIBILITIES**

NAME	AFFILIATION	RESPONSIBILITIES
Kevin J. Coppersmith	Geomatrix Consultants, Inc.	Project management and planning; methodology development; facilitating workshops; documentation
Roseanne C. Peman	Geomatrix Consultants, Inc.	Project planning and methodology development; organizing workshops and field trip; documentation
Robert R. Youngs	Geomatrix Consultants, Inc.	Project planning and methodology development
William Boyle	U.S. Department of Energy	Project oversight
Nicholas D. Francis	Sandia National Laboratory	Project planning and methodology development; workshop planning; documentation
Ernest L. Hardin	M&O/Lawrence Livermore National Laboratory	Project planning and methodology development; workshop planning; documentation
Peter A. Morris	Applied Decision Analysis	Project planning and methodology development; peer review of project direction; expert elicitation methodologies
Martha W. Pendleton	M&O/Woodward-Clyde Federal Services	Project planning and oversight; expert selection process; review of project direction

**TABLE 1-2  
EXPERT PANEL MEMBERS**

EXPERT	AFFILIATION
Derek Elsworth	Pennsylvania State University
John E. Gale	Fracflow Consultants, Inc.
Roger D. Hart	Itasca Consulting Group, Inc.
Benjamin Ross	Disposal Safety, Inc.
Robert S. Schechter	University of Texas (Emeritus)
Yanis Yortsos	University of Southern California

**TABLE 1-3  
TECHNICAL SPECIALISTS PARTICIPATING IN  
NFEW WORKSHOPS \***

<b>WORKSHOP 1 - SIGNIFICANT ISSUES AND AVAILABLE DATA</b>	
Robert Andrews	M&O/DESI
Stephen Blair	M&O/Lawrence Livermore National Laboratory
Jim Blink	M&O/Lawrence Livermore National Laboratory
Bo Bodvarsson	M&O/Lawrence Livermore National Laboratory
Nancy Brodsky	M&O/Sandia National Laboratory
Tom Buscheck	M&O/Lawrence Livermore National Laboratory
Larry Costin	Sandia National Laboratory
Lorraine Flint	U.S. Geological Survey
William Glassley	M&O/Lawrence Livermore National Laboratory
Kevin Knauss	M&O/Lawrence Livermore National Laboratory
Tim Kneafsey	M&O/Lawrence Berkeley National Laboratory
Wunan Lin	M&O/Lawrence Livermore National Laboratory
Annmarie Meike	M&O/Lawrence Livermore National Laboratory
John Nitao	M&O/Lawrence Livermore National Laboratory
Jeff Roberts	M&O/Lawrence Livermore National Laboratory
Chin-Fu Tsang	M&O/Lawrence Berkeley National Laboratory
Yvonne Tsang	M&O/Lawrence Berkeley National Laboratory
Brian Viani	M&O/Lawrence Livermore National Laboratory
Ralph Wagner	M&O/Woodward Clyde Federal Services
<b>WORKSHOP 2 - ALTERNATIVE MODELS AND INTERPRETATIONS</b>	
John Apps	M&O/Lawrence Berkeley National Laboratory
Stephen Blair	M&O/Lawrence Livermore National Laboratory
Thomas Buscheck	M&O/Lawrence Livermore National Laboratory
Fei Duan	M&O/Morrison-Knudsen
William Glassley	M&O/Lawrence Livermore National Laboratory
Peter Lichtner	Center for Nuclear Waste Regulatory Analyses/Southwest Research Institute
William Murphy	Center for Nuclear Waste Regulatory Analyses/Southwest Research Institute
Richard Nolting	M&O/Morrison-Knudsen
Eric Sonnenthal	M&O/Lawrence Berkeley National Laboratory
Carl Steefel	University of South Florida
Yiming Sun	M&O/Morrison-Knudsen

**Civilian Radioactive Waste Management System  
Management & Operating Contractor**

Chin Fu Tsang  
Thomas Woolery  
George Zyvoloski

M&O/Lawrence Berkeley National Laboratory  
M&O/Lawrence Livermore National Laboratory  
M&O/Los Alamos National Laboratory

- 
- Some members of the MDT and the expert panel also acted as technical specialists at the workshops; their names are not repeated here.

## 2.0 PROCESS FOR ELICITING EXPERT JUDGMENTS

### 2.1 INTRODUCTION

This section summarizes the methodology that was followed in carrying out the NFEE project. It is our belief that to be credible and useful, a technical analysis such as the NFEE must: (1) be based on sound technical information and interpretations, (2) follow a process that considers all available data, and (3) incorporate uncertainties into the assessments. A key mechanism for quantifying uncertainties in the NFEE is the use of multiple expert judgments. The *process* used to select the experts, facilitate their interaction and mutual education, and elicit their judgments is just as important as the technical content of their interpretations.

Because of the importance of the entire process, a methodology development team (MDT) was established at the outset. MDT members have experience in developing guidance for and implementing multi-expert studies, understanding technical aspects of near-field/alterd zone coupled effects, and performing TSPAs. For example, several members (K. Coppersmith, R. Perman, M. Pendleton, R. Youngs, and P. Morris) have conducted recent expert elicitations for the YMP pertaining to technical issues that include unsaturated zone flow, saturated zone flow and transport, and waste package near-field/alterd zone coupled effects processes. Drs. Coppersmith and Morris were members of the Senior Seismic Hazard Analysis Committee (SSHAC, described below); and Drs. Coppersmith and Youngs participated on the Electric Power Research Institute (EPRI) methodology team for seismic hazards assessment in the eastern United States (EPRI, 1986). Importantly, the MDT included representatives from performance assessment (N. Francis) and site characterization (E. Hardin) for the Yucca Mountain project. The site characterization program has developed most of the data related to near-field/alterd zone coupled effects for the Yucca Mountain project, and the TSPA will be the primary user of the results of the NFEE project.

### 2.1.1 Pertinent Guidance Regarding Expert Judgment

In the study of any complex technical problem—such as near-field/altered zone coupled effects at Yucca Mountain—expert judgment is used. The data themselves do not provide an interpretation of the processes or outputs needed for subsequent analyses. For example, experiments such the single heater test do not provide a direct estimate of the spatial distribution of fracture permeability changes. These data must be interpreted and combined with other data and analyses before they can be used in performance assessments. Through the scientific process, experts integrate and evaluate data to arrive at conclusions that are meaningful to assessments of near-field/altered zone coupled effects, including quantitative and qualitative expressions of the uncertainties. This process is the same regardless of the abundance or scarcity of data; the only difference is the level of uncertainty. In this sense, expert judgment is not a substitute for data; it is the process by which data are evaluated and interpreted. If data are scarce and uncertainties high, the uncertainties expressed by each expert and the range of judgments across multiple experts should reflect that high degree of uncertainty.

The procedures and approaches for eliciting expert judgments, developed through conducting many studies, have been formalized in guidance documents; the process followed in the NFEE project is consistent with these studies. The DOE recently developed guidance for the formal use of expert judgment by the Yucca Mountain Project (U.S. DOE, 1995), and the Nuclear Regulatory Commission (NRC) staff issued a Branch Technical Position on use of expert elicitation in the high-level waste program (Kotra et al., 1996). Comprehensive guidance on eliciting expert judgment for seismic hazards recently was set forth in a study produced by the Senior Seismic Hazard Analysis Committee (SSHAC) and sponsored by the DOE, the EPRI, and the NRC (SSHAC, 1995).

SSHAC (1995) defines the expert roles of *proponent*, *evaluator*, and *integrator*. A proponent advocates a particular technical view or interpretation; an evaluator weighs the relative merits of alternative views; and an integrator combines the alternative views into a composite distribution that includes uncertainties. The NFEE members were informed of their roles as evaluator experts and of the need to forsake the role of a proponent in



making their assessments and evaluating uncertainties. Expert interactions are deemed important in the SSHAC process and must be properly facilitated. Finally, the SSHAC process allows for aggregation or combining of multiple expert views. Equal weights are used in the NFEE study to combine the assessments of the experts.

The NFEE study closely follows the procedural guidance set forth in the SSHAC study, both in spirit (e.g., a belief in the importance of facilitated expert interactions) and, in many cases, in details of implementation (e.g., suggestions for conducting elicitation interviews). For example, the NFEE process was designed—in accordance with SSHAC guidance—to result in assessments that represent the “range of technical interpretations that the larger informed technical community would have if they were to conduct the study.” However, inasmuch as SSHAC professes to be “non-prescriptive” in specifying a single way of implementing the process, it would be inappropriate to say that the NFEE conforms exactly to the SSHAC process. In some cases, the NFEE process followed approaches that were more appropriate for a relatively modest multi-expert study than a larger, resource-intensive study. For example, after the elicitation interviews, feedback to the experts was accomplished by providing each expert with a feedback package that summarized all of their assessments and the implications of those assessments to certain key issues. The experts then were given an opportunity to revise their assessments in light of the feedback, as suggested in the SSHAC guidance. A more resource-intensive approach might have been to conduct a feedback workshop. Either process enables the experts to review the assessments of others on the panel and to examine the calculated implications of their assessments.

The goal of all of the guidance documents is not to establish a rigid set of rules for eliciting expert judgment; rather, it is to draw from experience—both successes and failures—criteria for when expert judgment should be used and to outline approaches to motivating, eliciting, and documenting expert judgments. Other documents in the literature provide alternative approaches to the formal or informal use of expert judgment (e.g., Meyer and Booker, 1991).

## **2.2 NFEE METHODOLOGY**

This section of the report summarizes the methodology implemented in the NFEE study. It begins with an overview of the important steps in the process, followed by a more detailed discussion of those steps.

### **2.2.1 Steps in the Methodology**

The principal steps followed in the NFEE project are described below.

1. **Development of Project Plan.** The MDT first developed a project plan that outlined the goals and key elements of the project, timing of significant activities such as workshops, topics to be covered at workshops, and significant milestones.
2. **Selection of the Expert Panel.** The MDT established criteria for participation on the expert panel. These criteria were intended to ensure that all expert panel members had significant professional stature and technical expertise. Highly regarded scientists and engineers were asked for their nominations to the panel, resulting in more than 35 nominations. From this list of candidates, six experts were selected and participated on the panel.
3. **Data Compilation and Dissemination.** The compilation and distribution of pertinent data, including published reference material, began early in the project. The experts were sent a number of data sets and publications throughout the project. Panel members were provided access, if requested, to all Yucca Mountain data gathered as part of the project.
4. **Meetings of the Expert Panel.** Structured, facilitated interaction among the members of the expert panel took place during three workshops. The workshops were designed to identify the significant issues, available data, alternative models, and uncertainties related to near-field/altered zone coupled effects. Debate and technical challenge of alternative interpretations were encouraged to provide that uncertainties were identified. At these meetings, researchers from a variety of

organizations, including LLNL, Lawrence Berkeley National Laboratory, Sandia National Laboratory, Center for Nuclear Waste Regulatory Analyses, and the Nuclear Regulatory Commission presented pertinent data sets and alternative models and methods.

5. **Elicitation of Experts.** One-day individual elicitation interviews were held with each member of the expert panel. Through discussions facilitated by the elicitation team (all of whom were members of the MDT), each expert provided his assessments of the key issues related to near-field/altered zone coupled effects, expressed the uncertainties, and specified the technical basis for the assessment. The elicitation team documented the elicitation during the interview. The experts subsequently reviewed, revised, and supplemented the summary prepared by the elicitation team.
6. **Feedback of Preliminary Results.** Based on the results of the elicitations, the elicitation summaries from all members of the expert panel were provided to each expert as feedback. This provided each expert with a broader perspective on the range of interpretations being developed.
7. **Finalization of Expert Assessments.** After reviewing the feedback package, the experts developed a final draft of their elicitation summary. The elicitation team reviewed this draft for completeness and clarity, then the experts finalized their summaries for this report (Appendix D).
8. **Preparation of Project Report.** This report was developed to document the process followed, the expert elicitation summaries, and the results.

The rest of Section 2.2 describes in more detail the key activities involved in implementing the NFEE methodology.

### **2.2.2 Selection of the Expert Panel**

The selection of members for the expert panel involved four steps: (1) developing selection criteria, (2) obtaining nominations from knowledgeable individuals, (3)

selecting and inviting candidates to participate, and (4) having candidates accept the invitation to participate.

Guidelines for selecting members of the expert panel were developed by the MDT. Candidates for the panel had to demonstrate the following characteristics.

1. Engineer or scientist having a good professional reputation and widely recognized competence based on academic training and relevant experience. Tangible evidence of expertise, such as written documentation of research in refereed journals and reviewed reports, is required.
2. Understanding of the problem area through experience in one or more of the following areas of technical expertise: ore deposit geochemistry specializing in oxidizing ore deposits; geothermal system geochemistry; low-temperature metamorphic petrology; hydrology with experience in thermally-elevated regimes; hydrochemistry of volcanic rocks; and rock mechanics. Individuals who have had a major role in the Yucca Mountain Site Characterization Project may be included on the expert panel; however, such experience is not a requirement for participation.
3. Availability and willingness to participate as a named panel member, including a commitment to devoting the necessary time and effort to the project and a willingness to explain and defend technical positions.
4. Personal attributes that include strong communication and interpersonal skills, flexibility and impartiality, and the ability to simplify. Individuals will be asked specifically not to act as representatives of technical positions taken by their organizations, but rather to provide their individual technical interpretations and assessments of uncertainties.

5. Ability to help create a panel of experts representing diverse opinions, areas of technical expertise, and institutional/organizational backgrounds (government agencies, academic institutions, and private industry).

The MDT conducted a broad search to obtain nominations for the expert panel. Letters requesting nominations were mailed to 17 scientists and engineers identified by the MDT. The letters requesting nominations contained a brief description of the project and included the above guidelines for selecting panel members. Thirty-five candidates for the expert panel were nominated and considered in the selection process.

The MDT carefully evaluated each nominee to ascertain whether the selection guidelines had been applied properly, and to balance the panel with respect to knowledge and experience. The list of candidates was narrowed to those individuals who met selection criteria 1 and 2; then the remaining criteria were applied. The professional reputation and publications of each candidate were discussed, and the number of nominations each candidate had received was reviewed. A total of about 14 individuals were considered to have the best qualifications for serving as members of the expert panel, and from this group a list of candidates to be invited to participate was developed.

The candidates were contacted by telephone and invited to participate. They were informed that the estimated level of participation was 20 to 25 days. Most accepted during the initial phone call; others requested time to consider potential conflicts of interest or schedule. Six accepted the invitation to become members of the expert panel.

The criteria for selecting the experts were reviewed with each expert before they made a commitment and throughout the project. Each expert had to commit a significant amount of time and would need to prepare for and attend all meetings. Information on potential sources of conflict of interest was provided by each expert and documented in the NFEE administrative files. The experts were informed of the role they would play in the NFEE assessment as an expert *evaluator* who considers a variety of viewpoints, challenges the interpretations of others, and arrives at a reasoned position that includes a representation of the uncertainties. The resulting panel consisted not only of experts of considerable stature and prominence in the professional community, but of individuals with

reputations as independent thinkers. The panel members clearly demonstrated that they were capable of evaluating all the data and hypotheses, and of providing the technical bases for their interpretations and uncertainties.

### **2.2.3 Review of Technical Issues/Expert Interaction**

Technical issues related to the NFEE project were identified in the first workshop and reviewed throughout the project. The workshops provided an opportunity for technical discussion and interaction, with an objective of providing a common understanding of the issues to be assessed and the data available to provide the technical basis for assessment.

Literature and data sets pertinent to assessing near-field/altered zone coupled effects were sent to members of the expert panel throughout the project. Some of the experts made available pertinent publications and reports based on their work at other sites; these publications were made available to the entire panel. A list of the references distributed is provided in Appendix B.

The following sections summarize the workshops and field trip conducted during the project. These activities are summarized under the topic of Review of Technical Issues/Expert Interaction, because the workshops and field trip were the primary vehicle for accomplishing this interaction. Summaries of the workshops and field trip are included in Appendix C.

#### ***2.2.3.1 Workshop on Significant Issues and Available Data***

The first of the three workshops conducted for the NFEE project was the Workshop on Significant Issues and Available Data. The goals of this workshop were to introduce the panel to the NFEE project; summarize the significant issues related to incorporating coupled process models in the TSPA, and summarize the available empirical data that indicate coupled processes are important to repository performance. The workshop included several introductory presentations on topics that included the reference repository design, repository-scale thermohydrology simulations, and the in-situ thermal tests being conducted by the YMP. Fifteen technical specialists then made presentations

on laboratory scale property measurements and coupled process experiments, field-scale coupled process experiments, and drift seepage calculations.

#### ***2.2.3.2 Workshop on Alternative Models and Interpretations***

This second workshop conducted for the NFEE project was designed to review the key issues and uncertainties associated with near-field/altered zone coupled effects at Yucca Mountain. Alternative models, modeling results, and interpretations related to thermal-mechanical, thermal-hydrologic, and thermochemical aspects of the potential repository system were described and discussed. Fifteen technical specialists made presentations at the workshop.

#### ***2.2.3.3 Workshop on Preliminary Interpretations***

The Workshop on Preliminary Interpretations, the third and final project workshop, was conducted prior to the elicitation interviews. This workshop provided an opportunity for the experts to present and discuss their preliminary interpretations and uncertainties regarding issues key to near-field/altered zone coupled effects. The experts presented their interpretations of each of six issues: mechanical stability of the host rock in the near-field/altered zone; impact of thermal loading on fracture porosity and permeability; impact of dissolution, precipitation, and mineral alteration on fracture porosity and permeability; multiply coupled effects from thermal, thermal-mechanical, and chemical processes on mechanical stability; and coupled effects from dissolution, alteration, and thermal and thermal-mechanical processes on the porosity, permeability, and mechanical stability of fracture pathways above the emplacement drifts, in pillars between drifts, and below the emplacement drifts.

#### ***2.2.3.4 Field Trip to Yucca Mountain***

A field trip was conducted that gave the experts an opportunity to observe field relationships and to discuss interpretations regarding coupled effects. Field trip stops included an overview of the region surrounding Yucca Mountain, the Drift Scale Test in the Exploratory Studies Facility, and the Large Block Test.

#### **2.2.4 Elicitation of Experts**

Through the elicitation process, the experts' interpretations of near-field/altered zone coupled effects at Yucca Mountain were obtained. The elicitations involved a series of activities, which can be grouped into three steps: (1) preparation for the elicitation, (2) the elicitation interview, and (3) documentation and review.

##### ***2.2.4.1 Preparation for the Elicitation***

Peter A. Morris of the MDT provided elicitation training at the third workshop. The objectives of the training were to demonstrate how to quantify uncertainties using probabilities, to recognize common cognitive biases and compensate for them, and to present examples of the types of assessments that would be made at the elicitation (e.g., continuous variables, discrete hypotheses, and associated weights). The training was designed to enable the experts to be comfortable with the *process* of eliciting their judgments, so that the elicitation interview could be focused on the *technical issues* of importance to the NFEE.

The specific topics to be covered in the elicitations were the subject of presentations at both Workshops 2 and 3. These topics are discussed in Section 3.0. The list of topics was intended to help the experts prepare for their interviews, to focus their data review on the issues of most significance, and to ensure that the important topics were addressed by all experts.

##### ***2.2.4.2 The Elicitation Interview***

The elicitations of the expert panel members took place in individual one-day interviews in the San Francisco office of Geomatrix. The interviews were conducted by members of the MDT; some interviews were also attended by a member of the YMP performance assessment staff (D. Sassani, M&O/DESI). The elicitation team members were K. Coppersmith (normative expert), and N. Francis, E. Hardin, and D. Sassani (specialists).

All data sets provided or made available to the experts during the project were present during the elicitation interviews. The elicitation interview followed a logical sequence from general to more specific assessments and proceeded through all of the technical



issues discussed in Section 3 of this report. Alternative models, approaches, and hypotheses were discussed and the basis for assessments of uncertainties were also given. The elicitation team took written notes of all assessments during the interviews.

#### ***2.2.4.3 Documentation and Review***

Documentation of the expert elicitations began with notes taken by the elicitation team during the interviews. Experience on several other expert assessment projects has shown this approach to be preferable to other documentation methods (for example, written questionnaires or experts writing their interpretations following the interview). During the one-day interview, each NFEE expert was asked to make many assessments, to quantify his uncertainties, and to provide the technical basis for his interpretations. By having the elicitation team take notes, the expert was free to focus on thinking through his answers and thoroughly expressing his interpretations. The elicitation team was able to be flexible in the elicitation sequence (i.e., following the logic comfortable to the expert) while providing that all elements were covered.

Following the interviews, the elicitation team provided each expert with written documentation of the interview, organized by model component. The experts were instructed to review, revise, and expand their preliminary assessments in this "First Draft" documentation summary so that it fully reflected their interpretations. The summaries revised by each expert became the "Second Draft" document. The "Second Draft" summaries from each expert were then distributed to all members of the panel as part of the feedback package so that each expert could review the judgments of others and the technical basis for each judgment.

After reviewing the feedback package, the experts made additional revisions to their elicitation summaries to reflect any resulting changes in their judgments. These revised summaries became the "Third Draft" set. The "Third Draft" summaries were reviewed by MDT members as part of the report review process. The experts responded to any requests for clarifications, and the summaries were finalized. The final elicitation summaries are provided in Appendix D.

#### ***2.2.4.4 Feedback and Sensitivity***

Feedback to the experts occurred throughout the NFEE project, primarily through interaction among experts. By presenting their ideas on models and interpretations at workshops, on the field trip and in general discussions, the experts both provided and received feedback from their peers on the panel.

More formally, feedback was provided to the experts in several other ways.

- At Workshop 3, the experts presented to the panel their interpretations of key issues. Discussions included the technical bases for the interpretations.
- Written elicitation summaries were provided to all panel members for their review.
- The MDT reviewed the First Draft written elicitation summaries for adequacy and completeness of documentation of the technical bases for judgments.

The feedback-revision process required the experts to defend/revise their assessments and provide appropriate documentation. In all cases, the experts on the panel responded positively to technical criticisms of their interpretations and to reviews of their documentation. The resulting assessments and finalized elicitation summaries reflect the significant effort expended by each member of the expert panel.

#### ***2.2.4.5 Aggregation of Expert Assessments***

The approach taken to combine, or aggregate, the expert assessments is equal weighting. Importantly, this approach was not a "default" but a goal throughout the project.

Accordingly, the proper conditions were created throughout the project to provide that a deliberate, defensible decision could be made to use equal weights (after SSHAC, 1995).

The actions that were taken to create these conditions included:

- carefully selecting highly qualified experts who represent diverse views and experience;

- establishing the commitment of each expert to provide the required effort throughout the project;
- identifying a comprehensive data base and disseminating it to all experts;
- educating the experts in issues important to NFEE and training them in elicitation methodologies and the role of experts as evaluators;
- facilitating interaction of the experts in workshops to foster a free exchange of data and interpretations and scientific debate of all hypotheses;
- providing feedback and sensitivity analyses to the experts; and
- providing an opportunity for experts to revise their assessments in light of feedback.

It should be noted that, in accordance with the guidance provided by the SSHAC study (1995), conditions could have been such that differential weights would have been necessary. For example, if a member of the expert panel had been unwilling to forsake the role of a *proponent* who advocates a singular viewpoint, for that of an *evaluator* who is able to consider multiple viewpoints, that expert may have been given less weight or removed from the panel entirely.

### 3.0 ASSESSMENT OF KEY ISSUES

#### 3.1 INTRODUCTION

The experts involved in the Near-Field/Altered Zone Coupled Effects Expert Elicitation (NFEE) project addressed a variety of technical issues related to the processes and implications of the thermal perturbation associated with emplacement of waste in the potential repository at Yucca Mountain. The key issues that the NFEE panel was asked to address are given in Table 3-1. Included are thermal (T), hydrologic (H), mechanical (M), and chemical (C) issues of potential importance to the Total System Performance Assessment (TSPA) as well as to the design of the potential repository (for example, stability of the liner and the drift wall through the thermal period; changes in hydraulic properties due to mechanical and chemical processes; durability of these changes as a function of time). In addition, the experts were asked to provide their perspectives on issues related to conceptual models (for instance, modeling of mechanical stresses and strains, conduction and convection heat transfer processes at the drift and mountain scales, influence of chemical precipitation on fracture/matrix interaction). Finally, the experts were asked for their perspectives on additional data collection or modeling activities that could reduce the uncertainties in the characterization of coupled THMC processes. The experts' evaluations are given in their elicitation summaries (Appendix D) and are summarized in Table 3-2 and this section.

It is important to remember the context of the experts' evaluations. First, the goal of this expert elicitation was to characterize the *uncertainties* associated with coupled effects in the near-field/alterd zone so that the TSPA-VA can incorporate a range of uncertainty when modeling important processes. As a result, the experts focused considerable attention on what is known from the available Yucca Mountain data and *what is not known*, and the reasons for that lack of knowledge. The reasons could include data gaps, complexities in mechanisms and processes, nonpertinent data, or multiple models consistent with the data. Rather than merely identifying and acknowledging the uncertainties, the experts were required to provide—to the extent possible—their characterization of the uncertainties for certain key issues with reference to the technical

literature when applicable. For example, the experts provided their assessments of the mechanisms and magnitudes of thermal stresses in the rock surrounding the drifts and their evolution through time during heat up and cooling. They utilized Yucca Mountain databases that they considered most pertinent as well as their own experience. Likewise, the experts characterized their knowledge and uncertainty regarding the mechanisms, magnitudes, and locations of changes in fracture permeability at various distances from the repository. In light of the sparse data gathered on this subject for the Yucca Mountain project, their assessments express a large degree of uncertainty.

It is also important to note that the experts' evaluations are, to a large extent, an expression of the professional judgment of each expert and are not based on extensive modeling or calculations carried out for this study. These judgments are derived not only from a consideration of Yucca Mountain data, but also data and observations from previous experience. Members of the panel were given a limited time in which to review Yucca Mountain data sets, test results, and models. Further, the experts were unable within the time frame of the project to conduct their own analyses and calculations. In many cases, the experts relied on the results of analyses presented in workshops by the Yucca Mountain researchers, their colleagues on the panel, or other researchers.

The results of the NFEE expert assessments have potential application in both the upcoming TSPA-VA and the ongoing site characterization program. Their evaluations will provide useful information on parameter uncertainties and will improve the models to make them more realistic and to better characterize the uncertainties. Likewise, comments made by the panel on the attributes and suggested alternatives to the models (e.g., the relative importance of mechanical and chemical permeability changes, processes of heat transfer) will help to improve those models as well. Several members of the panel who have considerable experience in collection of hydrologic and rock mechanical data provided advice regarding focused experiments that, they believe, could reduce significantly the present level of uncertainty. For example, most members of the panel applauded the Single Heater, Large Block, and Drift-Scale tests done to date, encouraged the continuation of these efforts, and provided ideas for additional associated activities to provide further insights.

### 3.2 SUMMARY OF EXPERT INTERPRETATIONS

This section summarizes the interpretations made by members of the NFEE panel regarding certain key issues related to coupled effects in the near-field/altered zone. The intent is to provide the reader with a perspective on the evaluations made by the experts, the manner in which each issue was addressed, an overview of the technical bases for the interpretations, the uncertainties identified by the experts, and the degree of convergence or divergence in the aggregate range of interpretations across the panel. The summary here is not intended to be exhaustive. For a more complete exposition of the interpretations made by the experts, the reader is directed to the elicitation summaries given in Appendix D.

The key issues shown in Table 3-2 are discussed below.

#### 3.2.1 Overall Processes

The NFEE experts provided their overview of the processes that they believe are most important to the TMHC effects and their coupling. The experts on the panel noted that the rock mass in the Yucca Mountain site is well fractured, and the processes occurring in this fractured system, particularly fracture permeability, are very important to mechanisms of heat transfer and fluid flow. The thermal loading will affect thermodynamic variables, thermal expansion, liquid-vapor phase changes, and possible chemical transformations. Overall heat transfer, countercurrent liquid-vapor flows, liquid-vapor phase change, and fracture-matrix interaction were identified as important processes that need to be understood and modeled. Changes in bulk fracture permeabilities associated with either the mechanical processes of thermal expansion and joint slip or the chemical processes of dissolution and precipitation were assessed to be the most important influences affecting dryout and reflux. These are time-dependent (i.e., they depend on the thermal history that develops during heat-up and cooldown) and will vary in space with distance from the drifts and with the geometry of the fractures. [The chemical changes in fracture permeabilities are associated with dissolution and precipitation of minerals and may affect fracture permeabilities, but it generally was judged that the more important influence of chemical processes will be the dissolution

and precipitation of minerals along fracture surfaces and the impact on fracture-matrix interaction.]

Thermal-mechanical issues include the pronounced change in the stress field around the drifts, including rotation of the principal stresses relative to the drift over time. The influence of the magnitude of these stresses, the response of the rock mass to strain (e.g., joint slip), and the consequent influence on the <sup>(3)</sup>stability of the drifts are important issues. The experts addressing the TM issue considered the influence of these stresses and the known rock properties in evaluating the <sup>(3)</sup>stability of the rock mass and the concrete liner.

*Stability of  
what period  
time? I do  
care if it's  
stable after  
it closes?*

The degree to which mechanical and chemically induced permeability changes counter or reinforce each other is another important issue. Further, large-scale processes (e.g., mountain-scale convection) and drift-scale processes (e.g., decrease in vertical permeabilities near the drifts and the effects on the location and stability of heat pipes) were identified as important. For example, Dr. Ross suggested that mountain-scale heat transfer and fluid flow are accomplished by two mechanisms: countercurrent gas-liquid flow and mountain-scale convective flow. He concluded that because of large uncertainties in the hydraulic properties at local scales, the only parameter significant to assessing mountain-scale convection is the bulk permeability of the rock mass. Dr. Ross considered the degree to which the thermal-hydrologic system will reach a steady state with zones of dryout, heat-pipes, and condensation over long periods an important issue. Some experts suggested that inherent instabilities in such a thermal system must be dealt with in the modeling. Several members of the panel suggested that changes in permeabilities at the drift scale can lead to significant changes in heat pipe development and convective heat transfer.

In addition to mineral deposition in fractures at the vaporizing ends of heat pipes, possible fracture healing due to dissolution of fracture asperities also was identified as a potential chemically induced issue. Both of these effects are postulated to result in reductions in fracture permeabilities.

### 3.2.2 TM—Thermal-Mechanical Effects: Induced Stresses

The experts provided their assessments of the impact that thermal loads would have on the stress field in the vicinity of the drifts. These thermally induced stresses are important because they affect drift stability and feedback mechanisms that have implications for thermal, hydrologic, and chemical fields. Dr. Elsworth noted that the thermal stresses are controlled by a small set of parameters defined at the scale of the rock mass: coefficient of thermal expansion, deformation modulus, Poisson ratio, and the form and magnitude of the induced temperature field. The experts noted that one important consideration in modeling the stress field is the displacement boundary conditions that should be applied to the repository as a whole (including the central part and the edges) and to the immediate area of the drifts. The possible conditions range from complete confinement (plane strain) to no confinement (plane stress). Dr. Gale believed that given the size and shape of the repository, the most likely condition will be one that reflects a combination of both boundary conditions.

For the repository block as a whole, relatively uniform horizontal stresses are expected, with shear stresses increasing from the repository center to the edges. Shear stresses/strains are expected to be largest in the zones of high temperature gradient, such as the repository edges and at the ends of heat pipes, and to migrate with these zones. As the rock mass heats, the thermally induced mechanical stresses will be both normal and shear stresses on existing fracture planes, and will change as the stress field changes.

For the ambient stress field at repository depth, the maximum stress will act vertically, and the ratio of vertical to horizontal stress  $s_v:s_H$  will be 7:3.5 megaPascals (MPa). With a temperature increase from 25° to 160°C, the initial field stresses will rotate from the maximum stress acting vertically to the maximum stress acting horizontally. Dr. Elsworth postulated a horizontal stress during peak thermal loading of about 14 MPa and an upper bound of about 20 MPa, with the vertical stresses essentially unchanged at 7 MPa. Considering a temperature rise up to 200°C, Dr. Gale postulated that the maximum horizontal stresses will be 20 to 40 MPa in the zone between the emplacement drifts at 200°C and the maximum extent of the 100°C isotherm. With heating from the drift, the radial and particularly tangential stresses will increase, leading to high roof and floor



stresses. Dr. Elsworth estimated that for a horizontal field stress of 14 MPa that is double the vertical stress, crown and springline stress concentrations would be on the order of 35 and 7 MPa, respectively. Dr. Gale estimated that the tangential stresses at the drift wall would be close to zero at the springline and range up to about 80 to 100 MPa at the crown of the drift, decreasing rapidly with decreasing temperature and increasing distance from the drift to about 20 MPa at the 100°C isotherm. Both Drs. Elsworth and Gale concluded that the stresses at the crown will exceed the computed rock mass strength of 18 to 19 MPa (Wilder, 1996) and lead to spalling of the drift. Dr. Elsworth postulated that induced, minor rock bursts may develop late in the thermal evolution, but their late timing means they are unlikely to affect drift stability.

As the stress field rotates, normal and shear stresses on fracture planes rotate through a 90-degree change. Dr. Gale estimated that normal stresses may range up to 40 MPa and shear stresses from zero to 15 to 20 MPa. Based on the expected combination of normal and shear stresses on the fracture planes, Dr. Gale expected that both dilatant and contractual behavior during shear displacement will be present in the perturbed rock mass.

### **a) 3.2.3 TM—Thermal-Mechanical Effects: Liner Stability**

The experts considered the mechanisms that might affect the stability of the concrete liner during the thermal period. Dr. Elsworth concluded that thermal liner stresses are controlled primarily by the composite liner properties of modulus, Poisson ratio, thermal expansion coefficient, and liner thickness; he found only a weak dependence on rock mass properties. He noted that liner stresses should increase up to the time of the drift thermal maximum, on the order of 50 years, and increase little after that. The liner elements surviving to the time of thermal maximum would be expected to fail from strength loss with time. He calculated that for a temperature change of 135°C, a hoop stress on the liner would be on the order of 40 to 80 MPa. If the liner is designed for long-term durability, then expectations of survival in the range of 50 to 100+ years may be achievable, depending on materials and fabrication methods. Dr. Gale suggested that local rock failures will result in movement of rock blocks and point loading at the contacts with the liner, leading to liner failure. He suggested that grouting the space

between the liner and the rock would integrate the liner and the rock mass, thus mitigating point load stresses and increasing the stability of the liner. Dr. Hart suggested that the long-term mechanical stability of the liner may be affected by material degradation processes, whereby progressive micro-fracturing occurs as the material experiences changes in stress. If such a process is operative, the long-term strength of the liner may be significantly lower than the short-term strength.

### 3.2.4 TM—Thermal-Mechanical Effects: Drift Stability

The experts were asked for their assessment of the manner in which thermal-mechanical processes would be expected to influence the stability of the drifts. Drs. Elsworth and Gale provided their estimates of the amount of drift (unlined) convergence or strain that would be expected from thermal loads. Dr. Elsworth estimated convergence of about 8 to 10 mm; Dr. Gale estimated strains of 2mm/m at 200°C. He concluded that the compressive strength of the rock mass is relative low (18 to 23 MPa) and that local failure of the rock mass should occur with strains of 1.5 mm/m.

Assuming the failure of the drifts, both experts assessed the bulking factor and porosities of the materials that will fill the drifts, as well as the amount of crown migration that would be expected. Dr. Elsworth estimated a bulking factor of about 35 percent, with a range of 20 to 65 percent, which represents drift-infill porosities in the range of 15 to 40 percent. In the case of complete failure of the drift by chimneying, this would represent failure to about 3 diameters above the initial drift, which is an upper bound. Expected drift elongation would be about one drift diameter, which is consistent with stable borehole breakout configurations. Dr. Gale estimated a bulking factor of about 30 percent, with a range of 15 to 45 percent, based on the blocky nature of the rock mass, which is equivalent to a porosity of 13 to 31 percent. For a five-meter drift opening, he would expect that the crown would migrate 10 to 12 m vertically. Dr. Gale noted that if backfill is placed in the drift, it will have only about 20 to 25 percent of the compressive strength of the rock, but should limit crown migration to about one meter, depending on how the backfill is placed.

The experts noted that the thermal and hydraulic properties of the rubble from drift collapse may be important. Dr. Gale, for example, concluded that the thermal conductivity of the rubble is potentially important to temperatures of the waste packages. He said that a reasonable range of permeabilities to use in the modeling is 1000 to 100,000 darcies given the low fragmentation. Dr. Yortsos noted that the rubble is a granular medium that may increase the heat transfer resistance (by conduction rather than radiation) and may affect the seepage in the drift. Dr. Ross noted that the presence of rubble may adversely affect ventilation design alternatives.

### 3.2.5 THM—Thermal-Hydrologic-Mechanical Effects

The experts considered the effects that the thermal perturbation would have on the mechanical properties of the rock and, in turn, the hydrologic properties. The most important hydrologic effect appears to be changes in fracture permeabilities from the thermal-mechanical load.

Dr. Elsworth provided his assessment of permeability changes around individual drifts related to excavation and subsequent heating. With excavation prior to the thermal period, radial permeabilities generally will decrease, and tangential permeabilities generally will increase within a zone about two drift radii into the wall and three to four drift radii into the roof. With heating to about 100°C, the effects of excavation-induced enhanced tangential permeabilities will be countered. He estimated that the development of shear stresses as horizontal field stresses build may increase permeabilities on the order of 2 to 10 times in diametrical lobes at 45°C from the horizontal and reach to three drift radii from the wall.

The experts generally concurred that, at the mountain scale, the increase in horizontal stresses with heating would increase normal stresses in the central part of the repository (away from the edges) on vertical fractures, reduce apertures, and decrease vertical permeabilities in the region near the drifts (2 to 5 drift diameters from the drifts, according to Dr. Gale) and toward the central part of the repository. The experts surmised that near the edges of the repository and at greater distances from the repository, opening of fractures and increased vertical permeability are possible. They

also estimated that horizontal permeabilities will increase due to shear stresses and displacements on horizontal fractures.

The magnitude of the reduction in vertical permeability was estimated by the experts to range from 1 to 3 orders of magnitude. Dr. Elsworth estimated a reduction of vertical permeabilities within the compressional envelope around the repository on the order of 10X. Assuming plane strain boundary conditions, Dr. Gale estimated that the magnitude of normal fracture closure should be about 0.1 to 0.3 mm depending on the roughness and the magnitude of the initial aperture, resulting in a change in vertical fracture permeability of 1.5 to 3 orders of magnitude. He noted that this magnitude of fracture closure is analogous to the permanent closure recorded from first-cycle data developed in laboratory tests. As noted by several experts, the fractures with the smallest initial apertures will experience the largest relative change in fracture aperture but the smallest absolute change. Dr. Yortsos estimated that the change in joint apertures will be in the range of 10 to 100  $\mu\text{m}$  (0.01 to 0.1 mm) and estimated a permeability change of about 10X.

Dr. Elsworth estimated the increase in horizontal permeabilities to range from 2X to 100X from the center of the repository outward. Dr. Yortsos also estimated that the increase in horizontal permeabilities may be on the order of 10X to 100X if dilation accompanies the slip on fractures. He noted, however, that it is also possible that slip will crush asperities and lead to a decrease in permeability. Dr. Gale concluded that the changes in vertical and horizontal permeability will occur at distance of 2 to 5 drift diameters, likely would occur within localized zones, and will be controlled to a large extent by the fracture geometry.

The experts provided their assessments regarding the durability of the permeability changes and the implications of the changes to fluid flow and other properties. In general, the experts concluded that the reductions in vertical permeability resulting from the increased horizontal thermal stresses will be reversible with cooldown, but the horizontal permeability changes associated with shear strains will not. They also concluded that although the permeability changes related to the thermal loading will be

significant particularly at a local scale, the changes in bulk rock permeabilities are expected to be comparable to or less than the ambient spatial variability. For example, Dr. Yortsos concluded that, given the uncertainty in fracture permeabilities, the variation due to thermal loading would be within the range of natural heterogeneity in the repository but skewed toward smaller permeability values.

The experts also concluded that the change in vertical and horizontal permeabilities—both during and following the thermal period—will lead to a permanent change in the anisotropy of the fracture network. For example, Dr. Yortsos suggested that the reduction in vertical permeabilities will lead to a reduction in the anisotropy of the fracture network and to a possible increase in lateral flow. Dr. Elsworth suggested that the final result will be that the permeability anisotropy of the Topopah Springs (TSw2) unit is switched from vertically dominant to horizontally dominant. Dr. Ross noted that buoyant gas flow will depend on permeability and, because under current conditions the vertical permeability is several times larger than the horizontal, the gas flux would be much more sensitive to changes in horizontal than in vertical permeability. Thus these thermal-mechanical changes in horizontal permeability could be important to gas flow. Dr. Gale also noted that the decrease in permeabilities could have a significant impact on the potential of the fractured rock mass to develop heat pipes, because of the increase in fracture contact area.

Dr. Ross asserted that mountain-scale convection is one of the most important processes affecting heat transfer and fluid flow, and depends only on the thermal loading and the bulk permeability of the rock mass. He favored a model of mountain-scale convection and countercurrent flow with irregular return flow of water, perhaps in local zones of condensate shedding. He concluded that instabilities will preclude a uniform zone of heat pipes and noted that convection can reinforce heat pipes above the repository and work against them below the repository.

### 3.2.6 THC—Thermal-Hydrologic-Chemical Effects

In providing their assessments of coupled thermal-hydrologic-chemical (THC) effects, the experts concluded that two principal processes may lead to significant effects:

fracture healing, and dissolution and deposition of minerals along fracture walls. Dr. Yortsos suggested that significant permeability reduction (on the order of 10X to 100X) is expected from fracture healing. The postulated mechanism is pressure solution, but typical pressure solution mechanisms require much higher stress levels than those expected in the thermal period, Dr. Yortsos noted, thus suggesting that the fracture healing is not well understood. Dr. Elsworth concluded that pressure solution would reduce permeabilities in zones of dissolution and precipitation by as much as 100X. Assuming a constant in situ stress magnitude, as the asperities are dissolved along the fracture walls, the stresses will also be reduced, leading to a reduction in the mechanically driven permeability reduction. He suggested that the net permeability reduction will be on the order of 10X. Dr. Gale also concluded that in the condensation zone, the walls of the fractures will be eroded during heating due to dissolution of fracture minerals, especially those that form the contact points or asperities, allowing for mechanical closure of the fracture.

Besides fracture healing, the second major THC process considered by the experts was the dissolution and precipitation of minerals within fractures.  $\text{SiO}_2$  and calcite dissolution in the condensate zone will lead to an increase in imbibition, Dr. Elsworth contended, and precipitation and coating of fractures in the dry-out zone will result in a decrease in imbibition. He suggested that the decrease in permeability due to mineral precipitation is on the order of 10X. Dr. Gale also concluded that in the vaporization/precipitation zone the permeabilities will be reduced as the solutes are precipitated. He also noted that the thermal-mechanical loading will also decrease the fracture permeability, but contact area is being added due to mineral precipitation. Thus the stresses on the asperities should not increase much, limiting the total amount of mechanical aperture closing. Mineral deposition following evaporation of the refluxing liquid at the end of the heat pipe zone would create a deposition zone of potential significance, Dr. Yortsos contended. Based on assumed kinetic data, the rate of growth of the deposition zone is on the order of 1 cm/yr for a heat pipe zone that is 20 m long. The zone, which would be characterized by a significantly reduced permeability, can be considered the equivalent of a "cap." Dr. Ross believed that changes in permeabilities due to dissolution or precipitation would not be significant to gas or water flow (because of the large permeability that exists) unless

they are large enough to change the flow regime. The development of an <sup>9</sup>impervious "caprock" could be significant enough to change the flow regime from conduction-dominated to conduction- and convection-dominated.

Dr. Schechter concluded that a principal effect of evaporation of pore fluids will be a reduction of matrix permeability, but this will not be a large effect because the matrix permeability is orders of magnitude smaller than the fracture permeability. Dr. Schechter suggested that mineral precipitation may occur in distinct bands of high crystal concentration, thereby increasing the potential for pore or fracture clogging. However, he concludes that mineral dissolution will be most active at those sites where condensate drops first form, which are the small fracture apertures. Therefore, as the narrow openings in a fracture are enlarged, condensation and dissolution will result in an increase in fracture permeability. He suggested that observations of fracture permeability decrease from the Single Heater Test may be due to clogging of the fracture permeability by colloidal particles or smoothing of the fracture surface.

The experts also assessed the implications of the changes in fracture permeability due to THC effects. For example, Dr. Yortsos concluded that reducing fracture permeabilities near the drift during heating will lead to diminished natural convection, increased local temperatures and gas pressure, a diminished heat pipe effect, and more symmetrical temperature profiles above and below the repository. Others on the panel also suggested that heat pipes may become ineffective below certain permeability values. It was also suggested that reduced permeability above the drift, particularly if an impervious cap develops, could affect seepage into the drifts.

Finally, the experts noted that the mineral dissolution and precipitation process could lead to significant effects on fracture-matrix interaction. Dr. Elsworth noted that the effects will vary spatially and during heat-up and cooldown. In the condensate zone, dissolution would remove the coating and increase fracture-matrix interaction, and deposition would occur in the matrix. In the dry-out zone, deposition would occur on the fracture walls, thus reducing coupling and retaining greater volumes of recirculating condensate. Dr. Yortsos concluded that the two issues related to fracture-matrix interaction are: the

degree to which water will flow in fractures versus being imbibed into the matrix; and the pattern of liquid flow along fracture surfaces, namely whether it will occur in the form of fingers or channels, or in an episodic manner.

### 3.2.7 Multiply Coupled Effects

Throughout the assessments discussed above, coupled temperature, hydrologic, mechanical, and chemical effects were considered in various combinations. The experts were also asked if there were considerations in fully coupled THMC processes that might not have emerged in their considerations of coupling of the various components. In general, the experts saw no strong need for a fully coupled model. For example, Drs. Hart and Ross suggested that because of the complexity of the system, a fully coupled model that accounts for all of the interactions is not feasible. Instead, they and Dr. Gale suggested that first the important processes be identified, then the linkages among processes be characterized. Dr. Gale suggested that computer simulations should allow processes to be weakly coupled and the interaction loops linked at appropriate time steps, temperatures, fluid/capillary pressures, and rock mass stresses. He also noted that these simulations of THMC effects will require some precise data sets for calibration and constraints on coupled processes.

Dr. Yortsos concluded that the important coupled effects were discussed in the context of coupling of the various components discussed above. He noted that fracture healing is expected to be the primary THMC effect. Dr. Elsworth summarized the relative importance of various coupled effects. He concluded that THC and THM changes in permeability work against each other, but result in a net decrease in vertical permeability. THM and THC changes in horizontal permeabilities also will work against each other, and the net result will be a decrease in horizontal permeability (10X) at the repository center and a net increase (100X) in horizontal permeability at the periphery. The net effect of combined THM and THC permeability changes is to suppress convective heat transfer at the center of the repository block and increase lateral diversion of condensate on the downdip portion of the repository periphery.



### **3.2.8 Durability of Effects**

The experts were asked to summarize their assessments of the durability of coupled effects over time, that is, the degree to which the significant changes will persist after the thermal period has ended. The general conclusion was that the mechanical permeability changes due to normal closure or extension will be largely recoverable. Dr. Yortsos pointed out that if fracture surfaces are not well mated, then the effects of normal stress and fracture healing will not be reversible. Mechanical changes involving shear displacements, which are expected to primarily affect horizontal permeabilities, were assessed to be irreversible. Likewise, chemical changes in permeability due to dissolution and precipitation, reactions leading to fracture healing, and formation of a zone of precipitation at the vaporizing end of heat pipes would be expected to be irreversible. This would include changes in fracture-matrix interaction due to precipitation along fracture walls.

### **3.2.9 Recommended Activities to Reduce Uncertainties**

Each member of the NFEE panel provided recommendations for activities that can be carried out to reduce uncertainties. These recommendations are given in their elicitation summaries in Appendix D.

**TABLE 3-1**  
**ISSUES ADDRESSED BY NFEE EXPERT PANEL**

**Thermal-Mechanical:**

1. Assess the mechanical stability of the host rock in the near-field environment, where rock mass failure can cause liner collapse, leading to rockfall into the emplacement drifts. Describe the processes in the thermal evolution of the repository, which will contribute to near-field mechanical instability, both during the period of increasing or stable elevated temperature, and during cooldown. For this assessment consider changes, if any, that would occur solely from thermal and thermal-mechanical causes.

**Thermal-Hydrologic-Mechanical:**

2. Assess the impact of thermal loading on the fracture porosity and permeability throughout the host rock, particularly near the emplacement drifts, and within the intervening pillars. Describe how these effects are likely to change upon cooling. For this assessment describe the changes, if any, that would occur solely from thermal-mechanical causes (e.g. air permeability in a dry rock mass).

**Thermal-Hydrologic-Chemical:**

3. Assess the impact of dissolution and precipitation in reflux zones, on the fracture porosity and permeability above the emplacement drifts, and in pillars between drifts where drainage occurs in thermal-hydrologic simulations conducted for the TSPA-VA base case. For this assessment describe the changes, if any, that would occur solely from these chemical causes, both during the period of maximum thermal-hydrologic activity before the reflux zone begins to contract, and during cool down.
4. Assess the impact of mineral alteration (to secondary forms with different physical and hydrologic properties) on fracture porosity and permeability above the emplacement drifts, and along pathways where drainage occurs in thermal-hydrologic simulations conducted for the TSPA-VA base case. For this assessment describe the changes, if any, that would solely occur both during the period of maximum thermal-hydrologic activity before the reflux zone begins to contract, and during cool down.

5. Assess changes in fracture-matrix coupling that may result from reflux activity. Describe the location, intensity, and reversibility of any such changes.

**Multiply Coupled:**

6. Assess multiply coupled effects from thermal, thermal-mechanical, and chemical processes, on the mechanical stability of the near-field environment, where rock mass failure can cause liner collapse, leading to rockfall into the emplacement drifts. Describe the multiply coupled processes in the thermal evolution of the repository, if any, which will contribute to near-field mechanical instability, both during the period of increasing or stable elevated temperature, and during cool down.
7. Assess multiply coupled effects from thermal, thermal-mechanical, and chemical processes, on fracture porosity and permeability above the emplacement drifts, and in pillars between drifts where drainage occurs. For this assessment describe the changes, if any, that would occur both during the period of maximum thermal-hydrologic activity before the reflux zone begins to contract, and during cool down.
8. Assess multiply coupled effects from dissolution and alteration, and from thermal and thermal-mechanical processes, on the porosity, permeability, and mechanical stability of fracture pathways for drainage below the emplacement drifts. For this assessment describe the changes, if any, that would occur both during the maximum thermal-hydrologic activity before the reflux zone begins to contract, and during cooldown.
9. Assess the durability of any fracture porosity and permeability changes caused by dissolution and precipitation, or by mineral alteration, as the host rock cools. Consider redissolution of precipitates and mechanical adjustment of the rock mass during cooling. Identify any processes that are likely to dominate the long-term hydrologic response of the rock mass.

TABLE 3-2  
SUMMARY OF KEY ISSUES

	Derek Elsworth	John Gale	Robert Hart	Benjamin Ross	Robert Schechter	Yanis Yortsos
Overall Processes	<ul style="list-style-type: none"> <li>+ Changes in permeability due to thermal, mechanical, and chemical (TMC) influences are likely to be important to the hydrology of Yucca Mountain.</li> <li>+ Changes in bulk fracture permeabilities are most important in controlling dryout and reflux; changes in matrix permeability are important in controlling the sequestering of condensate.</li> <li>+ Mountain-scale permeability changes from T(H)M and THC modes are of similar order and largely reinforce behaviors.</li> <li>+ Stresses developed in the thermal period will decrease vertical permeabilities and increase horizontal permeabilities, switching the regional permeability dominance from vertical to horizontal, and potentially suppressing the development of unthrottled convective energy transfer.</li> <li>+ Chemical dissolution products will coat fracture surfaces, reducing imbibition and recirculating larger volumes of reflux.</li> <li>+ Key uncertainties are permeability changes at the scales of interest, which range from the drift to the mountain scale. The processes controlling mechanical changes in permeability are reasonably understood; analogous chemical processes are significantly less well understood.</li> </ul>	<ul style="list-style-type: none"> <li>+ The rock mass at the Yucca Mountain site is well fractured; at least three fracture or joint sets have been mapped in the boreholes and tunnels.</li> <li>+ The impact of the fracture system on the near-field TMHC coupled processes must be evaluated.</li> <li>+ The most significant effects on repository performance will be those that are introduced by the full TMHC processes, primarily the permanent or near-permanent changes that the dissolution and deposition of minerals will have on the permeability of the fractures during thermal loading and the ability of the rock mass to dissipate the thermal load.</li> <li>+ The impact of shear displacement on fracture permeability during both the thermal loading and cooldown will both impact the development of heat pipes and provide the subhorizontal pathways for long-term flow and transport through the repository.</li> <li>+ The thermal-mechanical impacts, in terms of inducing roof migration, also will be significant.</li> <li>+ Agreement must be reached on the stress and displacement boundary conditions that should be applied to the repository as a whole and to the immediate area of the drifts specifically, as well as the edges of the repository.</li> </ul>	<ul style="list-style-type: none"> <li>+ The effect of the thermal pulse on the unsaturated flow regime and the influence of the partially saturated flow on the temperature profile in the host rock may be a very important coupled process.</li> <li>+ Of all the processes that have been identified, the one that appears to have received the least attention is geomechanical behavior, which may have a very important influence on the near-field environment. Specifically, thermally induced slip along joints within the host rock may strongly influence both the thermal-hydrologic response of the near-field environment (i.e., by affecting the intrinsic permeability of the joint structure) and also the mechanical response of the host rock around the emplacement drift (i.e., by affecting the mechanical stability of the drifts).</li> </ul>	<ul style="list-style-type: none"> <li>+ The combination of heat transfer and fluid flow is the most important coupled process related to the thermal perturbation of Yucca Mountain. Mechanical and chemical changes can also have large quantitative consequences, but they are less likely to move the system into a qualitatively different regime.</li> <li>+ Two different patterns of thermally driven liquid flow potentially could transfer significant amounts of heat: countercurrent gas-liquid flow, and mountain-scale convective flow.</li> <li>+ The most critical unknown about mountain-scale convection is whether it will make a significant contribution to heat transfer, which depends on only one parameter that is not well known: the bulk permeability of the rock mass.</li> <li>+ Countercurrent gas-liquid flow in some form is almost certain to occur at Yucca Mountain; the details are less clear.</li> </ul>	<ul style="list-style-type: none"> <li>+ Factors that tend to increase the rate of water influx into the drift and those that alter the composition of the water influx to increase its corrosiveness are of primary concern.</li> <li>+ Dissipation of heat into the environment by conduction will result in an endless chain of vaporization/condensation steps; these processes will not likely achieve a steady state, primarily because they cause a continuous alteration of the rock permeability; this alteration of permeability as a result of dissolution/precipitation processes represents one of the greatest uncertainties.</li> <li>+ One must anticipate the worst case—a greatly increased permeability in the rock surrounding the drift, extending out a distance beyond the point where substantial vaporization and condensation have taken place.</li> <li>+ Corrosion of the waste packages will be affected by the CO<sub>2</sub> and O<sub>2</sub> concentrations in the groundwater, which will be greatly enhanced by suction pressures.</li> </ul>	<ul style="list-style-type: none"> <li>+ The thermal loading will result in thermal effects on thermodynamic variables, thermal expansion in liquid-vapor phase changes, and possible chemical transformations.</li> <li>+ Predicting TM and TC effects requires the understanding and modeling of NFE processes, particularly: the overall heat transfer, the countercurrent liquid-vapor flows and the liquid-vapor phase change in a fracture-matrix system, and the matrix-fracture interaction. In particular, determining the flow path of the water following its vaporization from the matrix, and its subsequent condensation, is a key to the THC analysis.</li> <li>+ Important TM and THM effects should lead to a reduction in the apertures of vertical fractures near the center of the repository, with corresponding changes in fracture permeability depending on the original fracture values, the relative effect being smaller for larger-aperture fractures. Expected changes can be in the range of one to two orders of magnitude.</li> <li>+ Significant TC and THC effects should be expected mostly as a result of: (1) mineral deposition in fractures at the vaporizing ends of heat pipes, and (2) possible fracture healing due to dissolution of fracture asperities. Both of these THC effects will act to reduce fracture permeabilities, by one to two orders of magnitude in the fracture healing case, and perhaps by a greater degree in the case of deposition.</li> </ul>

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TABLE 3-2  
SUMMARY OF KEY ISSUES, (Continued)

	Derek Elsworth	John Gale	Roger Hart	Benjamin Ross	Robert Schreiter	Yanis Yortsov
TM - Thermal-Mechanical Effects: Stresses and Strains	<p>+ Thermally induced stresses, that in turn affect drift stability, and feedback on evolving thermal, hydraulic, and chemical fields, are controlled by a small set of parameters defined at the scale of the rock mass:</p> <p>+ Coefficient of thermal expansion, deformation modulus, Poisson ratio, and the form and magnitude of the induced temperature field.</p> <p>+ The repository block will be subject to relatively uniform TM horizontal stresses, with shear stresses increasing from the repository center outward, to a maximum at the edge. Shear stresses/strains will be largest in the zone of high temperature gradient, e.g., at the ends of heat pipes, and migrate with this zone.</p> <p>+ At the mountain scale, for a temperature rise from 25°C to 160°C, initial field stresses will rotate from the maximum stress acting vertically, with <math>\sigma_v : \sigma_h</math> initially as 7:3.5 MPa, to the maximum stress acting horizontally, with 7:14 MPa, with an upper bound on the order of 20 MPa. This transition from vertically dominant (2:1) to horizontally dominant (1:2) stress regimes, would be largely reversible on cooling in the post-thermal period.</p> <p>+ TM induced (minor) rock bursts may develop late in the thermal evolution; their late timing is unlikely to affect drift stability, and fluid volumes mobilized from the overlying condensate zone are unlikely to be greater than those currently in circulation.</p> <p>+ At the drift scale, with heating from the drift, radial and particularly tangential stresses will increase. At the thermal maximum, there will be high roof and floor stresses. For a resulting horizontal field stress of 14 MPa that is double the vertical stress, crown and springline stress concentrations would be on the order of 35 MPa and 7 MPa, respectively; these are sufficiently high to result in moderate scale spalling from the roof and springline.</p>	<p>+ As the thermally induced stresses change, they will produce a range of shear and normal stresses on existing fracture planes.</p> <p>+ Given the shape and size of the repository, the most likely condition will be one that reflects a combination of both boundary conditions but is weighted about 70% in terms of plane strain (complete confinement) and about 30% in terms of plane stress (no confinement).</p> <p>+ At peak thermal loading, the vertical stresses will remain close to 7 MPa, but the horizontal stresses will increase to about 20 to 40 MPa in the zone between the emplacement at drifts at 200°C and the maximum extent of the 100°C isotherm. The tangential stresses at the drift wall would be close to zero at the springline and range up to about 80 to 100 MPa at the crown of the drift, decreasing rapidly with decreasing temperature and increasing distance from the drift to about 20 MPa at the 100°C isotherm.</p> <p>+ The stresses at the drift crown will greatly exceed the computed rock mass strength of 18 to 19 MPa that is presented in Wilder (1996), leading to failure at the crown of the drift.</p> <p>+ With increasing thermal load, the normal stresses on the fracture planes will rotate through a full 90 degrees (i.e., the major principal stress will now be horizontal rather than vertical) and will range up to about 40 MPa for fractures that are outside of the zone of stress concentration. The shear stresses will range from zero up to 15 or 20 MPa. Based on the expected combination of normal and shear stress on the fracture planes, one can expect that both dilatant and contractant behavior during shear displacement will be present in the perturbed rock mass.</p>	<p>+ As the rock mass heats, thermally induced mechanical stresses will induce both normal and shear displacements along joints within the rock mass, depending on their orientation.</p> <p>+ Joint displacement is in both the normal and shear direction and is predominantly non-linear and irreversible.</p> <p>+ Opening and closing of the joint as a result of thermally and mechanically induced normal and shear displacements will have a strong influence on the intrinsic permeability of the joint.</p>	<p>+ It is possible that thermal mechanical effects could increase gas permeabilities around the rim of the repository, which would increase the strength of buoyant gas flow. Under ambient conditions, the vertical gas permeability is greater than the horizontal, based on barometric studies. If the thermal load enhances vertical permeabilities at some distance from the repository, this could reinforce mountain-scale convection.</p>		

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TABLE 3-2  
SUMMARY OF KEY ISSUES, (Continued)

	Derek Elsworth	John Gale	Roger Hart	Benjamin Ross	Robert Schechter	Yanis Yortsos
TM - Thermal Mechanical Effects: Liner Stability	<ul style="list-style-type: none"> <li>+ Thermal liner stresses are controlled primarily by the composite liner properties of modulus, Poisson ratio, thermal expansion coefficient, and liner thickness; there is only weak dependence on the rock mass parameters of modulus and Poisson ratio.</li> <li>+ Liner stresses should increase up to the time of the drift thermal maximum, on the order of 50 years, and increase little following that; liner elements surviving to the time of thermal maximum would be expected to fail from strength loss with time (THC: durability).</li> <li>+ For a temperature change of 135°C, a hoop stress in the liner of on the order of 40 to 80 MPa would result.</li> <li>+ If liner failure is predicated on durability, then expectations of survival in the 50- to 100-year range may be achievable, depending on materials and fabrication methods.</li> </ul>	<ul style="list-style-type: none"> <li>+ Local failures that result in movement of rock blocks would produce failure of the concrete liner due to point loading at the contacts with the rock. Grouting the space between the liner and the rock would integrate the liner and the rock mass and increase the area of the liner in contact with the rock, mitigating point load stresses and increasing the stability of the liner.</li> </ul>	<ul style="list-style-type: none"> <li>+ Material degradation implies that the long-term strength of a material is significantly lower than the short-term strength; this degradation can result from progressive micro-fracturing due to the change in stress experienced by the material. This may be an important process affecting the long-term mechanical stability of the concrete liner.</li> </ul>			
TM - Thermal-Mechanical Effects: Drift Stability	<ul style="list-style-type: none"> <li>+ Estimations of (unlined) drift convergence are about 8 to 10 mm.</li> <li>+ Reliable estimates of time to drift failure are infeasible; however, the liner should survive aggressive THC condition on the order of 50 to 100 years.</li> <li>+ Assuming failure of the drift, a bulking factor of about 35% may be expected, at the lower end of an anticipated 20% to 65% range (Church, 1981), representing drift-infill porosities in the 15% to 40% range. In the case of complete failure of the drift by chimneying, this would represent failure to about 3 diameters above the initial drift, which is an approximate upper bound to anticipated drift elongation to about one drift diameter, evaluated from stable borehole breakout configurations.</li> <li>+ TM-driven collapse will be largely complete by the time of maximum thermal stresses, in the range 100 to 300 years, with minor intermittent collapse thereafter.</li> </ul>	<ul style="list-style-type: none"> <li>+ Based on the measured and computed rock mass properties, strains of 2 mm/m seem reasonable at 200°C. The compressive strength of the rock mass is relatively low at 18 to 23 MPa, and local failure of the rock mass should occur with strains of 1.5 mm/m.</li> <li>+ When the drift fails, the crown will migrate with a bulking factor of about 30% (range of 15% to 45%), based on the blocky nature of the rock mass. This is equivalent to a porosity of 13% to 31%. For a 5 m drift opening, one would expect that the crown would migrate 10 to 12 m vertically.</li> <li>+ The thermal conductivity of the rubble is potentially important to temperatures of the waste packages; a reasonable range of permeabilities to use in the modeling is 1000 to 100,000 darcies given the low fragmentation.</li> <li>+ If backfill is placed in the drift, it will have only about 20% to 25% of the compressive strength of the rock, but should limit crown migration to about one meter, depending on how the backfill is placed.</li> </ul>	<ul style="list-style-type: none"> <li>+ Two processes are considered to have a dominant effect on mechanical stability: thermally driven stress change, and strength degradation of the host rock and liner materials. Thermally driven stress change can occur solely from thermal and thermomechanical causes. Strength degradation can occur from various coupled effects involving thermal, thermomechanical, and chemical processes.</li> <li>+ If the continuum failure of the rock blocks dominates the mechanical response of a jointed rock mass, then emphasis should be placed on characterizing the rock mass strength. If the discontinuum failure of the rock joint structure dominates the response, then the emphasis should be placed on characterizing the rock joint parameters.</li> <li>+ My analysis suggests that the observed behavior of the SFT is due to localized slip on favorably oriented joints within the rock block and is primarily responsible for the changing thermal expansion behavior. This also implies that the orientation of rock joints relative to the emplacement drift may be an important property for the assessment of mechanical instability.</li> </ul>	<ul style="list-style-type: none"> <li>+ If the natural ventilation alternative is selected for the repository, drift stability becomes important because blockage of air flow through the drifts by rockfalls would greatly reduce the ventilation air flow.</li> </ul>		<ul style="list-style-type: none"> <li>+ I expect that slip of joints would be important in evaluating drift stability, and simulations should be conducted to evaluate its effect.</li> <li>+ The collapse of the drift is important in the analysis of the viability of the project, given the effect of the granular medium to be created on increasing the heat transfer resistance (by conduction rather than radiation) and on the seepage in the drift.</li> <li>+ The flow properties (absolute and relative permeabilities) of the induced self-similar rubble packings can be studied using an Apollonian packing model.</li> </ul> <p><b>APERTURE CARD</b></p> <p>Also Available on Aperture Card</p>

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TABLE 3-2  
SUMMARY OF KEY ISSUES, (Continued)

	Derek Elsworth	John Gale	Roger Hart	Benjamin Ross	Robert Schechter	Yanis Yortsos
THM - Thermal-Hydrologic-Mechanical Effects	<p>+ Units having low initial permeability will exhibit the largest relative change in TM permeability and the smallest absolute change.</p> <p>+ At drift scale: With excavation prior to the thermal period, radial permeabilities will generally decrease, and tangential permeabilities will generally increase within a zone about two drift radii into the wall and three to four drift radii into the roof.</p> <p>+ With heating, permeabilities around the drift will decrease from post-excavation magnitudes. Temperature changes on the order of 100°C are estimated as sufficient to counter the effects of excavation-induced enhancement of tangential permeabilities.</p> <p>+ Development of shear stresses as horizontal field stresses build may induce permeability enhancement in diametral lobes at 45° from the horizontal and reaching to three drift radii from the wall. Permeability changes in these zones may be on the order of 2 to 10.</p> <p>+ Post-thermal drift collapse to a stable configuration, in the timeframe of 1000+ years, will result in a vertically elongate drift section, forcing TM permeability changes to migrate into the inter-drift pillar.</p> <p>+ At mountain scale: Conductive heating will decrease vertical permeabilities in the region closest to the drifts and will increase vertical permeabilities at the periphery of this zone. The reduction in vertical permeability within this compressional envelope may be on the order of 10X. Horizontal permeabilities will be increased from the center outward by a factor of 2 to 100.</p> <p>+ The vertical permeability changes associated with normal stresses will likely be reversible, while horizontal permeability changes associated with shear strains will not. A final result is that the permeability anisotropy of the TSw2 unit is switched from vertically dominant (<math>k_v \approx 5k_h</math>) to horizontally dominant. Shear-induced changes in permeability will reach a maximum of 100X at the periphery of the repository block.</p>	<p>+ Under thermal loading, all three modes of fracture displacement are expected: normal dilation and closure due to changes in normal stress, and dilation and contraction due to shear displacement.</p> <p>+ Assuming plane strain boundary conditions, the magnitude of normal fracture closure should be about 0.1 to 0.3 mm, depending on the roughness and the magnitude of the initial aperture. This is analogous to the permanent closure recorded from first-cycle data developed in laboratory tests.</p> <p>+ The overall fracture porosity change, which is a function of the fracture aperture and spacing, will be on the order of 0.0001 to 0.003. Assuming a range of initial apertures for the existing fractures, these aperture changes will result in fracture permeability changes of 1.5 to 3 orders of magnitude.</p> <p>+ Changes in normal and shear stresses would produce a significant increase in horizontal permeability and decrease in vertical permeability at distances of 2 to 5 drift diameters from the drifts; these changes would likely occur within localized zones and will be controlled to a large extent by the fracture geometry.</p> <p>+ Increases in local fracture porosity could be 0.0001 to 0.001, and increases in local fracture permeability could be by factors of 10 to 1000. Changes in bulk rock permeabilities due to THM coupling are expected to be less than the ambient spatial variability of this property if the fault zones are included.</p> <p>+ TMH changes could have a significant impact on the potential of the fractured rock mass to develop heat pipes; increase in contact area will minimize the development of heat pipes because the fractures will be filled.</p> <p>+ The reduction in fracture permeability due to the combined effect of dissolution at the contact points and fracture closure in the condensation zone followed by precipitation of solutes in the vaporization zone, which is expected to be associated with the advance of the front, is not expected to be reversed as the front retreats.</p>	<p>+ Thermal loading will affect both the intrinsic permeability and the relative permeability.</p> <p>+ Because of the strong dependency of intrinsic permeability on aperture, the effective permeability for the gas and the liquid may also be strongly influenced by aperture change.</p> <p>+ In the distinct element codes UDEC (in 2D) and 3DEC (in 3D), normal displacement of a joint is a direct function of normal stress, via joint normal stiffness, and joint shear stress, via joint dilation angle.</p> <p>+ The analyses identify dilation as a critical parameter in assessing the impact of thermal loading on fracture permeability; they also suggest that fracture permeabilities may increase (as a result of joint slip and dilation) along the sub-vertical joint structure and decrease (due to joint closure) along the sub-horizontal joint structure.</p>	<p><b>Thermal - Hydrologic: TH Effects</b></p> <p>+ Whether convection is important to heat transfer depends only on the thermal loading and the bulk permeability of the rock mass.</p> <p>+ Several numerical models point to a threshold of about 10 to 30 darcies for mountain-scale convection to be significant; gas permeability of fault zones seems to exceed the threshold.</p> <p>+ Mountain-scale convection is one of the most important processes affecting heat transfer and fluid flow. I am sure that it is important to water flow and think there is a good chance (more than 10% but less than 50%) that it is important to temperature.</p> <p>+ The manner in which fracture-matrix interactions are modeled in the presence of heat should be examined. Conceptual models available to explain the apparent discrepancy between incomplete saturation of the matrix and fast flow in fractures are a generalized ECM, DK, or a model that is based on fast-flow paths develop only near high-infiltration regions. This model is more like a discrete fracture model with transient flux boundary conditions.</p> <p>+ In deciding whether countercurrent flow will alter the heat transfer established by conduction, the key question is whether liquid water will flow back toward the heat source.</p> <p>+ When an ECM model describes countercurrent flow, it tends to depict a uniform heat pipe; an improved model would depict countercurrent flow occurring with irregular return flow of water, alongside mountain-scale convection and local zones of condensate shedding. 80% to countercurrent model; 20% to a model of uniform heat pipes and recycling.</p> <p>+ Local zones of shedding more likely pass downward through a few pillars between the drifts, where the temperatures are lower, than into the drifts, but seepage into the drifts is possible especially where there are cooler waste packages.</p> <p>+ Convective flow can reinforce heat pipes above the repository; below the repository a uniform heat pipe zone cannot coexist with convective flow.</p> <p>+ Calculations suggest there may be little gain from using backfill to reduce relative humidity.</p> <p>+ Suggest using passive ventilation to moderate the temperature and relative humidity.</p> <p><b>Thermal-Hydrologic-Mechanical (THM) Effects</b></p> <p>+ Buoyant gas flow will depend on</p>		<p>+ Because of symmetry-induced confinement and the planar heat source, I would expect a reduction in the aperture of vertical fractures near the repository (except for edge drifts), due to increased normal stresses. Near the edges (or for an isolated drift), the behavior might be different, and opening of fractures is possible.</p> <p>+ Stresses on the order of 10 to 20 MPa are expected as a result of thermal loading (<math>\Delta T = 75^\circ\text{C}</math>); changes in joint apertures in the range 10 to 100 <math>\mu\text{m}</math> can be expected.</p> <p>+ At the expected thermal stresses, horizontal fractures near the center of the repository and other joints near the edge of the repository may experience slip. It is not clear whether the slip will crush asperities or override them and cause dilation. If dilation occurs, permeability increases of one to two orders of magnitude are possible. But if asperities break, then the permeability may decrease. This effect is in need of further study.</p> <p>+ In vertical fractures away from the edge of the repository, the decrease in mechanical aperture will lead to a concomitant decrease in hydraulic aperture and, hence, fracture permeability. Given the uncertainty in fracture permeabilities, the variation due to thermal loading would be within the range of natural heterogeneity in the repository, but skewed toward smaller permeability values. Reduction in vertical permeabilities will lead to a reduction in the anisotropy of the fracture network and to a possible increase in lateral flow.</p> <p>+ The fracture geometry (roughness and aperture characteristics) will be affected by the thermal load. The effect of thermal load on 2-phase flow parameters would be an increase in the capillary pressure (decrease of the van Genuchten <math>\alpha</math> parameter) of the fracture and a decrease of the diffusion coefficient as fracture aperture decreases.</p>

**APERTURE  
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TABLE 3-2  
SUMMARY OF KEY ISSUES, (Continued)

	Derek Elsworth	John Gale	Roger Hart	Benjamin Ross	Robert Schechter	Yanis Yortsos
				<p>permeability, being strongest in high-permeability zones.</p> <ul style="list-style-type: none"> <li>+ Under current conditions, vertical permeability is several times greater than horizontal; therefore the gas flux would be much more sensitive to changes in horizontal than in vertical permeability.</li> <li>+ Faults are likely to be important in creating more permeable zones, but so are zones of enhanced permeability from the thermomechanical changes.</li> </ul>		
THC- Thermal-Hydrologic-Chemical Effects	<ul style="list-style-type: none"> <li>+ There are three permeability change mechanisms that appear to be feasible: (1) the potential for hyperalkaline fluids to develop as a result of dissolution of the concrete liner and formation of a precipitation zone beneath the drifts at the base of the dry-out zone; (2) <math>\text{SiO}_2</math> and calcite dissolution in the condensate zone leading to porosity changes, the primary influence likely being an increase in imbibition in the condensate zone and coating of fractures and decrease in imbibition in the dry-out zone; (3) pressure solution within contacting fractures, effect that would reduce permeabilities in zones of dissolution and precipitation. Assuming a constant in situ stress magnitude, there will be a net reduction in permeability of possibly two orders of magnitude. As the asperities are dissolved along fractures, the stresses will also be reduced, leading to a reduction in the mechanically-driven permeability reduction. Net permeability reductions on the order of 10X would be expected.</li> <li>+ Permeability changes that would be expected due to mechanical and chemical effects during the maximum thermal period and during the subsequent cooldown period are summarized in Figure DE-3; estimated reductions in permeability are likely to be on the order of no more than 10 and the increases in permeability on the order of no more than 100.</li> <li>+ Changes in permeability due to alteration to secondary forms are of low order, occurring at the upper range of expected repository temperatures.</li> <li>+ Fracture-matrix coupling effects vary spatially and during heat-up and cooldown.</li> <li>+ In the condensate zone, dissolution would remove the coating and increase the fracture-matrix interaction. Deposition would occur within the matrix. In the dry-out zone, deposits would occur on the fracture walls, thus reducing coupling and retaining greater volumes of recirculating condensate.</li> </ul>	<ul style="list-style-type: none"> <li>+ In the condensation zone, the walls of the fractures will be eroded during heating due to dissolution of fracture minerals, especially those that form the contact points or asperities, allowing for mechanical closure of the fracture. There probably will be a high degree of hysteresis or permanent fracture closure.</li> <li>+ In the vaporization/precipitation zone, the permeabilities are reduced as solutes are precipitated. Thermal/mechanical loading will also decrease the fracture permeability, but contact area is being added due to mineral precipitation. Thus the stresses on the asperities should not increase very much, thereby limiting the total amount of mechanical aperture closing. This increase in contact area will minimize the development of heat pipes because the fractures will be filled.</li> <li>+ The reduction in fracture permeability due to the combined effect of dissolution and fracture closure in the condensation zone followed by precipitation of solutes in the vaporization zone is not expected to be reversed as the front retreats.</li> <li>+ Precipitation of secondary minerals along the walls of fractures can have a significant effect on fracture-matrix interaction. Fracture mineralization impedes the interaction between fluids in the fractures and fluids in the matrix and adds to the contact areas, thus increasing fracture stiffness</li> </ul>		<ul style="list-style-type: none"> <li>+ At present, uncertainties about mechanisms of fluid flow are so great that even large changes in a flow parameter do not add significantly to the uncertainty; therefore, the processes of interest are only those that can cause large changes in parameter values and processes that can change parameters to which flow regime is highly sensitive.</li> <li>+ An impervious caprock would change parameters: change in gas permeability would change the system from a conduction to a conduction-and-convection heat transfer regime.</li> <li>+ Filling of fractures by chemical precipitates will not have a large effect on liquid flow, because the permeability far exceeds the amount of water available to flow through them. Fracture filling will also have a limited effect on gas flow.</li> <li>+ An impervious caprock is unlikely (5% to 10%), but would form at the interface between the boiling zone and condensate zone.</li> <li>+ Fracture "healing" would have little effect on liquid flow but could reduce gas flow. This mechanism has a low probability of occurrence in the unsaturated zone, because flow seems to concentrate in localized pathways.</li> <li>+ The primary chemical effect on fracture-matrix interactions is likely to be "armoring" of fracture surfaces by coatings of precipitate. This will have little effect on flow; the change is within the range of uncertainty from lack of knowledge about mechanisms of flow.</li> </ul>	<ul style="list-style-type: none"> <li>+ The precipitation attending the evaporation of pore fluids likely will result in a reduction of matrix permeability, but this permeability is orders of magnitude smaller than the fracture permeability.</li> <li>+ An important issue in terms of the effect of this adsorption or condensation on the fracture permeability hinges on the formation of liquid lenses or "droplets."</li> <li>+ An important observation is that the lenses will not, in general, occupy the full cross section of a fracture, thereby blocking the local flow of the gaseous phase.</li> <li>+ We must visualize the TH regime to be a dynamic one in which minerals are being continuously redistributed and the flow in the fractures is sporadic. Furthermore, there would be a net downward flow of condensate, not a true steady state.</li> <li>+ Mineral dissolution will be most active at those sites where condensate drops first form, which are the small fracture apertures. Therefore, as the narrow openings in the fracture are enlarged, condensation and dissolution will result in an increase in fracture permeability. The observed fracture permeability decrease could be due to clogging of the fracture permeability by colloidal particles or smoothing of the fracture surface.</li> <li>+ It is possible that mineral precipitation will occur in distinct bands of high crystal concentration, thereby increasing the potential for pore or fracture clogging.</li> <li>+ If the lifetime of a condensate lens is much less than the reaction time, the primary site of mineral dissolution will be at the condensation sites and within the matrix. My calculations suggest that the condensate will imbibe before reaction is complete. This implies that the dissolution that takes place in the fractures will tend to increase fracture permeability.</li> </ul>	<ul style="list-style-type: none"> <li>+ The change in the chemical composition of gases is mostly through <math>\text{H}_2\text{O}</math> and <math>\text{CO}_2</math> content; changes in the chemical composition of liquids occur due to evaporation and condensation and to transport and reaction with solid surfaces.</li> <li>+ Evaporation in the fractures from refluxing water will lead to precipitation of calcite and silica produced by dissolution of calcite and silica minerals lining fracture and pore walls during liquid flow return.</li> <li>+ Two THC processes may lead to non-trivial effects: (1) fracture healing and (2) the continuous deposition of minerals at specific locations, for example at the vaporizing ends of heat pipes.</li> <li>+ Significant permeability reduction (on the order of one to two orders of magnitude) is expected from fracture healing. The postulated mechanism is pressure solution; however, typical pressure solution mechanisms require much higher stress levels than those expected in the thermal period. At present, fracture healing is not a well-understood process.</li> <li>+ Mineral deposition following evaporation of the refluxing liquid at the end of the heat pipe zone would create a deposition zone of potential significance. Based on assumed kinetic data, the rate of growth of the deposition zone is on the order of 1 cm <math>\text{yr}^{-1}</math> for a heat pipe zone of length <math>L=20</math> m, which is a non-negligible rate of growth. This estimate will vary depending on the kinetic constants and the extent of the heat pipe zone. Fractures of lower permeability have a higher rate of growth. The zone would be characterized by a significantly reduced permeability, due to the small size of deposited grains, and can be considered as the equivalent of a "cap."</li> <li>+ Viscous fingering-type instabilities induced by dissolution reactions of the refluxing liquid are not expected to be important.</li> <li>+ Reducing fracture permeabilities near the drift during heating will lead to diminished natural convection, to increase local</li> </ul>



TABLE 3-2  
SUMMARY OF KEY ISSUES, (Continued)

	Derek Elsworth	John Gale	Roger Hart	Benjamin Ross	Robert Schechter	Yanis Yortsos
						<p>temperatures and gas pressure, to a diminished heat pipe effect, and to more symmetrical temperature profiles above and below the repository. Heat pipes may become ineffective for heat transfer below a critical permeability value. Development of a reduced permeability zone above the drifts will affect the seepage into the drifts.</p> <p>+ Fracture-matrix interaction: The first issue is the degree to which water will flow in fractures (advection) versus being imbibed into the matrix (diffusion). A second issue is the pattern of liquid flow along fracture surfaces, namely whether it will occur in the form of fingers or channels, or in an episodic manner. More correlated fractures will lead to a higher potential for channeling. In such cases, the fracture-matrix interaction reduction factor should be less than 1. At present this reduction factor is assumed to be proportional to the relative permeability between different parts of the fracture, but this needs to be justified.</p>
Multiply Coupled Effects	<p>+ The primary multiply coupled effect will be the interactions of THC and THM changes in permeability; these effects work against each other but result in a net decrease in vertical permeability.</p> <p>+ THM and THC changes in horizontal permeabilities will work against each other. The result will be a net decrease (10X) in horizontal permeability at the repository center and a net increase (100X) in horizontal permeability at the periphery.</p> <p>+ The net effect of combined THM and THC permeability changes is to suppress convective heat transfer at the center of the repository block and increase lateral diversion of condensate on the downdip portion of the repository periphery.</p> <p>+ A secondary multiply coupled issue relates to the durability of the concrete liner. Since the liner may be designed to withstand anticipated thermal loads, liner survival ultimately is defined by the rate of strength loss due to chemical weathering.</p> <p>+ <u>T, TM, THC Above the Drifts:</u> Mechanical and chemical effects largely work against each other in changing fracture permeability during the heating period. During cooldown, mechanical stresses will relax, if not already partially relaxed by dissolution processes. TM increases in vertical permeability will largely recover, but horizontal permeability enhancement and THC changes will not.</p> <p>+ <u>T, TM, THC Below the Drifts:</u> Low-permeability nonwelded units (CHn)</p>	<p>+ Given the complexity of the system, the best approach is to identify the key processes and then characterize the linkages among these processes.</p> <p>+ The only feasible approach to evaluating the coupling of these processes in a realistic time frame is to conduct computer model simulations in which the processes are weakly coupled and the interaction loops are linked at appropriate time steps, temperatures, fluid/capillary pressures, and rock mass stresses.</p> <p>+ Computer simulations of THMC effects will require some very precise data sets for calibration and to provide constraints on coupled processes.</p>	<p>+ A single method that incorporates the full coupling of all processes would be very difficult to develop; an alternative is to develop methods that partially couple processes, assuming that certain processes are more important than others.</p>	<p>+ Constructing a fully coupled THCM model that is deductive is too large an effort to be feasible.</p> <p>+ Success is much more likely if one tries first to identify important phenomena (e.g., fracture-matrix interaction, formation of a caprock) and then to develop the linkages that appear important.</p>		<p>+ Fracture healing is expected to be the primary THMC effect.</p> <p><b>APERTURE CARD</b></p> <p>Also Available on Aperture Card</p>

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TABLE 3-2  
SUMMARY OF KEY ISSUES, (Continued)

	Derek Elsworth	John Gale	Roger Hart	Benjamin Ross	Robert Schrechter	Yanis Yortsos
	underlying the repository are shown to be strongly hysteretic in thermal behavior, suggesting the potential for large permeability changes if temperatures significantly exceed boiling. However, anticipated temperatures at this depth are probably low enough ( $< 90^{\circ}\text{C}$ ) that this will not matter.					
Durability of Effects	<ul style="list-style-type: none"> <li>+ Durability of permeability changes depends on the causal mechanism.</li> <li>+ Mechanical permeability changes due to normal closure or extension will be largely recoverable.</li> <li>+ Changes involving shear displacements and irreversible mobilization of frictional forces are largely irreversible.</li> <li>+ Changes in fracture and matrix permeabilities due to dissolution and precipitation effects will be largely irreversible. Correspondingly, shear-induced enhancements of horizontal permeabilities, and dissolution/precipitation-driven reductions in permeabilities, are considered largely irreversible.</li> <li>+ T(H)M-driven reduction of vertical permeabilities in the thermal period is considered largely reversible.</li> <li>+ At the drift scale, permeability changes will be dominated by TM-driven redistribution of stresses and changes in drift geometry. Drift-local (to 5 radii) changes in permeability will be largely irrecoverable.</li> </ul>	<ul style="list-style-type: none"> <li>+ Normal stress effects are partly reversible, except for the hysteresis effects of fracture closure, which are essentially permanent. There will be very little opening of the fractures due to changes of normal stress during cooldown.</li> <li>+ The shear stresses and shear displacements that will be induced by the rotation of the stress field during the thermal loading will produce similar changes during both the thermal loading and the cooldown part of the repository lifecycle. The final changes in fracture permeability will be permanent.</li> <li>+ The TMHC effects can be considered permanent or very nearly so, except where the fracture is subject to high shear stresses at low normal stresses.</li> </ul>	<ul style="list-style-type: none"> <li>+ The displacements of joints within the host rock are primarily nonlinear and irreversible. If thermally driven shear displacement of the joints does occur, then I believe it is reasonable to expect an associated dilation that may also be primarily irreversible. I would also expect that if the joints dilate, there will be an increase in the intrinsic permeability of the joint.</li> </ul>	<ul style="list-style-type: none"> <li>+ Redistribution of water will, in the long term, be reversed.</li> <li>+ I do not expect the THC changes to be reversible. Caprocks are observed to persist in geothermal systems. Caprock precipitation occurs in the heat pipe; subsequent drainage occurs at lower temperatures. There is a large volume of rock and only small fractures, plus the precipitates would be silicates, not carbonates, and difficult to dissolve at lower temperatures. The chemical changes to the fracture-matrix interaction also seem likely to be largely irreversible and long-lasting.</li> </ul>	<p><b>APERTURE CARD</b></p> <p>Also Available on Aperture Card</p>	<ul style="list-style-type: none"> <li>+ The TM response is in general hysteretic. If the joint surfaces are not well-mated, there will be different and durable effects during the cooling period. If a fracture-healing process occurs, the surfaces will be better mated. Assuming that due to past thermochemical alteration the joints in the repository area are reasonably well-mated and that fracture healing will occur, the changes in the permeability of vertical fractures caused by normal displacement would be reversible. However, the changes in vertical and horizontal fractures due to shear slip and the response to normal stress of fractures with non-mated surfaces would not be reversible.</li> <li>+ The TC and THC response is reversible as far as phase change and the effect on thermodynamic, mechanical, and transport variables (e.g., solubilities, enthalpies) are concerned. However, effects on kinetics and extent of heterogeneous (solid-liquid) reactions are irreversible.</li> <li>+ Dissolution-precipitation reactions are hysteretic due to the need for nucleation in the second case.</li> <li>+ Dissolution and precipitation reactions leading to fracture healing and the formation of a zone of precipitation at the vaporizing end of heat pipes would be irreversible.</li> </ul>
Recommended Activities to Reduce Uncertainties (See Expert Elicitation Summaries in Appendix D)						

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#### 4.0 SUMMARY AND CONCLUSIONS

The Near-Field/Altered Zone Coupled Effects Expert Elicitation (NFEE) project is one of a series of projects that call on the elicitation of experts to characterize the knowledge and uncertainties in key inputs to the Yucca Mountain Total System Performance Assessment (TSPA). The objective of the NFEE project was to evaluate the temporal and spatial distribution of thermal, hydrologic, mechanical, and chemical effects associated with heating of the host rock from the emplacement of radioactive wastes at the potential repository at Yucca Mountain. An understanding of near-field coupled processes is important to evaluating the performance of the potential high-level nuclear waste repository at Yucca Mountain.

A major goal of the project was to capture the uncertainties involved in assessing near-field/alterd zone coupled effects. So that the analysis included a wide range of perspectives, multiple individual judgments were elicited from members of an expert panel. The panel members, who were experts from outside the Yucca Mountain project but included individuals with past project experience, represented a range of experience and specialization. A deliberate process was followed, consistent with procedural guidance regarding expert elicitation methodologies, to facilitate interactions among the experts, to train them to express their uncertainties, and to elicit their interpretations.

The NFEE experts evaluated several key technical issues related to near-field coupled effects. A brief summary of the expert interpretations is given below.

##### *Overall Processes*

The NFEE experts provided their overview of the processes that they believe are most important to the THMC effects and their coupling. The experts on the panel noted that the rock mass in the Yucca Mountain site is well fractured and that the processes occurring in this fractured system, particularly fracture permeability, are important to the mechanisms of heat transfer and fluid flow. Changes in bulk fracture permeabilities associated with either the mechanical processes of thermal expansion and joint slip or the chemical processes of dissolution and precipitation were assessed to be the most important

influences on dryout and reflux. These changes are time-dependent (i.e., they depend on the thermal history that develops during heat-up and cooldown) and will vary in space with distance from the drifts and with the geometry of the fractures. The chemical changes in fracture permeabilities, which are associated with dissolution and precipitation of minerals, may affect fracture permeabilities, but it generally was judged that the more important influence of chemical processes is the dissolution and precipitation of minerals along fracture surfaces and the impact on fracture-matrix interaction.

#### ***TM—Thermal-Mechanical Effects: Induced Stresses***

The experts provided their assessments of the impact that thermal loads would have on the stress field in the vicinity of the drifts. For the repository block as a whole, relatively uniform horizontal stresses are expected, with shear stresses increasing from the repository center to the edges. Shear stresses/strains are expected to be largest in the zones of high temperature gradient, such as the repository edges and at the ends of heat pipes, and to migrate with these zones. As the rock mass heats, the thermally induced mechanical stresses will be both normal and shear stresses on existing fracture planes, and will change as the stress field changes. For the ambient stress field at repository depth, the maximum stress will act vertically, and the ratio of vertical to horizontal stress  $\sigma_v:\sigma_h$  will be 7:3.5 MPa. With temperature rise, the initial field stresses will rotate from the maximum stress acting vertically to the maximum stress acting horizontally. With heating from the drift, the radial and particularly tangential stresses will increase, leading to high roof and floor stresses (assessed range of 35 to 100 Mpa for all panel members).

#### ***TM—Thermal-Mechanical Effects: Liner Stability***

The experts considered the mechanisms that might affect the stability of the concrete liner during the thermal period. Thermal liner stresses were judged to be controlled primarily by the composite liner properties of modulus, Poisson ratio, thermal expansion coefficient, and liner thickness; there is only a weak dependence on rock mass properties. Liner stresses are expected to increase up to the time of the drift thermal maximum, on the order of 50 years, and increase little after that. The liner elements surviving to the time of thermal maximum would be expected to fail from strength loss with time. Hoop stresses on the liner are estimated to be on the order of 40 to 80 Mpa. If the liner is

designed for long-term durability, then expectations of survival in the range of 50 to 100+ years were judged to be achievable, depending on materials and fabrication methods.

***TM—Thermal-Mechanical Effects: Drift Stability***

The experts were asked for their assessment of the manner in which thermal-mechanical processes would influence the stability of the drifts. The amount of drift (unlined) convergence or strain expected from the thermal loads ranged from 8 to 10 mm at 200°C. It was concluded that the compressive strength of the rock mass is relatively low (18 to 23 Mpa), and that local failure of the rock mass should occur with strains of about 7 mm (1.5 mm/m). The bulking factor and porosities of the materials that will fill the drifts, as well as the amount of expected crown migration, were estimated. The expected bulking is about 30 to 35 percent, with a range of 15 to 65 percent, which represents porosities of the rubble infill in the range of 15 to 45 percent. In the case of complete failure of the drift by chimneying, this would represent an upper bound failure to about 3 diameters above the initial drift, and an expected drift elongation of about one drift diameter. It was concluded that if backfill is placed in the drift, it will have only about 20 to 25 percent of the compressive strength of the rock but should limit crown migration to about one meter, depending on how the backfill is placed.

***THM—Thermal-Hydrologic-Mechanical Effects***

The experts considered the effects that the thermal perturbation would have on the mechanical properties of the rock and, in turn, the hydrologic properties. The most important hydrologic effect was judged to be changes in fracture permeabilities caused by the thermal-mechanical load. The experts generally concurred that, at the mountain scale, the increase in horizontal stresses with heating would increase normal stresses in the central part of the repository (away from the edges) on vertical fractures, reduce apertures, and decrease vertical permeabilities in the region near the drifts (2 to 5 drift diameters from the drifts, according to Dr. Gale). The experts surmised that near the edges of and at greater distances from the repository, opening of fractures and increased vertical permeability are possible. It also was estimated that horizontal permeabilities will be increased due to shear stresses and displacements on horizontal fractures. The experts estimated the magnitude of vertical permeability reduction to range from 1 to 3

orders of magnitude. The magnitude of normal fracture closure was estimated to be about 0.01 to 0.3 mm, depending on the roughness and the size of the initial aperture. As noted by several experts, the fractures with the smallest initial apertures will experience the largest relative change in fracture aperture but the smallest absolute change. The increase in horizontal permeabilities was estimated to range from 2X to 100X from the center of the repository outward. It also was concluded that although the permeability changes related to thermal loading will be significant particularly at a local scale, the changes in bulk rock permeabilities are expected to be comparable to or less than the ambient spatial variability.

#### ***THC—Thermal-Hydrologic-Chemical Effects***

When providing their assessments of coupled thermal-hydrologic-chemical effects, the experts concluded that two principal processes may lead to significant effects: fracture healing, and dissolution and deposition of minerals along fracture walls. A significant permeability reduction (on the order of 10X to 100X) was expected from fracture healing.  $\text{SiO}_2$  and calcite dissolution in the condensate zone will lead to an increase in imbibition and precipitation, and coating of fractures in the dry-out zone will result in a decrease in imbibition. It was suggested that the decrease in permeability due to mineral precipitation is on the order of 10X. It was judged that mineral deposition following evaporation of the refluxing liquid at the end of the heat pipe zone would create a deposition zone of potential significance, analogous to a "cap." Reducing fracture permeabilities near the drift during heating will lead to diminished natural convection, increased local temperatures and gas pressure, a diminished heat pipe effect, and more symmetrical temperature profiles above and below the repository. It also was suggested that reduced permeability above the drift, particularly if an impervious cap develops, could affect seepage into the drifts. Finally, the experts noted that the mineral dissolution and precipitation process could lead to significant effects on the fracture-matrix interaction. In the condensate zone, dissolution would remove the coating and increase fracture-matrix interaction, and deposition would occur in the matrix. In the dry-out zone, deposition would occur on the fracture walls, thus reducing coupling and retaining greater volumes of recirculating condensate.

### ***Multiply Coupled Effects***

The experts were also asked if there were considerations regarding fully coupled THMC processes that might not have emerged in their considerations of coupling of the various components. In general, the experts found no strong need for a fully coupled model. THC and THM changes in permeability work against each other, but result in a net decrease in vertical permeability. THM and THC changes in horizontal permeabilities also will work against each other, and the net result will be a decrease in horizontal permeability (10X) at the repository center and a net increase (100X) in horizontal permeability at the periphery. The net effect of combined THM and THC permeability changes is to suppress convective heat transfer at the center of the repository block and increase lateral diversion of condensate on the downdip portion of the repository periphery.

### ***Durability of Effects***

The experts were asked to summarize their assessments of the durability of coupled effects over time, that is, the degree to which the significant changes will persist after the thermal period has ended. The general conclusion was that the mechanical permeability changes due to normal closure or extension will be largely recoverable. Mechanical changes involving shear displacements, which are expected to primarily affect horizontal permeabilities, were assessed to be irreversible. Likewise, chemical changes in permeability due to dissolution and precipitation, reactions leading to fracture healing, and formation of a zone of precipitation at the vaporizing end of heat pipes were expected to be irreversible. These include changes in fracture-matrix interaction due to precipitation along fracture walls.

### ***Recommended Activities to Reduce Uncertainties***

Each member of the NFEE panel provided recommendations for activities that can be carried out to reduce uncertainties. These recommendations are given in their elicitation summaries in Appendix D.

## 5.0 REFERENCES

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**APPENDIX A**  
**BIOGRAPHIES OF EXPERT PANEL MEMBERS**

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### ***BIOGRAPHIES OF MEMBERS OF THE EXPERT PANEL***

***Dr. Derek Elsworth*** is Professor of GeoEnvironmental Engineering at Pennsylvania State University. His research focuses on the mechanical and hydraulic behavior of porous and fractured geologic media with application to poromechanics, penetrometer testing, geothermal reservoir engineering, igneous and volcanic processes, degradation of groundwater by mining activities, and contaminant hydrology. He has a particular interest in improving understanding of the mechanisms of permeability enhancement due to mechanical and thermal effects in fractured rock, and the role these mechanisms play in transport processes. In these areas, he has served as an adviser to the United Nations; the Power Reactor and Nuclear Fuels Development Corporation, Japan; and the U.S. Nuclear Regulatory Commission and its Advisory Committee on Nuclear Waste. The author of more than 100 professional papers, Dr. Elsworth received the Manuel Rocha Medal of the International Society for Rock Mechanics. Dr. Elsworth received a B.S. in Engineering Geology (1979) from Portsmouth Polytechnic, UK, and an M.S. in Engineering Rock Mechanics (1980) from Imperial College of the University of London. He received a Ph.D. in Engineering (1984) from the University of California at Berkeley.

***Dr. John E. Gale*** is Professor of Geological Engineering at Memorial University in St. John's, Newfoundland, and President of Fracflow Consultants Inc., also in St. John's. Dr. Gale's research focuses on the experimental and numerical study of the coupled hydraulic-mechanical response of discrete fractures and the impact that these coupled processes have on both single- and two-phase flow and transport properties of fractured rock masses. He has authored or co-authored more than 150 papers and reports for a variety of conferences and journals and has consulted with a range of industrial and government clients. Dr. Gale completed a B.S. in Geology (1968) from Memorial University of Newfoundland, an M.S. in Hydrogeology (1971) from the University of Western Ontario, and an M.S. and Ph.D. in Engineering Geoscience from the University of California at Berkeley in 1973 and 1975, respectively.

***Dr. Roger D. Hart*** is the director of software services at Itasca Consulting Group, Inc., in Minneapolis, Minnesota. Itasca specializes in geotechnical, mining, and civil engineering consulting and research and in developing computer software. Dr. Hart's duties include training client organizations in the operation of geotechnical software, coordinating code development and modifications, and consulting on civil engineering activities. He has been involved in the development, validation, and application of computer models in geomechanics since 1979. Dr. Hart has performed numerous rock mechanics studies associated with the underground isolation of radioactive waste in tuff, basalt, and salt, and he was the program manager for rock mechanics design reviews of U.S. Department of

Energy studies in connection with underground radioactive waste isolation. Dr. Hart holds a B.S. (1971) and M.S. (1972) in Civil Engineering-Soil Mechanics from Ohio University and a Ph.D. (1981) in Civil Engineering-Rock Mechanics from the University of Minnesota.

*Dr. Benjamin Ross* is president of Disposal Safety Incorporated, a consulting firm in Washington, D.C., that specializes in analysis of groundwater and soil contamination by radioactive and chemical waste. For the Department of Energy, he developed a coupled model of heat transfer and gas flow at Yucca Mountain that was used to predict the migration of carbon-14 from the potential repository. He currently analyzes near-field thermal effects at Yucca Mountain for the Electric Power Research Institute's Methodology Development Team. Dr. Ross also heads European Analytical Services, Inc., which represents Russian institutes selling technical services and products in the United States. Dr. Ross is a member of the Committee on Buried and Tank Waste of the National Academy of Sciences' Board on Radioactive Waste Management and served on the High Level Waste/Carbon-14 subcommittee of the EPA Science Advisory Board. He received his A.B. in physics from Harvard University and his Ph.D. in physics from the Massachusetts Institute of Technology.

*Dr. Robert S. Schechter* is Professor Emeritus of Chemical and Petroleum Engineering at the University of Texas at Austin. He has chaired the Departments of both Petroleum and Chemical Engineering. After beginning his tenure at the University of Texas in 1957, he held various Professorships and Chairs. He has been a visiting professor at several universities, including Kansas, Edinburgh, and Brussels. In 1976 Dr. Schechter was elected to the National Academy of Engineering; he was named Chevalier of the Order of Palmes Academiques in France in 1980. He has published 215 papers and 5 books. He has received a number of awards for his research, including the American Society of Engineering Educators Senior Research Award (1987), the Franklin Carll Award from the Society of Petroleum Engineers (1994), and the AIME Mineral Industry Faculty Award (1998). He holds a B.A. from Texas A&M University (1950) and a Ph.D. from the University of Minnesota (1957), both in Chemical Engineering.

*Dr. Yanis Yortsos* is Professor of Chemical Engineering and Petroleum Engineering at the University of Southern California, where he has also served as Chairman of the Chemical Engineering Department from 1991 to 1997. Since January 1995, he has held the Chester F. Dolley chair in Petroleum Engineering. His research and teaching interests are in the general areas of fluid flow, transport, and reaction processes in porous media. Dr. Yortsos has received several honors and awards, including the Rossiter W. Raymond Award of the AIME for Outstanding Technical Paper by an author younger than 33 years

of age (1985) and the Distinguished Service Award of the Pi Epsilon Tau (1984). He currently serves in the Editorial Boards of the journal *Transport in Porous Media* and of the *Society of Petroleum Engineers Journal*. He has been an invited or visiting professor or researcher at institutions that include the Universite Paris in Orsay, the Universite Pierre et Marie Curie in Paris, Stanford University, and Clarkson University. Dr. Yortsos has published more than 90 refereed publications, has given more than 60 invited presentations, and presented more than 90 conference papers. He received a B.S. degree (1973) from the National Technical University, Athens, and M.S. and Ph.D. degrees from the California Institute of Technology (1974 and 1979, respectively), all in Chemical Engineering.

## **APPENDIX B**

### **REFERENCES DISTRIBUTED TO EXPERT PANEL MEMBERS**

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## **APPENDIX C**

### **WORKSHOP AND FIELD TRIP SUMMARIES**

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**SUMMARY**  
**WORKSHOP ON SIGNIFICANT ISSUES AND AVAILABLE DATA**  
**NEAR-FIELD/ALTERED ZONE COUPLED EFFECTS**  
**EXPERT ELICITATION PROJECT**

November 5-7, 1997  
Clarion Hotel - San Francisco Airport  
Millbrae, California

The Workshop on Significant Issues and Available Data was the first of three workshops to be conducted for the Near-Field/Altered Zone Coupled Effects Expert Elicitation (NFEE) for the Yucca Mountain project. The purposes of this workshop were to introduce members of the expert panel to the goals and context of the NFEE project and to outline the available data and significant issues. Copies of the handouts and overhead transparencies from the workshop can be found in the administrative files for the project.

**DAY 1 - WEDNESDAY, NOVEMBER 5**

Debra Bryan of the Department of Energy (DOE) welcomed workshop participants. Kevin Coppersmith of Geomatrix then introduced the workshop, identifying the project's Methodology Development Team, describing the purpose and procedure for performing an expert elicitation, and summarizing how panel members were nominated and selected. He described the process and guidelines for the elicitations, what will be covered in the workshops, and the meetings of the expert panel. The members of the expert panel were asked to introduce themselves: Derek Elsworth, an expert in fluids in porous media, deformation of porous media, geothermal features, and dewatering of wells related to volcanism; John Gale, expert in the hydrogeology of fractured rock, two-phase (gas/liquid) flow, and effects at high temperatures; Roger Hart, expert in geomechanics, rock mechanics, and stress analysis for underground structures; Benjamin Ross, expert in physics, hydrodynamics, and coupled processes (including previous experience with Yucca Mountain through studies with EPRI); Robert Schechter, expert in chemical and petroleum engineering and colloid and interface science; and Yanis Yortsos, expert in chemical engineering, flow reaction in porous media, and steam injection for oil recovery.

Martha Pendleton, Woodward-Clyde Federal Services, then gave an overview of the Yucca Mountain project. She described the site and the work completed to date, noting a layout of the tunneling and locations of boreholes. She outlined the strategies for waste

containment and isolation based on interim performance guidance from DOE. She described plans for a viability assessment, final Environmental Impact Statement, site recommendation, and application for a license from the Nuclear Regulatory Commission by the year 2002. She highlighted the goals of the NFEE and how the expert elicitations fit into and support viability and performance assessments.

James Blink, Lawrence Livermore National Laboratories (LLNL), completed the introductory remarks by presenting a reference repository design and outlining a conceptual understanding of the evolution of repository processes over time. He provided design numbers: numbers and sizes of waste packages and drifts, locations in relation to rock types and groundwater, allowances for ventilation, and anticipated temperatures. He then outlined the anticipated performance of the waste packages, other engineered barriers, and the near-field and altered-zone environments over periods extending to 100,000 years.

After a short break, workshop participants reconvened to hear four overview descriptions of the site and project findings to date. The first, by Thomas Buscheck of LLNL, described work done to simulate thermal-hydrologic conditions in the near-field environment at the scale of the drifts. He discussed the duration of boiling in the drifts (which will last as long as 7000 years) and the modes of water contact on the canisters. The LLNL methodology utilizes both drift-scale and mountain-scale models of temperature and relative humidity at different times and locations for different waste package designs. They have found that the use of backfill would have a strong influence on both temperature and humidity. Bo Bodvarsson, Lawrence Berkeley National Laboratory (LBNL), gave the next talk, "Overview of Repository-Scale Thermohydrology Simulations." He described the geologic framework of Yucca Mountain, locations of perched water, and infiltration rates for the area, then presented LBNL's conceptual model of water, gas, heat, and chemical transport at Yucca Mountain and described thermohydrologic simulations conducted to date. Topics discussed included percolation flux, fracture and matrix flow, effects of faults and major features, effects of gas flow, effects of perched water, and temperature changes.

After a break for lunch, two more overview presentations were made. The first, by Ernest Hardin of LLNL, focused on coupled effects, the gradients and magnitudes of processes in the near field, and the interaction between the engineered barriers and surrounding rock. The extent of the altered zone, he noted, will depend on both thermohydrologic and thermochemical conditions. The next presentation, by Ralph Wagner of Woodward-Clyde Federal Services, was titled "Overview of In-Situ Thermal Testing at Yucca Mountain." Wagner described several scales for in-situ thermal tests at Yucca Mountain's Exploratory Studies Facility (EFS): a large-block test (about 40 square

meters); a single-heater test performed in a thermal alcove; and a drift-scale test that will test predicted versus actual isotherms through four years each of heating and cooling. The goals of all tests are to develop a better understanding of the coupled processes (thermal-mechanical-hydrological-chemical, or T-M-H-C). He discussed the history and evolution of the studies.

Next began a series of presentations on laboratory measurements of and experiments with material properties. The first talk, given by Nancy Brodsky of Sandia National Laboratories, focused on the thermal and mechanical properties of Yucca Mountain site materials. She described methods and results for laboratory tests of thermal conductivity (which is related to moisture content, temperature, and porosity), thermal expansion (at various temperatures and moisture contents), heat capacity (for various temperatures and moisture contents), unconfined strength and confined strength, changes in unconfined strength under various strain rates and constant stress, and mechanical properties of fractures at room and elevated temperatures.

After a short break, Lorraine Flint of the U.S. Geological Survey (USGS) discussed the laboratory tests her group has performed to identify the hydrologic properties of the rock matrix in the repository host rock and the effects of elevated temperature on the physical and hydrologic properties of the tuff matrix. Her group measured the hydrologic properties of rock units at the repository site with the goal of identifying unique hydrogeologic units for use in numerical models of flow. They have identified matrix properties for distinct hydrogeologic units that can be identified readily from borehole data. Flint noted that changes in parameters representing matrix capillarity can cause significant differences in calculated hydrologic response. The last talk of the day, by Brian Viani of LLNL, was titled "Integrated Testing." His laboratory studies are aimed at obtaining estimates of ways in which fluid composition and temperature affect sorption and radionuclide transport through the near field. There were no comments from observers, so the workshop adjourned for the day at 6 pm.

## **DAY 2 - THURSDAY, NOVEMBER 6, 1997**

The second day began with two more presentations on laboratory measurements of material properties for the near field at the Yucca Mountain site. William Glassley of LLNL discussed mineral alteration in the near field. He used results from the single-heater test at the ESF to help establish parameters for studies of the engineered barrier system (EBS). He identified hydrothermal processes as driving mineral alteration, and described several types of reactions that could be associated with boiling. Glassley's work leads him to conclude that mineral alteration will significantly modify properties along flow paths. Interaction among condensate, fracture, and matrix drives a chemical

"evolution," forming secondary minerals, modifying material properties along the flowpaths, and modifying fracture porosity. He found that the precipitate produced at the vaporization front may seal fractures: in their laboratory tests, about one-half of the porosity was filled by secondary minerals. He predicts a notable increase in porosity above and below the drifts.

Annemarie Meike, LLNL, gave the second talk of the day. She discussed the changes to be expected from materials introduced to the repository. Materials introduced to date include construction materials that range from water to diesel fuel and concrete to extruded polystyrene. These materials could introduce nutrients that would be useable by microbes. Microbes, which operate through extremely diverse metabolic modes, can dissolve metal, cement, and ceramic materials and can generate byproducts that will change the chemical parameters of the near field. By altering their environments, microbes could alter the permeability beneath the repository and produce changes in pH and water chemistry that would affect radionuclide transport. In addition, she said, colloids may derive from degradation of greases, wood, and other introduced organic matter such as grouts, cements, and shotcrete.

After a short break, the workshop addressed the next area: laboratory experiments of coupled thermal, hydrologic, and geochemical processes. Kevin Knauss of LLNL gave the first presentation, on physical and conceptual modeling of reactive transport experiments. His group has performed reactor experiments to study the dissolution and precipitation of the minerals found at Yucca Mountain. Experiments used a plug flow reactor to simulate reactive transport. They then compared experimental results with those from computational modeling of reactive transport. They found basic agreement between results, achieving qualitative validation of their modeling approach and identifying ways to refine both the physical and computational models. In the next presentation, Annemarie Meike continued her discussion of LLNL's laboratory studies of alteration of introduced materials, focusing in this talk on cementitious materials. Her group studied the concrete used in the invert of the ESF. Having identified stages in the evolution of concrete, they intend to tie those stages to the time history of environmental conditions in the potential repository. Among the factors to be considered: some components of concrete, when heated, become amorphous, affecting strength; other, mineralized components go through shrink-swell changes that may cause irreversible mechanical changes. After this presentation, workshop participants stopped for lunch.

After the lunch break, the workshop continued the discussion of laboratory experiments of coupled processes. Wunan Lin of LLNL began with a talk on fracture and matrix permeability at elevated temperatures. The laboratory tests he has participated in indicate that permeability of fractured samples decreases with time and drops rapidly at high

temperatures. Results suggest that a redistribution of calcite and silica is the mechanism for "healing" fractures. Lin described ongoing experiments to study how a small amount of flowing hot water affects fracture healing and future experiments on the effects of flowing steam and of alternate hot water/drying out. Stephen Blair, LLNL, gave the next presentation, which concerned ongoing multiple coupled process experiments at 0.5m scale. The experiments focus on coupled processes and behavior at elevated temperatures over long periods.

Jeff Roberts, LLNL, gave the next presentation, titled, "X-ray Radiography of Fracture Flow and Matrix Imbibition in Topopah Spring Tuff Under a Thermal Gradient." He described experiments using X-ray radiography to evaluate water content and to track its movement within a fractured sample of Yucca Mountain tuff. His group is studying the effect of thermal gradient, initial water content, type of fracture, and aperture. Their experiments varied the amount of water, the temperature, and other parameters. Noting that X-ray radiography permits the examination of active coupled processes, Roberts showed a video of a transient flow experiment.

After a short break, workshop participants returned to hear Timothy Kneafsey (LBNL) describe work that he and Karsten Pruess have done. His presentation, titled, "Liquid Flow in Fracture Models under Vaporizing Conditions," also included a video to demonstrate heat pipes and patterns of water and vapor flow. Kneafsey and Pruess have identified liquid flow occurring in films, intermittent rivulets, and continuous rivulets; identified rapid evaporation events; and noted that the region near a heat pipe is altered by the aperture structure.

The next four presentations concerned field experiments on coupled processes. Wunan Lin began the series with his second talk of the workshop, describing interim results from the single-heater test performed in the ESF. His group collected results for various boreholes at various distances from the heater using an automated data-collection system. They placed electrodes in four holes around the heater and measured moisture content using a neutron probe. After mapping changes in resistivity, they found a region of decreasing resistivity around the heater. They also studied changes in saturation, which they previously had simulated using various models. In the test, drying occurred around and above the heater; wetting occurred primarily below and to the sides of the heater; and some re-wetting occurred on cooling.

Several observers asked presenters technical questions regarding their presentations, then Kevin Coppersmith adjourned the workshop for the day.

**DAY 3 - FRIDAY, NOVEMBER 7**

Larry Costin, Sandia, opened the third day of the workshop with a continuation of the discussion of field experiments on coupled processes. He described thermomechanical results from the single-heater test at the ESF. His group used the tests to check field data against pre-test predictions of thermohydrologic and thermomechanical effects. They looked at alternative ways of modeling permeability, comparing measured permeabilities to those predicted by low- and high-permeability models. They obtained thermal expansion data and measurements of rock mass temperatures, displacements, modulus, and saturation. Costin's group found that conduction is the primary mode of heat transfer, and that large increases in rock mass modulus occurred at elevated temperatures. The predictions from their computational model compared well with data at first, but diverged after about 100 days. Yvonne Tsang, LBNL, gave the next presentation, also based on results from the single-heater test. She focused on thermal-hydrologic processes, again comparing simulations and predictions to field data. Her group used both passive and active monitoring to observe vaporization and condensation. Passive monitoring involved measurements of temperature, gas pressure, and relative humidity; active testing involved neutron logging and cross-hole radar tomography, plus electrical resistivity tomography and air permeability tests. Tsang's group found good agreement between data and three-dimensional simulations. They found heat conduction to dominate, but noted that more information is needed regarding hydrologic properties of the matrix and fractures.

Dale Wilder, LLNL, gave the last talk on field studies, describing interim results from the large-block test (LBT) at the ESF. He first described the objectives of the LBT: to study coupled processes, test instruments and techniques, and test proposed waste package materials. The block, heavily instrumented through both vertical and horizontal boreholes, received full-power heating until 10/06/97, after which power began to ramp down. Power will be turned off in January of 1998; cool-down is expected to be complete by August 1998. The initial state of the LBT was characterized—borehole cores were logged and samples tested, fractures mapped, and initial moisture content measured. Samples were tested for resistivity, porosity, and air permeability. The block was heated by five heaters, while moisture and heat losses were controlled and measured. Wilder's group measured liquid-phase saturation and water volume, then compared predicted and measured data.

After a short break, workshop participants returned to hear two presentations on drift seepage. The first, by Chin-Fu Tsang of LBNL, was titled, "Drift Seepage Calculations with Spatial Heterogeneity." Seepage of water into the drifts that hold the waste packages is important because water will affect the rates of package corrosion, waste mobilization,

and radionuclide transport. His group developed a model of the drifts based on data from the ESF (data on fractures, permeability, hydraulic parameters); performed both two- and three-dimensional simulations; and produced contours showing fracture continuum saturation at various depths and locations under various assumed conditions. They found it important to model the heterogeneity of the matrix to simulate seepage.

The second presentation on drift seepage, by John Nitao of LLNL, focused on seepage under altered conditions. He related drift seepage to percolation, and noted that current estimates of percolation are higher than originally thought and that fracture flow is recognized as more prevalent than previously thought. Nitao described seepage from percolation, condensation of water boiled from rock, and liquid films on waste packages produced by high relative humidity. He then described the available approaches to modeling flow in the fracture-matrix system: all flow in a single continuum; fractures modeled separately; or a combination of fracture and matrix continua. The code his group uses combines all three methods. Nitao described the way their three-dimensional model represents spatial heterogeneity using random fields randomly distributed. He presented calculation results at various times under pre- and post-emplacement conditions given variable saturation conditions with and without ventilation at various relative humidities and rates of percolation. Their conclusions: small amounts of seepage into drifts are expected at Yucca Mountain; filling fractures can inhibit seepage significantly; and condensate can form within the drift before the rock reaches the boiling point, after which it will stop until temperatures again decline below boiling. Nitao's presentation ended the technical descriptions for the workshop.

Returning to the task facing expert panel members, Robert Andrews of TRW Environmental Safety Systems Inc. described the role of the NFEE in supporting model abstractions for the total system performance assessment-viability assessment (TSPA-VA). He described the key issues to be addressed in the expert elicitations, focusing on the role of thermal hydrology and the effects of coupled processes (T-H-M or T-H-C) on thermal hydrology. He summarized what is known about the physical and chemical processes in the near field and the proposed make-up of the waste packages. He asked the experts to consider thermohydrologic effects at both the mountain and drift scales over time. Andrews referred to information (from reports that will be distributed to the expert panel) provided by the ongoing TSPA peer review and by the Nuclear Regulatory Commission, along with lists of the issues they consider important. He also identified important issues that surfaced at the workshop on thermohydrology held for the Yucca Mountain unsaturated zone expert elicitation. Mr. Andrews reviewed the reasons for having an expert elicitation (to quantify the uncertainty for incorporation into the TSPA); outlined what was expected in the elicitation (definition of key processes and properties, their temporal evolution, and uncertainty in that evolution); and highlighted some of the



properties of special importance and some observations that to date have been made about those properties.

Then Kevin Coppersmith outlined future plans and schedules for the NFEE project, took comments from observers, and adjourned the workshop.

**SUMMARY**  
**WORKSHOP ON ALTERNATIVE MODELS AND INTERPRETATIONS**  
**NEAR-FIELD/ALTERED ZONE-COUPLED EFFECTS**  
**EXPERT ELICITATION PROJECT**

**December 3 and 4, 1997**  
**Alexis Park Resort**  
**Las Vegas, Nevada**

The Workshop on Alternative Models and Interpretations was the second of three workshops to be conducted for the Near-Field/Altered Zone Coupled Effects Expert Elicitation (NFEE) for the Yucca Mountain project. The purposes of this workshop were to review the key issues and uncertainties associated with coupled effects in the near-field at Yucca Mountain; to present and discuss alternative models and interpretations related to the thermomechanical, thermohydrologic, and thermochemical aspects of the potential repository system; and to identify any additional data needed to conduct the elicitations. Copies of the handouts and overhead transparencies from the workshop can be found in the administrative files for the project.

**DAY 1 - WEDNESDAY, DECEMBER 3**

Kevin Coppersmith of Geomatrix Consultants introduced the workshop, outlining its purposes and reviewing the ground rules for the workshops, which focus on enabling the members of the expert panel to participate effectively in expert elicitation. He emphasized again the role of the experts as evaluators of various models and interpretations, rather than proponents of any particular approach.

Nicholas Francis, M&O/Sandia National Laboratories (SNL), gave the first presentation, defining the key issues surrounding coupled effects in the near-field. He distinguished between issues related to the thermal and the post-thermal periods. During the thermal period, the key issues of fracture porosity and permeability apply both near to and away from the emplacement drifts. Other issues concern the nature (extent and permanence) of changes to matrix properties. During the post-thermal period, key issues include the possibility of rockfalls into the drifts and potentially permanent changes to the hydrologic properties of Yucca Mountain. Francis discussed the application of and limitations on models of these changes. Noting that it is unlikely that a fully coupled thermal-hydrologic-mechanical-chemical (T-H-M-C) flow and transport model can be developed, he discussed ways in which the upcoming total system performance assessment (TSPA) for viability assessment (VA) can use information about the near-field to evaluate the

intensity, extent, and importance of changes to properties of the fractures and matrix and the uncertainty associated with thermal alterations. The discussion of key issues was continued by Ernest Hardin of M&O/Lawrence Livermore National Laboratory (LLNL), who gave a presentation titled, "Summary of Near-Field Environmental Conditions." He summarized the environmental changes expected to occur in the near-field, showing projections of ambient and mobilized fluxes and fluxes resulting from episodic flows. He showed projected changes in temperature and relative humidity based on stipulated conditions of drift layout, backfill, flux, and so forth. Hardin also showed projections of the evolution of pH, ion concentrations, and mechanical load and the period during which the waste packages would be susceptible to crevice corrosion.

The last general discussion of key issues was given by Chin-Fu Tsang of M&O/Lawrence Berkeley National Laboratory (LBNL). His presentation was titled, "A Discussion of Coupled T-H-M Processes Associated with a Nuclear Waste Repository" and he described the importance of coupled processes in fractured rock around a geologic nuclear waste repository over long periods. He presented a conceptual model of H-M coupled processes on a single fracture, then outlined coupled T-H-M processes through the stages of the repository's excavation, operation, and containment/isolation. Tsang went on to describe an international research project termed DECOVALEX, which is attempting to develop computer models of coupled processes and validate them against experimental data. The models studied combine thermal, hydrologic, and mechanical effects in geologic media as related to performance assessment of nuclear waste repositories. Among tests to support modeling of T-H-M effects in the near-field are some under way in Kamaishi, Japan. Tsang highlighted issues revealed by DECOVALEX and others surrounding the unsaturated system at Yucca Mountain, such as changes to fracture permeability and heterogeneity of the media. He described the thermal testing facility at Yucca Mountain's Exploratory Studies Facility (ESF), the Drift-Scale Test, and borehole data from liquid injections. Tsang also indicated data needed for site characterization and noted that the modeling must consider three stages corresponding to the three stages of repository development, but each stage would provide the next with more data and more sophisticated modeling.

Richard Nolting, M&O/Morrison-Knudsen Company, introduced the next two talks on drift-scale modeling of thermomechanical effects. He outlined the topics: thermal models, thermomechanical models, and results of numerical models. He detailed the plan of the drifts and the placement of packages in drifts. He gave preliminary property values (for density, porosity, thermal conductivity of rock, compressive and tensile strength of rock, and properties of the concrete or steel lining) for evaluating alternative designs. All these values, he noted, need to be verified. He also gave parameters for the waste packages (dimensions, waste content, and heat output) and average heat flux values for the

packages. Nolting also presented details on the thermal/mechanical properties of the rock units. Y. Sun, also of Morrison-Knudsen, continued the discussion by describing thermal (ANSYS) and thermomechanical (FLAC) computer models, their geometries and boundary conditions. He provided time histories of various factors, such as principal stresses, compressive stresses and strains, and temperature. All modeling, he noted, has been performed for dry rock mass.

After a short break, the workshop reconvened to hear F. Duan, also of Morrison-Knudsen, discuss the seismic analysis of rock mass response at the drift scale. He summarized results from models using the FLAC code for analysis of seismic loading of emplacement drifts, concluding that although seismic loading is noticeable, displacement would be less than 10 percent and therefore insignificant. He also showed results of UDEC modeling for multiple emplacement drifts, in particular the stresses on an unsupported drift under seismic loading. After Duan's presentation, workshop participants took a break for lunch.

After the lunch break, panel members returned to hear a presentation titled, "Modeling of T-H-M Effects in the Drift-Scale Test." The presentation, by Stephen Blair of M&O/Lawrence Livermore National Laboratory (LLNL), reviewed his group's development of a conceptual model of thermomechanical effects on permeability. He showed a schematic of the Drift-Scale Test at the Yucca Mountain ESF and projections of the temperature field at various times (using FLAC). He showed models of the stress field and summarized two- and three-dimensional stress-displacement calculations. Blair's group also simulated uniaxial compression tests and resulting crack development. They used FLAC3D, a three-dimensional finite-difference model for temperature, stress, and displacement calculation.

In his second presentation of the workshop, Nicholas Francis discussed analysis of coupled T-H-M effects. The key issues he is studying are whether mechanical changes to host rock will alter flow fields or predictions of state variables. He applied the two-dimensional thermomechanical model developed by Mack and others (1989) to simulate altered zones at discrete times and used one-dimensional TOUGH2 simulations (1) of unaltered ambient hydrologic properties and (2) altered conditions at discrete times. He showed zones of compression and tension predicted according to Mack and others (1989). Simulations for both the altered and unaltered near-field produced similar trends in liquid flow in fractures, liquid saturation, and temperatures.

Francis was followed by Thomas Buscheck (M&O/LLNL), who described thermal-hydrologic (T-H) simulations for analyzing the performance of the engineered barrier system (EBS). He gave a two-part presentation, the first part of which identified key issues related to developing a model of T-H behavior. Key issues include distribution of

the heat source (whether a point or line source); magnitude and spatial distribution of percolation flux; and the magnitude of capillary-driven matrix imbibition and wicking in fractures. He described properties used to model the Single-Heater Test and Large-Block Test at the ESF and the field and laboratory results used to calibrate model parameters. Buscheck has developed a thermal-hydrologic (T-H) abstraction methodology to provide a "detailed description of the T-H variables affecting EBS performance throughout the repository area" (for TSPA-VA). Buscheck then presented drift-scale results for the T-H model. The first part of his presentation ended with several conclusions: (1) The spatial and temporal extent of dryout, superheated conditions, and reduction in relative humidity are extremely sensitive to the magnitude of capillary-driven matrix imbibition; (2) It is important to use hydrologic parameter sets that produce values of the matrix imbibition diffusivity that are consistent with thermal tests in the field and with laboratory imbibition tests; and (3) The spatial and temporal extent of dryout, superheated conditions, and reduction in relative humidity are very sensitive to the distribution of percolation flux (when matrix imbibition does not limit dryout). Workshop participants took a short break after the first part of Buscheck's presentation.

After the break, Buscheck gave the second part of his presentation, titled, "Multi-Scale Model-Abstraction Method for Representing Variability in Thermal-Hydrological Conditions in the Repository." His method, designed to estimate near-field T-H conditions based on analysis of the reference design, incorporates a range of complementary T-H models at the mountain and drift scales. He described four models: a three-dimensional model of thermal conduction only, at the mountain scale; a two-dimensional model that describes thermal hydrology for a line heat source at the drift scale; a one-dimensional model that covers thermal conduction at the drift scale; and a three-dimensional model that applies to thermal conduction for discrete heat sources at the drift scale. The model abstraction methodology incorporates aspects of all the models to construct distributions of temperature and relative humidity and to determine the variability resulting from location within the repository and from waste package type and sequencing. Model results predict temperature and relative humidity at the drift wall and on the waste package as a function of variables such as location, infiltration flux, heat source distribution, backfill, and type of waste, using TSPA-VA parameter sets. Results indicate that temperature and relative humidity along drifts are very sensitive to local heating conditions and that the reduction of the gas-phase air-mass fraction depends strongly on the duration of boiling.

There were several questions for Buscheck from observers, for instance regarding properties and effectiveness of the backfill, after which the workshop adjourned for the day.

**DAY 2 - THURSDAY, DECEMBER 4, 1997**

The second day of the workshop focused on thermochemical modeling of the near-field. Thomas Wolery (M&O/LLNL) opened the topic by describing a chemical modeling code, EQ3/6, used for modeling the geochemistry of aqueous systems, including aqueous solutions, water/rock systems, and water/rock/waste systems. The code, which has been used by LLNL, LBNL, LANL, the USGS, and the PA organization, is being applied to several areas of the Yucca Mountain project. Wolery described the features of the program and compared program results with experimental results for hydrothermal interactions between the Topopah Springs tuff and J-13 water. He described solid-solution models and models that simulate cation exchange, comparing model results with experimental results. Current developments of EQ3/6 include improving the connection between EQ3/6 and TOUGH2, and updating the thermodynamic database.

Next, John Apps (M&O/LBNL) gave a presentation titled, "Modeling of Tuff-Water Interaction at Elevated Temperature." Knowing the composition of pore water, he said, is essential to understanding ambient conditions. His studies began as input to LBNL's modeling of the unsaturated zone. His group collected pore waters from different geologic units and analyzed their compositions. The process they used (a triaxial press) is ineffective on the welded tuffs in the middle of the stratigraphic section, so results from above and below must be interpolated. Apps showed plots of water chemistry at various depths. His very recent work involves EQ3 modeling of evaporation and condensation in the zone of boiling.

The third presentation of the day, given by Carl Steefel (University of South Florida), was titled, "Overview of Modeling of Coupled Reactive Transport Processes." He described the capabilities of the OS3D and GIMRT modeling codes he uses, such as the inclusion of multicomponent geochemical reactions; advective, dispersive, and diffusive transport; and multiple spatial dimensions. The codes can accommodate porosity-permeability feedback and temperature-dependent thermodynamics and mineral-fluid kinetics. Steefel went on to describe work performed with P. Lichtner of the Center for Nuclear Waste Regulatory Analyses (CNWRA), to apply the codes to near-field processes around a cementitious repository and to compare analytical and numerical solutions. Steefel described diffusion-reaction simulations with and without feedback of porosity change due to chemical reactions, and he discussed results of preliminary dual porosity simulations of fractures at Yucca Mountain. He described software developments in OS3D/GIMRT—capabilities added for handling intra-aqueous kinetic reactions (e.g., microbially mediated reactions) and for gas-phase diffusion.

A short break followed Steefel's presentation, after which William Glassley, LLNL, discussed simulating reactive transport on the drift scale. He emphasized (1) that the near-field studies define the starting point for studies of the engineered barrier system (EBS): important factors include the water composition and amount entering the EBS, the mineral alteration along flow paths out of the EBS, and the transformation of physical properties; and (2) that hydrothermal processes drive mineral alteration: formation of condensate leads to chemical conditions that are far from equilibrium; the extent and location of effects depend on design and operation. He described how thermal and hydrologic conditions may evolve as reactive transport modifies the physical system, then outlined the key parameters that define mineral alteration. He has performed reactive transport modeling with OS3D/GIMRT, and reaction path modeling with EQ3/6, concentrating on the processes within fractures. His group compared computed results with measurements from the Single Heater Test and Drift-Scale Test, checking the computed versus measured flow distance, water chemistry, and time evolution. His group found that preliminary two-dimensional simulations of drift-scale changes are consistent with one-dimensional fracture-flow models. The group also modeled changes in porosity and pH below the drift after one year of heating. The implications of their work: (1) precipitation at the vaporization front may seal fractures (a finding consistent with laboratory experiments); (2) mineral evolution during reactive transport modifies fracture porosity; and (3) there is a notable increase in porosity projected to occur above and below the drifts where condensate forms. After this presentation, workshop participants took a break for lunch.

The workshop reconvened after lunch with a talk by Peter Lichtner of CNWRA titled, "Modeling Coupled Thermal-Hydrologic-Chemical (T-H-C) Processes." He outlined important aspects of the near-field chemistry: salinity, pH, oxygen fugacity, mineral alteration, changes to porosity and permeability, and the influence of microbes. He then described MULTIFLO, a multiphase, multicomponent reactive transport model that can interface with METRA, a code that describes sequentially coupled mass and energy transport (two-phase fluid flow and heat flow), and GEM, which pertains to the reactive transport of aqueous, gaseous, and mineral species. Lichtner described the attributes of the METRA and GEM codes and their application to near-field conditions. He showed the MULTIFLO prediction of chloride enrichment and various mineral alterations, which depend on the surface area of minerals in fractures and matrix and on characteristic mineral dissolution times. His conclusions included: (1) near-field chemistry produced by a partly saturated environment differs significantly from that of a fully saturated environment; (2) in some cases, T-H-coupled models may provide reasonable estimates of increases in salinity; and (3) given high areal mass loading, the waste packages may be expected to be in contact with small amounts (drips, thin films) of highly saline fluid for relatively long periods depending on the rate of rewetting.

Next, George Zyvloski of M&O/Los Alamos National Laboratory (LANL) gave a presentation titled, "Near-Field Reactive Flow and Transport," based on work he has done with Bruce Robinson, also of LANL, and others. He described their modeling efforts and goals, which include ensuring model validity and producing a usable model for TSPA-VA. He described the approach taken and software employed. Their purpose was to predict the transport of  $^{237}\text{Np}$  through the unsaturated zone of Yucca Mountain as affected by hydrologic processes (infiltration rate, temperature, and stratigraphy of the unsaturated zone); reactive transport processes (advection, dispersion); and geochemical reaction (the dissolution of the radionuclide inventory and the aqueous speciation of  $^{237}\text{Np}$  and how it sorbs to zeolite minerals). They simulated a base case, then varied infiltration rates, pH, fracture or matrix domination of flow, and climate changes. Their results indicated that higher infiltration rates result in faster dissolution of the inventory and in larger peak fluxes at the water table. However, Zyvloski said, pH increases in the near-field due to  $\text{CO}_2$  degassing appear not to affect the zeolitic layers 150 meters from the repository.

After a brief break, the workshop reconvened to hear William Murphy of CNWRA discuss geochemical models of gas-water-rock interactions at the proposed repository. He described the differences in chemistry between water in fractures and in matrix, noting that many conclusions rest on water chemistry. Murphy discussed key concepts for geochemical modeling for the proposed repository: system components (calcite, feldspar, etc.); the natural system model (for example, that water recharge from the soil zone is saturated with calcite); and the nonisothermal model (in which temperature-time relations are derived from heat flow modeling, reaction progress-time relations are derived from kinetic modeling, etc.). Conclusions included: the transient thermal regime associated with high-level waste disposal requires geochemical models that relate time, temperature, and rates of chemical reactions; and modeling to date suggests that repository heating would cause alteration of feldspar to aluminosilicate minerals, precipitation of calcite, and increases in pH and in the concentrations of most other aqueous species except calcium.

The last speaker of the workshop, Eric Somenthal of LBNL, gave a presentation titled, "Preliminary Drift-Scale Thermo-Hydro-Chemical Modeling of Reaction-Transport Processes." After acknowledging his co-workers in the fields of modeling, geochemistry, and isotopic chemistry, he summarized important aspects of reaction-transport processes: the chemical modification of pore waters that may seep into drifts; mineral precipitation/dissolution that may modify permeability, porosity, and imbibition at fracture walls; and mineral species that may retard radionuclide transport in the unsaturated zone. He described the computer codes and models used and experiments



done to understand reaction-transport processes in the near-field, and the preliminary drift-scale T-H-C model developed. He showed simulated distributions around a heated drift of, among others, temperature, chloride, calcite in fractures and matrix after 2.5 months of heating. Dual permeability models yield strikingly different mineral dissolution/precipitation patterns and pore fluid chemistry in matrix versus fractures.

Kevin Coppersmith ended the workshop by outlining future plans and schedules for the NFEE project, emphasizing the importance of this expert elicitation because the base case for the TSPA-VA risk assessment currently does not include T-H-C coupled effects. This elicitation provides the opportunity for identifying alternative models and parameters, he said, possibly even ranking the importance of T-H-C processes, which likely will vary over time. Both the changes over time and changes within different areas (boiling versus condensation zones, etc.) are important to understanding this problem, which, he emphasized, requires a multidisciplinary approach. Coppersmith reviewed the purpose of Workshop 3, which will be a forum for expert panel members to present and consider their preliminary interpretations, receiving feedback from other panel members. After the elicitations, additional opportunities will be provided for review of assessments and documentation of the process. There were no comments from observers, so Coppersmith thanked all speakers and adjourned the workshop.

## **SUMMARY FIELD TRIP TO YUCCA MOUNTAIN**

### **NEAR-FIELD/ALTERED ZONE COUPLED EFFECTS EXPERT ELICITATION PROJECT**

**December 5, 1997**

The field trip to Yucca Mountain and the surrounding region was organized to enable the NFEE expert panel members to observe the general setting of Yucca Mountain, visit the Exploratory Studies Facility (ESF) tunnel, and the locations of the major heater tests. The primary goal of the field trip was to provide expert panel members with an opportunity to observe and discuss with the principal investigators the tests that are being conducted to provide a more in-depth understanding of the coupled processes anticipated in the rock mass surrounding the proposed repository. The field trip was led by YMP principal investigators Stephen Beason (ESF overview), Moon Lee and Mark Peters (Single Heater Test and Drift Scale Test), and Dwayne Chestnut (Large Block Test). The informal atmosphere and small size of the group allowed extensive debate and discussion.

#### **Exploratory Studies Facility**

The group entered the ESF through the South Portal via a man-train. The group observed fracture patterns and features such as faults within the tunnel, and learned how fracture data were collected and compiled as part of the detailed ESF line survey. The group walked into Alcove 5, the thermal test facility alcove. The Single Heater Test was visited, and the purposes, test apparatus, and status and results obtained to date for the test were described and discussed. A focus of the discussion was the evidence for the movement and accumulation of moisture during heat-up. The group then walked farther into the alcove to observe the Drift Scale Test, which had commenced testing two days previously on December 3. The characteristics of this large-scale test, which is planned to run for eight years, were also discussed.

#### **Yucca Mountain Crest**

After leaving the ESF, the group traveled to the crest of Yucca Mountain. The geography and geology of the region were summarized, including the location of major landforms, the stratigraphy of the volcanic tuffs comprising the repository horizon, major fault zones and structural features, infiltration mechanisms and their spatial variability, and the regional groundwater flow pattern.

### **Large Block Test**

The group visited the location of the Large Block Test. The apparatus used in this heater test, and the results of the test obtained to date were described. Discussion centered around the possible evidence for the development of heat pipes, instabilities in the thermal and hydrologic system, possible permeability changes due to heating, and the applicability of the test results to understanding thermal, hydrologic, and mechanical behavior at Yucca Mountain.

Following this discussion, the field trip ended, and the group returned to Las Vegas.

**SUMMARY**  
**WORKSHOP ON PRELIMINARY INTERPRETATIONS**  
**NEAR-FIELD/ALTERED ZONE COUPLED EFFECTS**  
**EXPERT ELICITATION PROJECT**

January 6-7, 1998  
Embassy Suites  
South San Francisco, California

The Workshop on Preliminary Interpretations was the last of three workshops to be conducted for the Near-Field/Altered Zone Coupled Effects Expert Elicitation (NFEE) for the Yucca Mountain project. The purposes of this workshop were to provide an opportunity for the experts to present and discuss their preliminary interpretations and uncertainties regarding issues key to coupled effects in the near field/altered zone; to provide the experts with feedback from their colleagues on the panel regarding their preliminary interpretations before the elicitation sessions; and to provide the experts with elicitation training. For each of six key issues, two experts presented their preliminary interpretations, after which all of the experts discussed the issue. The focus was on understanding the interpretations, their technical bases, consistency with data, and expression of uncertainty. Copies of the handouts and overhead transparencies from the workshop can be found in the administrative files for the project.

**DAY 1 - TUESDAY, JANUARY 6**

Kevin Coppersmith of Geomatrix Consultants welcomed workshop participants and introduced Peter Morris of Applied Decision Analysis, Inc., member of the project's Methodology Development Team and specialist in decision analysis, who provided elicitation training. Morris spent the morning discussing using probabilities to quantify uncertainty, representing and manipulating probabilities, and assessing probabilities. Probability, he said, is a formal quantification of uncertainty, and probabilities can be assessed either objectively (if the uncertainty pertains to a property of the physical world) or subjectively (if the uncertainty is a degree of belief about the real world). A probability assessment can be viewed as a qualitative assessment of a person's knowledge. Morris reviewed the terminology and calculations used in probabilistic analysis, defining probability density functions, cumulative probability distributions, and expected values. He went on to discuss quantifying uncertainty with probability and using probabilities to

support decision-making. He also described the motivational and cognitive biases that can creep into probability assessments. He then described the six-phase process of probability assessment and the technique of aggregating expert assessments. After Morris's training, workshop participants took a break for lunch.

After lunch, Coppersmith reviewed the ground rules and purposes of the workshop, which are geared toward enabling the members of the expert panel to undergo effective elicitations. He emphasized the need for each expert to be able to re-examine his thinking in light of others' interpretations. He ended by reviewing the schedule for the NFEE, noting the opportunities for feedback and revision.

Then Ernest Hardin (Lawrence Livermore National Laboratory) summarized why and which coupled effects are likely to be significant at the proposed Yucca Mountain repository. He outlined some of the questions surrounding thermal mechanical (TM), thermal hydrologic mechanical (THM), and thermal hydrologic chemical (THC) coupled effects. The experts, he said, are being asked to assess multiply-coupled effects on the mechanical stability of the near-field zone; on fracture porosity and permeability above the emplacement drifts; and on the porosity and permeability of fracture pathways below the drifts. Hardin directed experts in how best to address coupled effects with the tools available to provide useful inputs to the performance assessment group. After Hardin's presentation, Coppersmith reiterated that the performance assessment group needs certain inputs formulated in specific ways, although those who have worked on characterizing near-field conditions may approach the problem differently.

Next began the experts' presentations of their preliminary interpretations. Derek Elsworth gave the first of two presentations regarding the mechanical stability of the host rock in the near-field/alterd zone. He reviewed the available data and the drift- and mountain-scale models being considered for representing TM issues. He described the anticipated magnitude of thermal stress changes at the drift scale and for the package liners, noting the maximum stresses predicted to occur at maximum drift temperatures. He described the potential for developing wedges and linear creep. He described post-thermal behavior and the possibility of seismicity, either natural or induced by mining or by thermal stresses. Elsworth provided his preliminary conclusions and uncertainties. Stability problems, he believes, will be greatest during the thermal period, when the concrete liners will be especially stressed. He discussed alternative support methods such as rock bolts, and alternative designs such as use of concrete shells and backfill. His uncertainties focus on the properties of the liners and the rock mass.

There was a short break after Elsworth's presentation, after which Roger Hart gave the second preliminary interpretation regarding mechanical stability issues. Hart provided a

preliminary definition of mechanical stability as it relates to properties of the host rock and of the liner. He believes that the Single-Heater Test (SHT) at Yucca Mountain provides the best available data for assessing properties. He looked at data from specific locations of the SHT and estimated properties based on data reported in the literature. Hart concluded that the thermal numbers reported seem reasonable, although he believes that a higher thermal expansion coefficient for the rock mass is indicated from three-dimensional thermoelastic analysis than is reported for the SHT. In addition, he noted that the thermal expansion coefficient for the rock mass may be influenced by localized joint slip. If joint slip occurs and the joint dilates, he said, fracture permeability may increase, an effect that may explain the surface displacement observed at two locations and the water flow observed at two boreholes in the SHT.

The next issue to be examined was the impact of thermal loading on fracture porosity and permeability. First John Gale gave his preliminary interpretation. He reviewed what is known of conditions in the drifts and the bases for his interpretation. He discussed the effect of thermal expansion and the thermal loading that is anticipated at the proposed repository. Gale went on to describe a conceptual model of the fractures and matrix. He showed estimates of apertures, the aperture being the control on fracture stiffness and saturation levels within a fracture. He outlined the effects of thermal expansion and anticipated thermal loading. Gale expects all three modes of fracture displacement: dilation, closure, and shear. He also examined plane strain boundary conditions, offering his preferred interpretation that change caused by mechanical closure is permanent. Regarding plane strain and new fractures, Gale expects increases in local fracture porosity and permeability. He expressed uncertainty about the applicability of available data to other scales.

The second preliminary interpretation of the effects of thermal loading on fracture porosity and permeability was given by Yanis Yortsos. He described the key effects of thermal load at Yucca Mountain, noting which effects were reversible and which irreversible. He described TM effects at Yucca Mountain in general, on the mechanical aperture of a single fracture, on the hydraulic aperture/single-phase permeability of a fracture, and on other transport properties of a fracture. Yortsos predicts that regions of significantly reduced permeability will be produced in the near field. He predicts fracture opening above the repository (within the range of natural variability). The scarcity of data, he said, makes it difficult to reduce the uncertainty that surrounds the TM effect. Yortsos summarized his preliminary interpretation as follows. (1) Thermal stresses in the near field will decrease mechanical fracture aperture. (2) There is an expected concomitant decrease in hydraulic aperture, hence fracture permeability (but not below a "residual" value), and a concomitant increase in fracture capillary pressure. (3) The variation falls within the range of natural heterogeneity, although restricted to a narrower

range of smaller values (by one to two orders of magnitude). Uncertainty still exists regarding this effect. (4) The effect is likely to lead to smaller natural convection, higher repository temperature, and shorter heat pipes.

Derek Elsworth then gave a short presentation on the thermal loading topic. He referred to continuum approaches to changes in permeability. These approaches can relate changes in strain in the block to changes in fracture apertures, controlled by the variation in stiffness of the materials. This work takes data from the SHT and an LBNL Niche-3650 study regarding changes around a borehole and applies it to changes around a drift. This work indicates that the affected zones are small—perhaps 10 meters around a drift—and within these zones permeability can change by a factor of two.

After this discussion, observers offered comments. Chin-Fu-Tsang said he liked Elsworth's approach, then made a suggestion regarding measurements of permeability and fracture orientations. There was also a general discussion regarding slippage on joints. The workshop was then adjourned for the day.

## **DAY 2 - WEDNESDAY, JANUARY 7**

The second day of the workshop opened with two preliminary interpretations regarding the impact of dissolution, precipitation, and mineral alteration on fracture porosity and permeability. Ben Ross gave the first interpretation, finding enormous uncertainties regarding the coupled effect of heat transfer and fluid flow. He described three possible heat transfer regimes: one dominated by conduction; one controlled by convection and conduction; and a heat pipe regime. Whether convection may be important to heat transfer is determined, Ross said, by the bulk permeability of the rock mass. There is a threshold at which permeability will activate, but it is uncertain whether the bulk permeability of the Yucca Mountain welded tuff exceeds that threshold, except for fault zones, where it seems to. Many uncertainties surround the role of convection, which is not well addressed by modeling to date, Ross said. The consequences of convection, should it occur, are (1) a greater temperature difference between the center and rim of the repository, and (2) more water above the repository, which eventually will flow down. Ross then examined a heat pipe regime, noted the uncertainties and modeling associated with it, and looked at interactions between convective gas flow and heat pipes. He concluded that the hydrothermal system itself is complex and difficult to predict. Also, heterogeneities in the system add to the complexity for direct assessments. Estimating the uncertainty in each component of the system and synthesizing these uncertainties into an overall uncertainty of water movement is unlikely to be a fruitful approach, Ross said. He

said it might be better to elicit the quantities of interest directly—how many wet packages there are, what the temperature is, etc.

Next Robert Schechter presented the second preliminary interpretation of the impact of dissolution, precipitation, and mineral alteration on fracture porosity and permeability. He believes that much uncertainty derives from complex issues related to the vaporization and condensation processes over an extended period in the proposed repository. Schechter listed six of the complex processes related to vaporization and condensation of pore waters resulting from the heat generated by the waste deposited in the drift. Any or all of these processes may alter permeability in the near field and the quantity of the seepage into the drift. He looked at etch patterns obtained by researchers in the oil industry. The etch pattern produced in laboratory experiments in which acid was injected into rock is a single preferred flow path. Oil industry studies provide no evidence that fracture permeability decreases as a result of dissolution of carbonate from the fracture surface; in fact, it increases. Schechter believes the dissolution of minerals will increase fracture permeability at Yucca Mountain; permeability may decrease because fractures become clogged with colloidal particles. He went on to discuss the reduction in permeability caused by injections of fresh water—again using oil industry experience. Fracture permeability decreased when condensation occurred. Colloidal particles became trapped, but the use of salt water restored the original permeability.

After the break, the experts returned to hear two preliminary interpretations of multiply-coupled effects from thermal, mechanical, and chemical (TMC) processes on mechanical stability of the drifts. John Gale was first to present his preliminary interpretation of the issue, which he said relies on TMC data reported by Wunan Lin at NREE Workshop 1. He concluded that permeability changes with changes in confining pressure and temperature. Pore space evolves over time because of stress and fluid dissolution effects. After a metastable equilibrium is established, there is an increase in load due to TM effects, and ultimately a new metastable equilibrium is established. There is evidence of changes to fluid chemistry, he said, but the uncertainty is high because the available data sets do not give good information on TMC. He showed a graph for the transmissivity of a concrete sample over time and other graphs of transmissivity over time for N<sub>2</sub> degassing at different stress values. Profile sections made through samples after shear failure demonstrate that there is a TMC response by the rock. Still, he concluded, the dataset is small.

Roger Hart gave his second presentation of the workshop, offering the second preliminary interpretation of multiply-coupled TMC effects on mechanical stability, focusing on the mechanical stability of the drift. Clearly, he said, there are major uncertainties in the data regarding mechanical stability. He based his preliminary



interpretation on the assumption that localized rock joint slip controls mechanical stability, then addressed the question, "How does thermal loading affect this stability?" He first examined results of modeling with the computer program UDEC (Version 3.0): when heat was applied from below initial small failures, stresses increased and rock blocks began to move, demonstrating the coupling of heating with mechanical issues. Hart described his group's efforts to examine a URL tunnel that developed notching within 12 to 24 hours after the initial, circular, carefully mined opening. The need for a different approach to modeling responses to a high stress regime led to the so-called particle flow code (PFC) model. Hart described efforts to develop and verify this numerical model for predicting excavation-induced rock-mass damage and long-term strength. The model is designed to incorporate precracking ahead of the advancing tunnel face, stress corrosion, and thermal loading. He described the model's capabilities and conclusions derived from the first three phases of model development. The workshop took a break for lunch after Hart's presentation.

After lunch, participants returned to hear two preliminary interpretations regarding coupled effects from dissolution, alteration, and thermal and mechanical processes on the porosity, permeability, and mechanical stability of fracture pathways above the emplacement drifts, in pillars between drifts, and below the drifts. Ben Ross gave the first presentation. He discussed his diagram of significant influences, referring to the influences as "straw men" that are based on the assumption that Yucca Mountain offers well-drained conditions and that the mountain-scale convection and heat pipes described in his first presentation apply. He concluded that the uncertainties about the mechanisms of fluid flow are so great that a fairly large change in a parameter would not add significantly to the uncertainty. Thus the focus needs to be on potential changes in flow parameters so large that they change the nature of the fluid flow or parameters which, if moderately changed from measurable values, will change the flow regime. The only TM or TC processes that contribute significantly to uncertainty in fluid flow or temperature is the possible formation of an impervious caprock by precipitation of dissolved minerals, or the possible thermal mechanical enhancement of gas permeability.

Yanis Yortsos gave his second presentation of the workshop, focusing on the same issue as Hart, but emphasizing coupled TM and TC effects on permeability. The key effects of thermal load he had discussed the previous day. He reviewed the effect of thermal load on chemical alteration and the composition of chemicals at Yucca Mountain. The effect of chemical dissolution-precipitation under applied stress will differ in the matrix and in fractures, he said. Yortsos considers the effect of thermal load on chemical alteration through evaporation in the matrix to be insignificant. He sees TMC coupling as most important in fractures because of condensate flux. He expects fracture healing, the primary effect of TMC coupling, to occur in heat pipes or around the repository and

believes it could reduce permeability permanently in those areas. He regards the healing as a gradual filling in of areas, rather than a process that takes the form of fingering. Yortsos outlined implications a reduction in permeability would have for repository performance: (1) an increase in gas pressure near the repository; (2) a reduction in natural convection; (3) a reduction in the length of heat pipes; (4) higher and more symmetric profiles for temperature; and (5) achievement of an equilibrium state in which reduced permeability creates less heat pipe activity, which mitigates further reductions in permeability. Workshop participants took a short break after this presentation.

When the workshop reconvened, participants heard two preliminary interpretations of the final issue to be discussed: the durability of fracture porosity and permeability changes caused by dissolution and precipitation, or by mineral alteration, as the rock cools. Derek Elsworth was first to give his preliminary interpretation, focusing on thermomechanical changes during the cool-down period. He identified three mechanisms involved in THC changes to permeability: the creation of hyperalkaline fluids, dissolution of  $\text{SiO}_2$ , and pressure solution. Elsworth described conceptual stress changes on the mountain and drift scales during different thermal periods, including the post-thermal period. He described stress changes due to cooling, emphasizing the importance of stress paths and hysteresis. In the cool-down process, it is assumed that there is a large volume of water above the repository that enters as the temperature drops. The mechanical behavior (TM calculations) of the rock mass during cool-down is better constrained than are the THC conditions of initial porosity. Thus calculations of TM effects in the early thermal period are more dependable; there even are some large-scale data available. But because initial conditions are not well understood, TM effects in the later periods are not well understood.

Robert Schechter gave his second presentation, the last of the workshop and the last one on the durability of fracture porosity and permeability changes caused by dissolution and precipitation, or by mineral alteration, as the host rock cools. He made three comments based on information presented in previous workshops. First, he said, the anticipated  $\text{CO}_2$  concentration in water is higher than it should be. Then, that the chemistry of water in pores is not the same as in fractures. He noted that, based on Henry's constant, the quality of water will be affected as the dried-out zone is re-invaded by water. Henry's constant for  $\text{CO}_2$  absorption is increased by 20 percent in water contained in a partly saturated tuff compared to its absorption in bulk water. Increased  $\text{CO}_2$  absorption can be expected to alter mineral solubility. In conclusion, he noted that we cannot model everything, for instance the Liesegang rings that form in supersaturated solutions. Strange spatial patterns of precipitates have been observed from diffusion occurring in gels; similarly strange patterns could result from advection and mineral dissolution. He identified this as one of the complex issues that have not been studied; nor has a way to model it been

developed. He also mentioned wettability and the possibility that a hydrophobic system might develop. The very process of heating rock near the drifts may alter water wettability. If the wettability of the matrix is altered, Schechter noted, the rate of water imbibition from the fractures into the matrix also will be altered.

A general discussion of the issues followed Schechter's presentation. John Gale referred to a viewgraph on the scales of interest and the three different stress loading conditions (ambient, peak thermal, and cooling). Expert panel members decided to define spatial and temporal conditions that all experts will use so that effects can be described in uniform temperature steps.

Kevin Coppersmith referred the experts to the list of nine questions discussed in the previous workshop that they are to consider prior to and during the elicitations. He also outlined the schedule for the elicitations and the feedback, review, and documentation steps that follow them. Because there were no comments from observers, Coppersmith thanked all who presented their preliminary interpretations and adjourned the workshop.

**APPENDIX D**

**ELICITATION SUMMARIES**

## TABLE OF CONTENTS

Derek Elsworth

John E. Gale

Roger D. Hart

Benjamin Ross

Robert S. Schechter

Yanis Yortsos

## **ELICITATION SUMMARY**

### **DEREK ELSWORTH**

#### **OVERALL PROCESSES**

Changes in permeability due to thermal, mechanical, and chemical (TMC) influences are likely to be important to the hydrology (H) of Yucca Mountain. Changes in bulk fracture permeabilities are most important in controlling dry-out and reflux. Changes in matrix permeability are important in the sequestering of condensate. Mountain-scale permeability changes from T(H)M and THC modes are of similar order and largely reinforce behaviors. Stresses developed in the thermal period will decrease vertical permeabilities and increase horizontal permeabilities, switching the dominant regional permeability from vertical to horizontal and potentially suppressing the development of unthrottled convective energy transfer. Chemical dissolution products will coat fracture surfaces, reducing imbibition and recirculating larger volumes of reflux.

Key uncertainties surround permeability changes at the scales of interest, which range from the drift to the mountain scale. The processes that control mechanical changes in permeability are reasonably understood, and anticipated form, distribution, and ranges of magnitude are reasonably constrained. Analogous chemical processes are less well understood, not only the processes but also the sense of permeability change. The highest uncertainty surrounds these chemical processes.

TM drift stability is more definable than many of the hydraulic processes. The growth of liner stresses will mirror liner temperatures, peaking in the definable short term, with drift survivability controlled largely by liner durability. The timing of drift collapse will be modulated by loss of the liner. Drift stability, in the early thermal regime, may be maximized by adopting readily implemented design measures.

## THERMAL-MECHANICAL (TM) EFFECTS (DRIFT STABILITY)

Mechanical stability can be viewed at two scales, the drift scale and the mountain scale. At the mountain scale, natural seismicity can occur and lead to instability at any time. During the pre-thermal and early thermal periods, mechanical rock bursts are unlikely because the anticipated excavation-induced drift-local stresses are relatively minor (see following). During the late thermal period and cooldown, minor thermal rock bursts or induced seismicity may affect the stability of the drifts and the condensate zone. By this time, the failed drifts are expected to have reached equilibrium, with little further potential for collapse. Seismically induced reflux from disturbance of the overlaying condensate zone depends on the relative volumes laterally diverted and those held in the matrix and fracture system. Reflux volumes potentially released from the matrix or fractures under anticipated stress drops, or from the fracture system by changes in capillary characteristics, should be no more significant than those already in circulation.

Thermally induced stresses, which in turn affect drift stability, and feedbacks on evolving thermal, hydraulic, and chemical fields are controlled by a small set of rock mass parameters. Key parameters are the coefficient of thermal expansion,  $\alpha_m$ , deformation modulus,  $E_m$ , Poisson ratio,  $\nu_m$ , and the form and magnitude of the induced temperature field,  $T_r$ . Importantly, these parameters must be defined at the scale of the rock mass, to account for scale effects. Data from the Single Heater Test at Yucca Mountain (presented by L. Costin at NFEE Workshop 1) provide predictions for response at the scale of one to a few meters. Estimated rock mass thermal expansion coefficients (L. Costin, NFEE Workshop 1),  $\alpha_m$ , are close to laboratory-measured magnitudes (presentation by N. Brodsky at NFEE Workshop 1), on the order of  $5 \mu\epsilon/^\circ\text{C}$ , and Poisson ratios have a small and predictable range. The greatest scale effect is for mass modulus,  $E_m$ , related to intact modulus,  $E_r$ , through a reduction coefficient, as  $R_m = E_m/E_r$ . For the lower TSw2 unit, intact moduli are on the order  $E_r = 25$  to  $40$  Giga Pascals (GPa) with a porosity of about 10 percent. Borehole jack evaluations of modulus ( $E_m$ ) in the SHT are in the range 3 to 6 GPa at ambient temperatures and 6 to 20 GPa under maximum thermal loading ( $145^\circ\text{C}$ ), corresponding to  $R_m$  magnitudes in the range 0.1 to 0.5. Independent confirmation of

these data is provided by laboratory testing of a large block (S. Blair at NFEE Workshop 1) with  $E_r$  in the range 4 to 6 GPa ( $R_m = 0.1$  to 0.25), and from the rock mass classification studies (Pye et al., presentation at NFEE Workshop 2). Rock mass rating values from the TSw2 unit, along the course of the Exploratory Studies Facility (ESF), are in the range 45 to 65, excluding the upper and lower 10 percentiles. These values correspond to  $R_m$  magnitudes (Nicholson and Bieniawski, 1990) in the range 0.1 to 0.3, yielding three independent corroborations of  $R_m$  that impart some degree of confidence in the use of these magnitudes for preliminary estimates of TM and TMH response at Yucca Mountain. Modulus reduction magnitudes,  $R_m$ , are rock quality and stress dependent, the upper magnitudes of the 0.1 to 0.5 range being applicable for "stiffened" conditions likely at temperatures of the order of 160°C.

### Mountain Scale

Thermal-mechanical response at the mountain scale depends on the lateral constraint applied to the external boundaries of the repository block as it heats. If the block is unrestrained laterally, expansive displacements will reach a maximum, resulting in horizontal shear and vertical doming above the repository, but stresses will remain close to ambient. If the block is laterally restrained, horizontal stresses will build to a maximum, but overlying shear will be minimized. Response will, in reality, be a mixture of these models, most closely representing full restraint in the center of the repository block, and unrestrained toward the periphery. This understanding enables the response to be bounded by order-of-magnitude estimates.

The thermal stress regime will evolve following emplacement of high-level waste. Initial response will be dominated by conductive heat transfer outward from the drift wall. Based on a thermal diffusivity in the range of 28 m<sup>2</sup>/yr, the thermal aureoles around the drifts will penetrate about five drift radii in 3 years and coalesce in the ensuing 50 years and beyond to form a contiguous heated block, perhaps 200 m deep. Assuming full lateral (but not vertical) restraint, the magnitude of induced lateral stress,  $s_H$ , may be estimated as



$s_H = \frac{\alpha_M (E_R R_m) \Delta T}{(1 - \nu_M)}$ , yielding  $s_H = 3$  to 10 MPa, for a temperature rise from 25° to

160°C, and using the previous data from the SHT. This effect essentially would rotate initial field stresses from the maximum stress acting vertically, with  $s_v:s_H$  initially as 7:3.5 MPa, to the maximum stress acting horizontally, with 7:13.5 MPa. The observed "stiffening" of rock mass moduli at higher temperatures (see SHT results) may inflate these estimates of stress increase by perhaps 20 to 80 percent, resulting in upper bound horizontal stresses of the order of 20 MPa. This transition from vertically dominant (2:1) to horizontally dominant (1:2+) mountain-scale stress regimes would be largely reversible on cooling. Anticipated doming displacements for a 200-m-thick block, subject to the same temperature rise, are on the order of 0.1 to 0.15 m.

Although mapping data from the ESF (Pye et al., NFEE Workshop 2) and TM data from the SHT suggest that these mechanical properties are broadly applicable to the TSw2 unit, variations in TM properties in units beyond this may produce different induced stress magnitudes. Specifically, mismatches in mass thermal expansion coefficients,  $\alpha_M$ , will increase the potential for horizontal shear along sub-horizontal lithologic boundaries.

### Drift Scale

The response of the drift is controlled by the separate or combined response of the rock mass and liner to thermally induced loads. These loads are controlled by mechanical interactions and, in turn, modulated by certain rock mass parameters. The important parameters are identified in Appendix 1 and referenced in the following discussion.

**Unlined response.** Initially, at ambient temperatures, there will be mild compression in the roof and floor of the drift. The largest stresses will be in the drift wall. Intact rock compressive strengths on the order of 100 MPa, and rock mass strengths perhaps an order of magnitude lower than this, obviate significant ground control problems under ambient conditions. This conclusion is clear from ESF studies.

Stresses: With heating from the drift, the radial, and particularly the tangential, stresses will increase. The magnitude of stress increase is proportional to the parameter

$$\Delta s_H \approx \Delta \sigma_\theta \approx \frac{\alpha_M (E_R R_m) \Delta T}{(1 - \nu_M)} \quad (\text{see Appendix 1}), \text{ describing the principal dependencies.}$$

Of these parameters, the thermal expansion coefficient,  $\alpha_M$ , Poisson ratio,  $\nu_M$ , and conductive temperature change,  $T_x$ , are most robust; the mass modulus,  $E_M = E_R R_m$ , and its spatial variability, are more speculative. Confirmatory data at relevant scales and temperatures will be available from the Drift Scale Test.

In the very early thermal period (1 to 5 years), compressive tangential stresses will develop in the drift wall, controlled by the thermal loading and TM parameters. The induced stresses will be approximately radially symmetric around the drifts before the coalescence of the thermal aureoles between drifts. For a temperature rise of 135°C, maximum induced drift wall stresses will be on the order of 3 to 10 MPa, and comparative to anticipated rock mass strengths, which are in the range of 10 MPa. Scaling and spalling, in the absence of ground support, are likely. The release and sliding of unfavorably oriented blocks, unrestrained by bolting or other support, also is likely.

At the thermal maximum, there will be high roof and floor stresses, as the major principal field stress rotates from the vertical to the horizontal. For a resulting horizontal field stress of 14 MPa that is double the vertical stress, crown and springline stress concentrations would be about 35 and 7 MPa, respectively. This estimate assumes a circular-section drift. Although no data are available for the TSw2 unit, mass strengths are estimated in the range 10 to 30 MPa for fair to good rock, suggesting that stresses are sufficiently high to result in moderate spalling from the roof and springline.

Convergence: The closure or convergence of the drift wall, assuming an unlined drift, will directly follow the drift wall temperature. This effect will reflect the relatively rapid thermal communication between adjacent drifts, which will produce a largely uniform thermal field in the drift pillar. Thus, as temperatures rise from 25° to 160°C, the vertical extension and horizontal closure of the drift will mirror closely the temperature change at

the drift wall (R. Nolting et al., NFEE Workshop 2). Importantly, the displacement behavior is conditioned by the thermal expansion coefficient and Poisson ratio of the rock mass alone, without significant dependence on the mass modulus, as apparent in Appendix 1. Correspondingly, because these parameters are considered relatively robust, convergence estimates will reflect this assurance.

The asymmetry of convergence will occur in response to lateral restraint from the adjacent drift geometry. The vertical extension of the drift will approximate the horizontal closure. This behavior conserves the cross-sectional area of the drift with deformation and is a manifestation of the zero-convergence response anticipated for a single drift that is not constrained laterally (see Appendix 1). Back-of-the-envelope estimates of drift convergence are confirmed by more sophisticated calculations (Nolting et al., NFEE Workshop 2) that define convergence of about  $\pm 8$  to 10 mm, irrespective of a fourfold increase in the rock mass modulus,  $E_m$ , from 6 to 23 GPa.

**Liner response.** Where a liner is placed in intimate contact with the drift wall, ground reaction stresses will build as the rock mass marginally loosens. The observed fair to good quality of the rock mass in the TSw2 unit suggests that these ambient loads will be low to moderate and readily accommodated in liner design, fabrication, and installation. With increasing temperature in the drift, additional compressive thermal stresses will develop in the liner. For a solitary lined drift, heated from ambient temperature, the liner and ground reaction stresses may be approximated (see Appendix 1) and used as an analog to define anticipated response of a multiple drift system. The key results from this are repeated here from Appendix 1.

1. Thermal liner stresses,  $\sigma_\theta$ , are controlled primarily by the composite liner properties of modulus,  $E_L$ , Poisson ratio,  $\nu_L$ , thermal expansion coefficient,  $\alpha_L$ , and liner thickness,  $w$ . These parameters are controllable, to some degree, during design and fabrication, by means that include compressible lagging or blocking, backfill, or compressible joints to control the indeterminate influence of liner creep, and thereby the magnitude of thermally induced stresses.

2. There is only weak dependence of liner stresses on the rock mass parameters of modulus and Poisson ratio.
3. Liner thermal stresses are surprisingly independent of the coefficient of thermal expansion of the rock mass,  $\alpha_r$ , depending only on the instantaneous liner temperature differential above ambient,  $T_L$ .

In the evaluation of potential drift stability, the most significant aspects are that liner behavior depends largely on properties of the liner, not the rock mass, and that liner stresses will largely mirror the drift wall temperature history. Correspondingly, liner stresses should increase up to the time of the drift thermal maximum, about 50 years, and in the absence of significant creep or other unaccounted effects, increase little following that. Liner elements that survive to the time of thermal maximum are expected to fail from strength loss with time rather than as a result of increasing mechanical load. In this regime, liner survival depends on anticipated rates of strength deterioration, controlled largely by durability of the concrete. If the liner undergoes creep at a rate that exceeds the rock creep, the stresses will be reduced, and liner longevity potentially extended.

In terms of liner stresses, the ambient rock load on the liner is expected to be trivial, a few MPa maximum, and will be controlled by intimacy of liner-drift placement. The thermal load, however, will be substantial. This load may be estimated from the simplified relations in Appendix 1. For a temperature change of 135°C in a liner of  $E_L = 27$  GPa,  $\nu_L = 0.21$ ,  $\alpha_L = 10 \mu\epsilon/^\circ\text{C}$  of 0.12 m thickness, a hoop stress of 40 MPa would result. This result compares with the range from a more sophisticated analysis including rock mass failure (R. Nolting et al., NFEE Workshop 2), with pre-creep stresses in the range 60 to 80 MPa, also largely independent of rock mass parameters. These stresses are high compared to nominal concrete strengths on the order of 35 MPa, and likely would result in liner failure. Designing the liner for yield or creep, or fabricating it from high-strength concretes, may circumvent this problem. Silica fume "powder" concretes are available (Dallaire et al., 1998) that have low pH, routine strengths on the order of about 200 MPa,

and potential lifetimes of about 100 years, all outcomes having apparent advantage at Yucca Mountain.

**Discontinuum response.** Although generally so highly fractured that it can be represented as a continuum, the underlying sub-vertical and sub-horizontal discontinuity (fracture) structure in the TSw2 unit may produce discontinuous deformations. Under ambient conditions, mobile rock wedges may be bolted in place and fixed behind the concrete liner. Under thermal conditions, the large tangential stresses in the drift wall may further expel these wedges, deforming the emplaced liner. The process will be controlled by the frictional strength, stiffnesses, and orientations of the discontinuities. Available calculations (Nolting et al., NFEE Workshop 2) show these thermal displacements to be on the order of 4 mm at a thermal maximum of 160°C, probably insufficient to cause liner rupture. These calculations are performed with fracture stiffnesses consistent with current knowledge of mass moduli and fracture spacings,  $s$ , in the range<sup>1</sup> of 5 to 50 GPa/m, and friction angles of 35 to 45 degrees. The potential for this form of liner rupture will be indicated by the Drift Scale Test (DST) at Yucca Mountain and, if apparent, readily mitigated by the selection of appropriate ground control measures.

### Long Term Response

Reliable estimates for the time to failure of the drifts currently are not feasible. Survival estimates for the liner may be rationalized on the observation that (in the absence of creep) liner stresses do not increase following the thermal maximum. If liner failure is predicated on durability, then expectations of survival in the 50 to 100+ year range may be achievable, depending on materials and fabrication.

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<sup>1</sup> Normal and shear stiffnesses may be estimated from  $k_n = \frac{E_R / s}{1/R_m - 1}$ ,  $k_s = \frac{G_R / s}{1/R_m - 1}$ , and with

$$G_R = \frac{E_R}{2(1 + \nu_R)}$$

Assuming failure of the drift, a bulking factor of about 35 percent may be expected, at the lower end of an anticipated 20 to 65 percent range (Church, 1981), representing drift-infill porosities in the 15 to 40 percent range. In the case of complete failure of the drift by chimneying, this would represent failure to about three diameters above the initial drift, based on geometric constraints alone. This geometric constraint of three diameters provides an approximate upper bound to anticipated drift elongation to about one drift diameter. This is based on observations of wellbore sections containing stable breakouts (Ewy et al., 1987), where wall stresses reach equilibrium with available rock mass strength.

The equilibrium, vertically-elongated shape will be stable during and after cooldown as field stresses reduce and the maximum principal field stress rotates to align parallel to the vertical long-axis of the drift section. Loosening and relaxation of the rock mass in this period of mountain-scale stress reduction likely will produce additional block failures in the drift walls.

In terms of timing, unfavorably oriented roof blocks are expected to fall by about 100 to 200 years, within the period of maximum temperature, and depending on failure of the liner. This situation will allow stable configurations to develop rapidly, within the first few hundred years, conditioned by kinematics of release from existing fracture planes. TM-driven collapse will be largely complete by the time of maximum thermal stresses, in the range of 100 to 300 years, with minor intermittent collapse thereafter. The locally conductive and largely invariant temperature, with its corresponding constant thermal stress, at drift level in the 200 to 1000+ year range will result in only minor intermittent collapses. Intermittent collapse will continue, with stress rotation, in the post-thermal regime.

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## THERMAL-HYDROLOGIC-MECHANICAL (THM) EFFECTS

The anticipated primary coupling in the THM triplet will be the TM response, with convective thermal fluxes potentially influencing the early conductive temperature distribution, which in turn impacts mechanical response. Virgin permeabilities of the TSw2 unit are recorded in the 1  $\mu$ d (micro Darcy) range for the matrix, between 1 to  $10^{-2}$  d in the SHT and DST areas, and between 10 and  $10^{-1}$  d elsewhere. Fault permeabilities are on the order of 100d. The reported bulk permeability data have a surprisingly narrow distribution. The higher measurements of bulk permeability span the threshold between anticipated non-buoyant and buoyant convection ( $k \approx 5$ d) (T. Buscheck, NFEE Workshop 1), with important implications for the form, size, and persistence of the dry-out zone. The following text focuses on bounding the anticipated form and extent of changes in permeability, neglecting the other parameters of relative permeability and capillary pressure. Accepted models for scaling relative permeabilities and capillary pressures with saturation are expected to be broadly applicable. Specifically, the scaling of capillary pressures with the inverse square root of permeability ( $p_c \propto k^{-1/2}$ ) will apply.

### TM Response

**Anticipated Permeability Changes.** Approximate magnitudes of the changes in TM permeability may be estimated from initial permeability distributions, defined above, together with observed rock mass structure and anticipated magnitudes of excavation- and heat-induced stress or strain. Assuming the creation of no new fractures, the ubiquitous nature of jointing observed in the TSw2 unit, approximated linear stiffness of discontinuities over a small applied stress range, and parallel plate flow, enables permeability enhancement to be estimated (Ouyang and Elsworth, 1993). The ratio of permeability,  $k$ , to initial permeability,  $k_0$ , may be estimated as  $\frac{k}{k_0} = (1 + \frac{\Delta b}{b_0})^3$ , where  $b_0$  and  $b$  are the initial and final mean fracture aperture, respectively. Accordingly, decoupling Poisson effects in describing strain changes enables the magnitudes of

permeability changes to be determined as  $\frac{k}{k_0} = \left[ 1 + \left( \frac{1}{R_m} - 1 \right) \frac{s_0}{b_0} \left[ \frac{\Delta\sigma}{E_R} + \frac{|\Delta\tau|}{G_R} \tan i \right] \right]^3$ , where  $s_0$

is the initial spacing between adjacent fractures,  $i$  is the dilation angle for the fracture surfaces in shear,  $\Delta\tau$ , is the change in shear stress, and changes in compressive normal stresses,  $\Delta\sigma$ , are defined positive in extension. Clearly, many assumptions are included in this expression, but it remains useful in evaluating order-of-magnitude estimates of effects. The appropriateness of this expression may be benchmarked with existing Yucca Mountain data, most usefully the Exploratory Studies Facility (ESF) niche experiments.

**Niche Experiments.** Pre- and post-construction in situ air permeabilities are reported for the roof rocks of Niche 3650 (J. Wang, presentation by C.-F. Tsang at NFEF Workshop 2; J. Wang, personal communication, 1998). Substantial permeability increases are recorded (averaging 10× to 100×) from a mean permeability of 0.06d, with excavation of the niche adjacent to packer holes approximately 1 m from the niche roof, and running parallel to the niche axis. These are interpreted (by this respondent) as evidence of TM enhancement of permeability, although disturbance by mechanical excavation, saturation changes, and the imposition of a closer pressure boundary may also have influenced the response.

Evaluating anticipated stress changes in the niche roof using a linear elastic boundary element model yields maximum radial stress drop at the packer location on the order of  $\Delta\sigma \approx +6$  MPa. This reduction in radial stress will induce an increase in permeability in the tangential direction, the magnitude of which will depend on the previously defined  $k/k_0$  relation. This, together with a modulus of  $E_R = 40$  GPa; rock mass reduction ratio of  $R_m = 0.15$ ; initial permeability,  $k_0$ , defined (through packer testing) along the hole; and local fracture aperture evaluated from the parallel plate law as  $b_0 = \sqrt[3]{12k_0s_0}$ , enables the modified permeability magnitudes,  $k$ , to be determined. These magnitudes are evaluated for assumed initial fracture spacings,  $s_0$ , of 0.2, 0.5, and 1.0 m, as illustrated in Figure DE-1. Notably, the distribution of evaluated post-excavation to pre-excavation permeability ratio,  $k/k_0$ , exhibits the same structure as that observed, both in form and



magnitude. Zones having low initial permeabilities exhibit the largest change in  $TM\ k/k_0$ , and those having high initial permeabilities, the smallest. The most favorable match is for five fractures per meter, consistent with observed fracture spacings in the TSw2 unit.

With appropriately defined material parameter magnitudes, representative of the TSw2 unit, and assumed response in the evolution of drift- and mountain-scale thermal stress fields, TM changes in permeability may be estimated.

#### Drift Scale

Magnitudes of bulk permeability will change with the excavation of the drifts, with matrix permeabilities remaining largely unchanged. Relative changes in permeability ( $k/k_0$ ) are expected to be largest for zones of initial low permeability, as changes in fracture aperture contribute a proportionally large change in permeability. Absolute changes in permeability will be largest in zones of initial high permeability. The following discussion distinguishes between isothermal changes in bulk permeability that accompany excavation and subsequent non-isothermal changes in the thermal period.

**Isothermal.** With excavation, radial permeabilities generally will decrease, and tangential permeabilities generally will increase. This excavation-disturbed zone is relatively thin, decaying rapidly within about two drift radii into the wall and three to four drift radii into the roof. The relative effect ( $k/k_0$ ) will be greatest in zones of low initial permeability (0.01 d), where enhancements may be on the order of  $10\times$  to  $100\times$ . Radial permeabilities (theoretically) will be decreased, perhaps on the order of  $10\times$ , but overall response will be dominated by the permeability increases, due to the potential communication with inclined cross-cutting fractures. Changes in shear-induced permeability enhancement will be essentially confined to within the predefined influence zone (two to four radii into the drift wall), arranged in lobes 45 degrees above and below the horizontal, and be on the order of  $1\times$  to  $10\times$ .

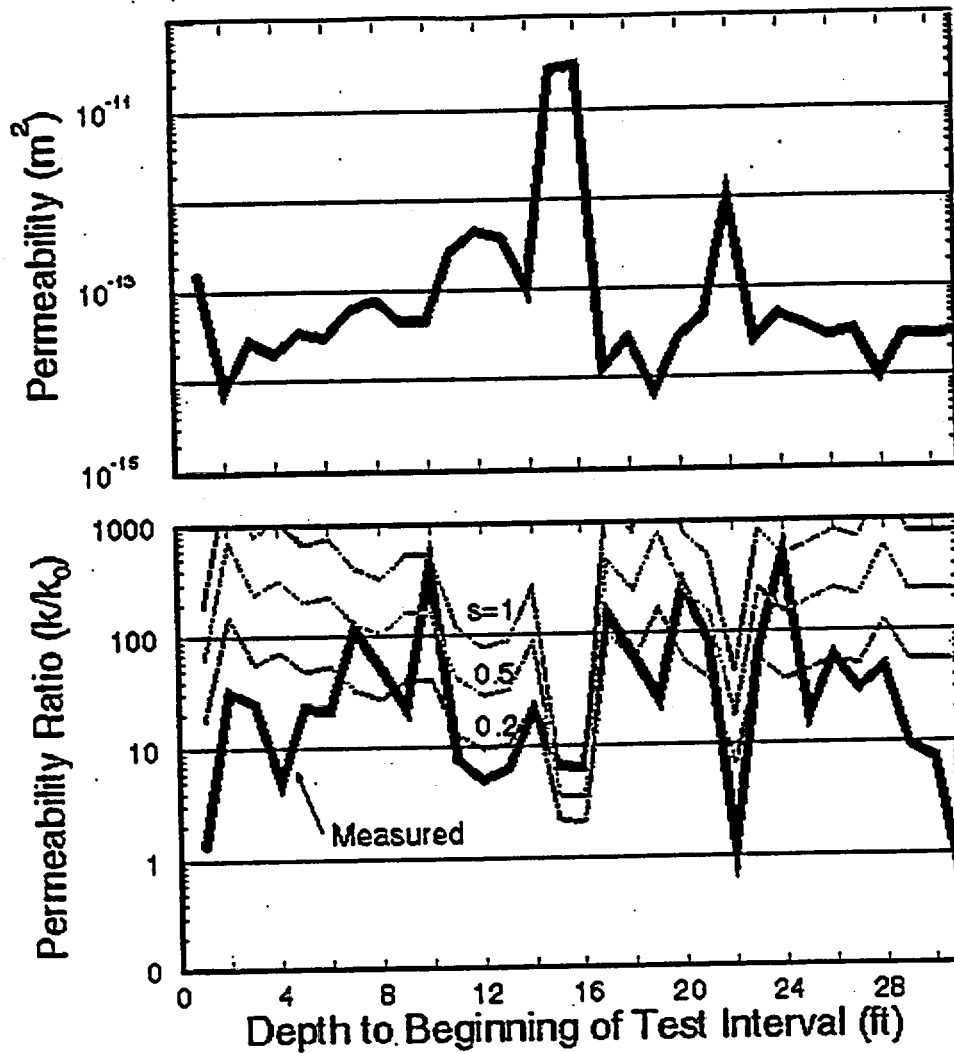


Figure DE-1 Upper: Initial permeability magnitudes, pre-excavation, for the Niche 3650 central borehole. Lower: Post-excavation to pre-excavation permeability ratios, solid. Estimates for relative change in permeability ( $k/k_0$ ) derived.

$$\text{from } \frac{k}{k_0} = \left[ 1 + \left( \frac{l}{R_m} - l \right) \frac{s_0}{b_0} \left[ \frac{\Delta\sigma}{E_R} + \frac{|\Delta\tau|}{G_R} \tan i \right] \right]^3.$$

**Thermal.** With heating, permeabilities around the drift will decrease from post-excavation magnitudes. Temperature changes on the order of 100°C will be sufficient to counter the effects of excavation-induced enhancement of tangential permeabilities, resulting in substantial recovery of these permeability changes. As horizontal field stresses build during the thermal period, stresses may develop and enhance permeability in diametral lobes at 45 degrees from the horizontal, reaching to three drift radii from the wall. Permeability increases in these zones may be on the order of 2× to 10×, reinforcing those shear-induced changes apparent under isothermal conditions.

The above TM estimates anticipate the reactivation of displacements on and across existing fracture planes, rather than development of significant new fracture area. Significant quantities of reflux to the drift may add to permeability enhancement through thermal quenching, and resultant fracturing.

**Post-thermal.** Drift collapse to a stable configuration, in the time frame of 1000+ years, will result in a vertically elongate drift section, forcing TM permeability changes to migrate into the inter-drift pillar. Similar patterns of increased tangential permeabilities and decreased radial permeabilities will endure, zone dimensions scaling approximately with equilibrium drift dimension.

#### **Mountain Scale**

At the mountain scale, as the repository is heated, conductive heating will decrease vertical permeabilities in the region closest to the drifts and will increase vertical permeabilities at greater distances, approximately beyond the 50°C isotherm. Permeability decreases occur within the zone of increased compressional stresses in the thermal envelope encompassing the drifts, and will migrate outward as this zone spreads. These permeability changes, which are due to fracture compression, will be largely recoverable on cooldown. At the repository center the reduction in vertical permeability within this compressional envelope may be on the order of 10×, with horizontal permeabilities remaining substantially unchanged. Horizontal permeabilities will be increased from the repository center outward by a factor of 2 to 10×, potentially reaching

100× at the periphery. This effect reflects the shear strain that develops on existing horizontal fractures in response to the thermal gradient between the zone of thermal expansion near the drifts and the zone of extension at greater distances. If there is a heat pipe zone, the local thermal gradient at the edge of this zone will be higher, and shear will be enhanced. The changes in vertical permeability associated with normal stresses likely will be reversible, while changes in horizontal permeability associated with shear strains will not. A final result is that the mountain will exhibit a lower vertical permeability and a higher horizontal permeability at the peak of the thermal period, with the permeability anisotropy of the TSw2 unit switched from vertically dominant ( $k_v = 5k_h$ ) to horizontally dominant. Shear-induced changes (increases) in permeability will reach a maximum of 100× at the periphery of the repository block.

Changes in bulk permeability due to fracture-normal loading (i.e., changes in  $k_v$ ) are expected to be largely recoverable, and those due to shear loading (changes in  $k_h$ ) will be largely irrecoverable. Fracture wall strengths are sufficiently high, and induced stresses sufficiently low, that shear effects will be largely dilational, with minimal creation of gouge, and with shear displacements resulting in expected increases in permeability.

### **THERMAL-HYDROLOGIC-CHEMICAL (THC) EFFECTS**

The following discussion focuses on the physical effects (i.e., changes in fracture porosity/permeability) due to chemical changes, specifically comparing these effects with porosity/permeability changes due to mechanical effects. There are three mechanisms for changes to permeability that appear to be feasible based on discussions at the NFEE workshops. These three principal mechanisms are illustrated in Figure DE-2, two of them constituting TMC behavior, and the third with a strong coupling to mechanical effects (TH(M)C).

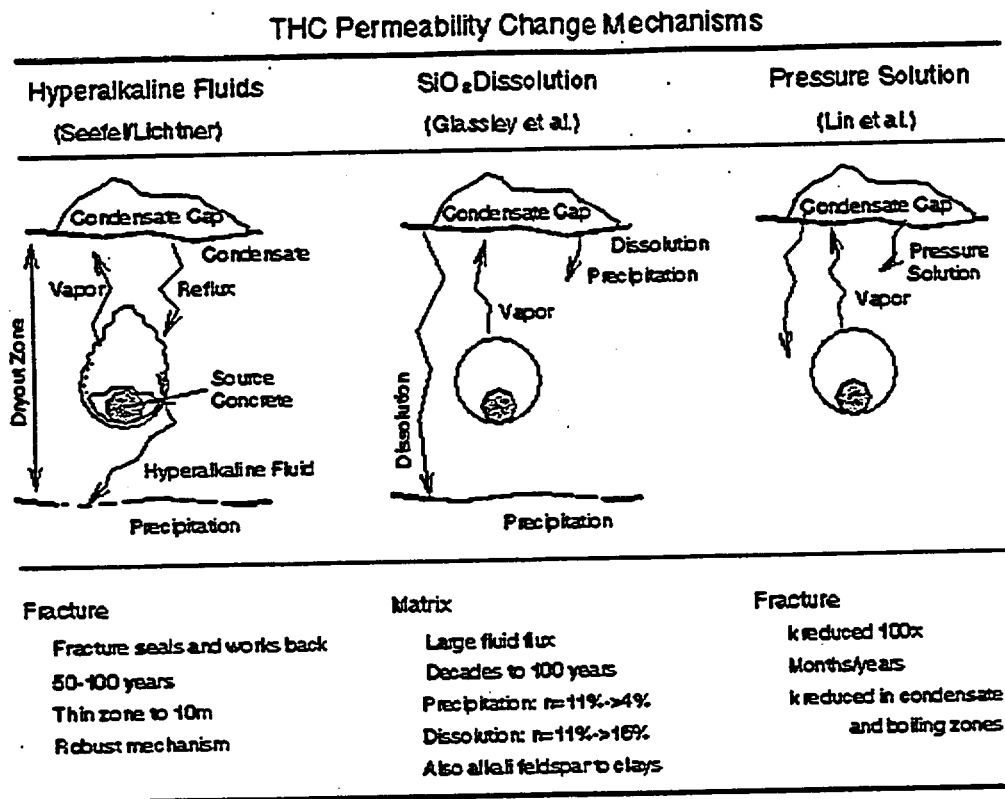


Figure DE-2 Schematic showing mechanisms for permeability change resulting from thermal-hydrologic-chemical (THC) effects.

The first mechanism is the potential for hyperalkaline fluids to develop as a result of dissolution of the concrete liner (C. Steefel and P. Lichtner, NFEE Workshop 2). Percolating water from the condensate zone would dissolve the concrete liner and form a precipitation zone beneath the drifts at the base of the dry-out zone. A thin zone is postulated to develop, a few to ten meters thick, within 50 to 100 years. Precipitation would plug the fractures, and the zone would propagate back toward the drifts, the ensuing process appearing robust, as secondary pathways seal and hyperalkaline fluids plug remaining pathways. This seal would develop after the transient permeability-changing THM effects had largely passed, leaving the zone little threatened by mechanical rupture. If capable of developing, this underseal would prevent the downward escape of water, keeping the repository wetter than otherwise, but lessening

contact of reflux with the underlying saturated zone. It is not known whether this process can be anticipated for this site, although geologic analogs support the general principle. Further studies of the scope and potential for this process to develop are needed from the drift-scale test (DST) to provide appraisal of this effect.

A second process is  $\text{SiO}_2$  and calcite dissolution as discussed by W. Glassley (NFEE Workshops 1 and 2). Dissolution, which would occur in the condensate zone, reportedly would lead to (fracture) porosity changes on the order of a fraction of a percent, with a 100-year penetration of 3 m under a reflux of magnitude of  $1000 \text{ m}^3/\text{m}^2/\text{yr}$ . This effect appears small, despite the assumed reflux corresponding to an anticipated upper bound in the TSw2 unit, corresponding to a permeability of 1 d under an applied unit hydraulic gradient. The increase in porosity in the condensate zone and decrease in porosity in the dry-out zone is unlikely to have a large effect. The primary influence likely is an increase in imbibition in the condensate zone and coating of fractures and decrease in imbibition in the dry-out zone. Analogous reduction of porosity in the matrix adjacent to fractures is observed in the palaeocirculation systems of tuff units that are locally (to Yucca Mountain) intruded (Matyskiela, 1997), lending credence to this anticipated behavior.

Other analyses (W. Glassley, NFEE Workshop 2) indicate dissolution and precipitation driven changes in (matrix) porosity from the ambient 11 percent, increasing to 16 percent in zones of dissolution, and reducing to between 10 and 4 percent in below-drift zones of precipitation. If restricted to the matrix, these changes will increase imbibition rates in the condensate zone, potentially sequestering more of the recirculating water and preventing its return to the boiling zone. If the effect becomes concentrated in the wall rock of fractures, moderate changes in matrix permeability may result. These effects are likely transitory as the front moves through the system. The most important effects probably will be the change in fracture permeability, more storage in the condensate zone, and the formation of more rivulets as water moves through the dry-out zone. It is also possible for a precipitation zone to develop at the bottom of the dry-out zone beneath the drifts.

A third permeability-change mechanism is the potential for developing pressure solution within contacting fractures (W. Lin et al., NFEE Workshop 1). Permeability reductions in laboratory tests were greatest for the passage of water (four orders of magnitude permeability decrease from  $k_0 = 1d$ ), compared to a modest decrease for steam circulation, suggesting the effect will be greatest in the condensate zone, but also present in the boiling zone. This effect would reduce permeabilities in zones of dissolution and precipitation, because of the structure sensitivity of the asperity-to-asperity contact across fractures. Assuming a constant magnitude of in situ stress, there will be a net reduction in permeability of possibly two orders of magnitude, from  $1d$  to  $10^{-2}d$ . The postulated asperity dissolution process, contributing to the permeability reduction mechanism, will tend to reduce TM stresses and TM-driven reductions in permeability, thereby constituting a complex TH(M)C process. Correspondingly, where pressure solution and TM effects act to reduce permeability, their combined effect will be less than their expected summed influence (i.e., the chemical and mechanical effects will work against each other). Pressure solution will tend to reduce the TM stresses driving TM reductions in permeability. The magnitude of this effect is uncertain. However, as the asperities are dissolved along fractures, the stresses will also be reduced, leading to a reduction in the mechanically driven permeability reduction. Net permeability reductions on the order of  $10\times$  would be expected. This effect could be operative in both the condensate and dry-out zone.

Permeability changes expected due to mechanical and chemical effects during the maximum thermal period and during the subsequent cooldown period are summarized in Figure DE-3. The effects are given both for an unthrottled, high-permeability system characterized by a heat-pipe zone, and for a low-permeability system driven primarily by conduction. The diagram enables comparison of the nature and spatial location of permeability changes from mechanical and chemical effects. The boundaries between zones of changed permeability differ for the THM and THC mechanisms because of the different driving mechanisms. THC changes are delimited by the boiling isotherm, and THM changes are delimited by a lower isotherm, shown in previous analyses (Mack et al., 1989) to approximate an isotherm  $25^\circ\text{C}$  above ambient (i.e., approximately  $50^\circ\text{C}$ ).

The changes in permeability shown for the maximum thermal period are relative to ambient conditions, and for the cooldown period are relative to the maximum thermal period. Magnitudes of THC-induced changes in permeability are more difficult to predict than for THM, because of the greater uncertainty in mechanisms of permeability change. However, estimated reductions in permeability are likely to be of no more than on the order of 10 $\times$ , and the increases in permeability no more than on the order of 100 $\times$ .

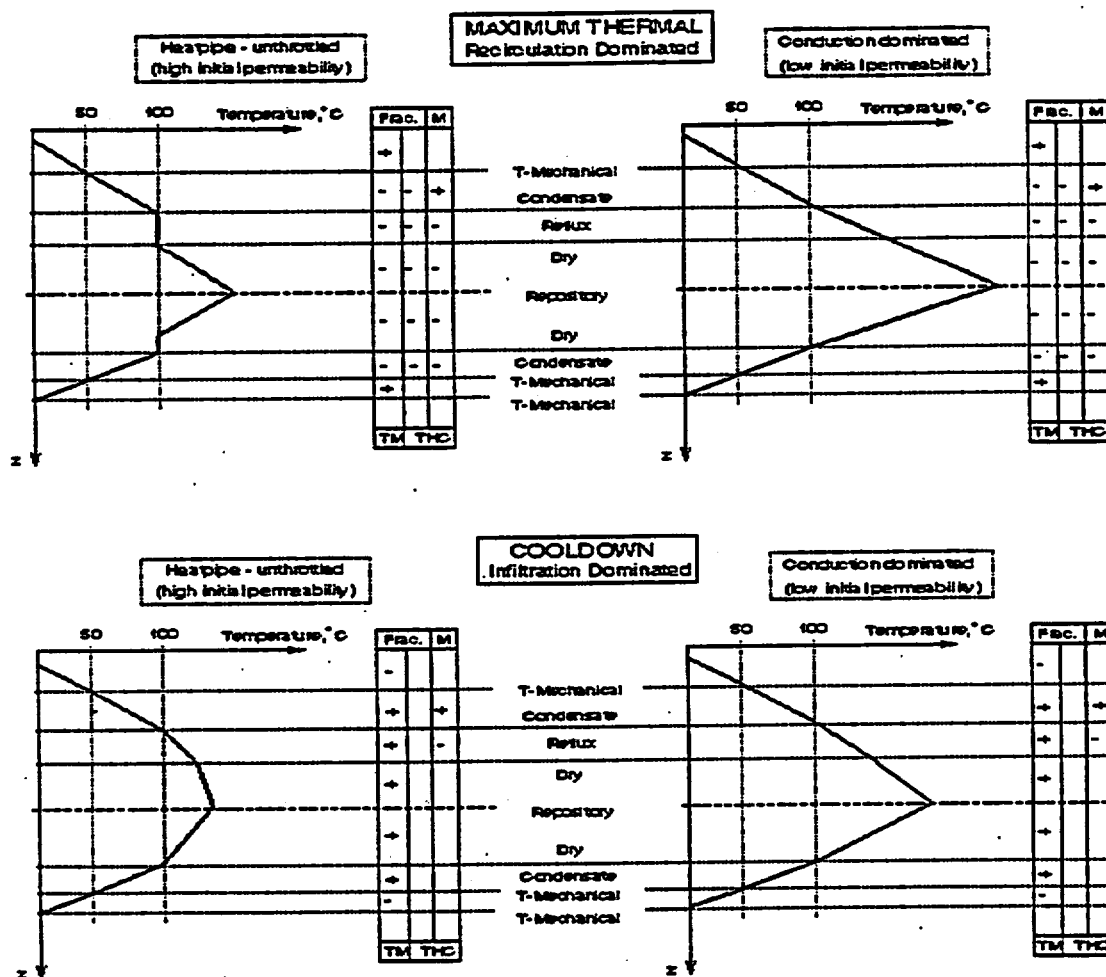


Figure DE-3 Schematic view of anticipated mountain-scale changes in permeability due to THM and THC processes. Major influences are on fracture permeabilities (Frac.), with minor influence on matrix permeabilities (M). Permeability change during the maximum thermal period is relative to



initial ambient permeability. Permeability change during cooldown is relative to the maximum thermal permeability. Increases in permeability are denoted as '+', decreases as '-', and null as blank. Magnitudes of permeability change are 10× in reduction and 100× in enhancement. THC changes are relative to the boiling front ( $T = 100^{\circ}\text{C}$ ), and THM changes are relative to the ambient temperature front (approximately  $T = 50^{\circ}\text{C}$ ). Temperature profiles are for illustration and not scalable above  $100^{\circ}\text{C}$ .

Changes in permeability due to alteration to secondary forms are of low order, occurring at the upper range of expected repository temperatures, and therefore limited to the core of the mountain. Changes from  $\alpha$ - to  $\beta$ -cristobalite generally happen at about  $220^{\circ}\text{C}$  and result in a 1 to 2 percent volume change. For the temperatures expected here, imbibition into the matrix should increase, and the volume change could increase the permeability in the matrix and minimally decrease the fracture permeability.

In terms of fracture-matrix coupling, the effects vary spatially and temporally. In the condensate zone, dissolution will remove the coating and increase the fracture-matrix interaction. Deposition will occur within the matrix. In the dry-out zone, deposits will occur on the fracture walls, thus reducing coupling. During heat-up, the condensate zone will expand, with fracture coating allowing fingers or rivulets to penetrate more deeply into the boiling zone. This behavior will be tempered by permeability reduction from mutually reinforcing THM and THC effects. During cooldown, the dry-out zone will collapse, enabling water to penetrate more deeply into the dry-out zone through coated fractures. If the process occurs slowly, the system could at least partly recover through dissolution, although THC-induced permeabilities are unlikely to approach their pre-thermal state. It is more likely that the process will happen quickly, and THC-induced changes will be largely irrecoverable. If water is laterally diverted around the dry-out zone, there will be less water to dissolve the coatings during refluxing.

## MULTIPLY COUPLED EFFECTS

The primary multiply coupled effect will be the interactions of THC and THM changes in permeability. In this regard,  $\text{SiO}_2$  dissolution in constant stress tests (W. Lin et al., NFEE Workshop 2) illustrates the potential for decreasing fracture permeabilities. In a natural system, where stresses are controlled partly by displacements, this will reduce the stress driving THM reductions in permeability. These effects work against each other but result in a net decrease in permeability. This coupling was discussed in detail in the section on THC effects.

THM and THC-driven changes in horizontal permeabilities will work against each other. The result will be a net decrease in horizontal permeability ( $10\times$ ) at the repository center and a net increase in horizontal permeability ( $100\times$ ) at the periphery. Anticipated decreases in vertical permeability will reduce convective heat fluxes and result in increased temperatures at the repository level. Increases in horizontal permeabilities will increase the potential for lateral division of refluxing fluids, particularly at the downdip periphery of the repository.

A secondary multiply coupled issue relates to the durability of the concrete liner. Because the liner may be designed to withstand thermal loads, liner survival is constrained by the rate of strength loss due to chemical weathering. Very low-permeability concretes may be anticipated to have structural lifetimes approaching 100 years. Only with the removal of the liner will substantial portions of the drifts be free to collapse. Progressive collapse will develop from the sequential release of roof blocks, resulting from progressive strength loss on existing fractures. Fracture strength loss will be from the combination of stress redistribution with block rotation and release, thermal microcracking, spalling, and chemical alteration.

### **T, TM, and THC Above the Drifts**

Mechanical and chemical effects will partially work against each other in changing fracture permeability during the heating period. Pressure solution will decrease the permeability, but also reduce the stress, lessening the decrease in permeability due to THM effects. Shear-induced increases in horizontal permeability will work against TM and THC decreases above the drifts. Shear strains and corresponding permeability enhancements will increase in magnitude from null effect at the repository center to a maximum at the edges. Dissolution of the matrix in the condensate zone will work against the thermal stresses in the same zone, but this will probably not have a large effect on mountain-scale circulation, except by potentially increasing matrix imbibition and in sequestering fluids from recirculation. During cooldown, mechanical stresses will relax, if they are not already partly relaxed by dissolution processes. TM increases in vertical permeability will largely recover, but horizontal permeability enhancement and THC changes will not. These effects are summarized in Figure DE-3.

### **T, TM, and THC Below the Drifts**

Low-permeability nonwelded units (CHn) underlying the repository are shown (N. Brodsky, NFEE Workshop 1) to be strongly hysteretic in thermal behavior, suggesting the potential for large permeability changes if temperatures significantly exceed boiling. Collapse of this structure may also affect permeabilities in adjacent units, through loss of mechanical support or confinement. However, anticipated temperatures at this depth are probably low enough ( $< 90^{\circ}\text{C}$ ) that this will not be an important effect.

### **DURABILITY OF EFFECTS**

The durability of permeability changes depends on the causal mechanism. Mechanical permeability changes due to normal closure or extension will be largely recoverable. Changes involving shear displacements and irreversible mobilization of frictional forces are largely nonreversible. Changes in fracture and matrix permeabilities due to

dissolution and precipitation effects will be largely irreversible. Correspondingly, shear-induced enhancements of horizontal permeabilities and dissolution/precipitation-driven reductions in permeabilities are considered largely irreversible. T(H)M-driven reduction of vertical permeabilities in the thermal period is considered largely reversible. The durability of these coupling effects at mountain scale is summarized in Figure DE-3. At the drift scale, permeability changes will be dominated by TM-driven redistribution of stresses and changes in drift geometry. Drift-local (to five radii) changes in permeability will be largely irrecoverable.

## RECOMMENDED ACTIVITIES TO REDUCE UNCERTAINTIES

Uncertainties exist in the evaluation of TM stability of the drifts and of permeability changes from THM and TH(M)C couplings. Of these behaviors, drift stability is least uncertain, TH(M)C permeability-coupling most uncertain, and THM effects intermediate to these two.

Determination of material parameters, anticipated response, and the presence of unexplained processes, all at the requisite large scale, are adequately provided in the completed SHT and ongoing DST. Although the DST will not be completed by the time of the Yucca Mountain license application, ongoing data recovery and analysis are expected to significantly reduce uncertainties in the anticipated TM, THM and TH(M)C response at scales of interest. This is proposed as the primary vehicle for reducing uncertainties discussed in this summary.

Although crucial in reducing uncertainties, the anticipated nonuniform distribution of the DST thermal pulse will be quite different from that expected for "in-drift" heating alone, because of wing heaters. The DST should not be viewed as a direct analog for individual TM or THM drift behavior. Rather, important processes will be represented and appropriate characterization of these processes will be the primary contribution of the DST.

### **TM Drift Stability**

The processes affecting drift stability are well understood. Parameters defining the response are well defined.

The primary drift-scale parameters that control stability in the short term (to 100 years) are available from the SHT. These mechanical and structural parameters provide adequate, robust input to calculations of TM stability. The expectation that liner stress history will mirror drift temperatures, together with predictions for liner stresses and displacements, will be testable in the DST. The DST will yield supplemental data, and observed response of a candidate drift, albeit over a short time. This observed response should confirm the importance of controlling processes and of validating straightforward mechanistic models and designs. Because drift TM processes are expected to progress close to the rate of drift temperature change, these confirmatory data should be significant in reducing uncertainties, even for the relatively short test.

The potential to retain the liner in-place through the initial short-term thermal period (to 100 years) depends on narrowly constrained physical parameters, predictable processes, and a variety of design options. No significant data acquisition beyond routine site characterization and the observed DST response are suggested. Available data are adequate to support worthwhile scoping calculations (continuum and discontinuum) to assess liner and support options, propose durable solutions, and define the anticipated form of the drift profile, post-failure. Ancillary surveys of liner (concrete) durability, including creep, and historical survival of drifts in similar anticipated stress/strength regimes, are appropriate.

### **THM Permeability Changes**

The processes affecting THM response are moderately well understood. Parameters defining the response are moderately well defined.

The SHT results and niche tests provide important evaluations of THM effects. The DST data and subsequent benchmarking analyses will provide additional data, at a

progressively larger scale. These data largely obviate the need for extensive small-scale (T)HM testing of single fractures. However, limited testing specifically to define the potential for gouge formation, fracture-sealing stresses, and residual apertures would be useful. These could be obtained through laboratory testing of fractures. Further measurement of rock moduli under increasing thermal stresses (during the DST) would enable reconstruction of a more complete fracture stiffness curve, better defining coupled THM effects on permeability, at large scale.

Field characterization is sufficiently advanced that meaningful scoping (modeling) studies of TM response to varying rock mass structural conditions would be useful. The estimates used in this report (Mack et al., 1989) are a decade old and represent a different emplacement configuration. Continuum and discontinuum analyses would enable refined evaluations of boundaries between zones of thermally-induced extension and compression, thereby defining the sense of permeability changes. Mass moduli, fracture stiffnesses and knowledge of rock mass structure are sufficiently constrained to enable the evaluation of improved estimates of the magnitudes of permeability change. These evaluations would especially improve estimates of THM changes in horizontal permeability magnitudes, both in the center and at the edge of the repository.

The niche "mine-by" studies continue to be useful in defining important HM responses, at moderate scale, and for projection to THM effects. The permeability enhancement processes operating in these studies could be confirmed through additional visible-dye tracer testing, mechanical instrumentation, and resin impregnation and exhumation.

Estimates of rock mass creep behavior are needed to define the durability of THM changes to permeability, but no feasible method is available to recover these data at appropriate size and time scales, except perhaps in the DST, where dissolution/precipitation effects are anticipated to dominate over creep behavior.

### TH(M)C Permeability Changes

The processes affecting TH(M)C coupling are the most poorly understood, including such basic issues as whether dissolution will increase or decrease permeability. Parameters defining this TH(M)C response represent the greatest uncertainty for the couplings evaluated in this report. Fundamental to this uncertainty is the observation that fracture permeabilities may decrease with  $\text{SiO}_2$  dissolution, whereas the non-structure sensitive matrix is anticipated to increase in permeability with dissolution. The primary difference is the structure sensitivity of fractures to stresses, and the effect that dissolution may exert on stress reduction, potentially checking THM permeability reduction. Key to this process is a fundamental understanding of whether dissolution occurs primarily at contacting asperities, where wetting fluid components are attracted by capillarity, or in the void structure where rivulets may propagate. Flows driven alternately by capillarity or gravity may exhibit fundamentally different permeability-change responses for similar magnitudes of energy and mass flux. Laboratory testing to better define the sense of this response to dissolution is recommended, necessarily including control on stresses and displacements of a natural fracture (from the TSw2). Sequential application of both constant stress and constant (external) displacement boundary conditions should identify the ranges of permeability response. Pressure solution effects develop sufficiently rapidly within fractures (150 days, W. Lin et al., NFEE Workshop 2) to yield definitive results in a timely manner. The proposed DST should be used to provide quantification of these important dissolution/precipitation processes. Resolving the processes controlling structure-sensitivity of the fracture and matrix is key to reducing uncertainties in the evaluation of TH(M)C permeability enhancement.

More speculative models for permeability transformation, such as the effect of hyperalkaline fluids, have yet to be validated experimentally. If a concrete liner will be retained in the evolving final design, the likelihood of this response must be confirmed through use of analogs, reaction vessel experiments, and modeling.

Determining field-scale imbibition properties that affect matrix-fracture interaction is important in defining depths of reflux penetration (boiling zone) and volumes of fluid

sequestration (condensate zone). These behaviors are strongly affected by dissolution/precipitation, and are difficult to determine because of the extended time scale of formation. Natural imbibition behavior, at the scale of tens of meters, will be obtained from the observed DST response. Predictions over repository lifetime may be aided by relevant analog studies (e.g., Matyskiela, 1987) that quantify the reduction in fracture wall permeability magnitudes resulting from the circulation of hot fluids. Post mortem observations from the proposed laboratory pressure solution studies may also be useful in defining the influence of precipitation/dissolution on imbibition behavior.

## APPENDIX

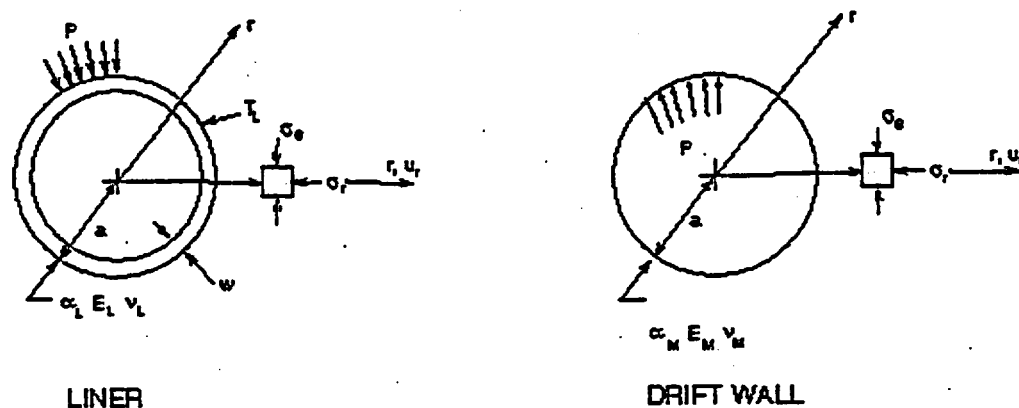


Figure DE-4 Liner and drift wall geometries used in the analysis.

## APPENDIX 1 - LINER STRESSES AND DRIFT STABILITY

Liner stresses and displacements from uniform heating of the surrounding rock mass may be evaluated by considering a thin liner embedded within a circular-section drift.



### Liner Behavior

The liner is of external radius,  $a$ , thickness,  $w$ , with material coefficients representing thermal expansion,  $\alpha_L$ , deformation modulus,  $E_L$ , and Poisson ratio,  $\nu_L$ . Under uniform temperature change in the liner, relative to ambient,  $T_L$ , for the radially symmetric geometry, the tangential strain,  $\epsilon_\theta$ , is defined in terms of the radial displacement of the liner,  $u_r$ , with radius,  $r$ , as

$$\epsilon_\theta = -\frac{u_r}{r} \quad (1)$$

where displacements are positive outward, as shown in Figure DE-4. Summing the components of the tangential strain in the liner due to the application of a tangential stress,  $\sigma_\theta$ , resulting from ground reaction pressure,  $p$ , and due to the thermal load, yields

$$\epsilon_\theta = -\frac{u_r}{r} = \frac{\sigma_\theta}{E_L}(1 - \nu_L^2) - (1 + \nu_L)\alpha_L T_L \quad (2)$$

where axial displacements along the drift are zero, corresponding to plane strain conditions. Tangential stresses,  $\sigma_\theta$ , in the liner are related to the ground reaction pressure,  $p$ , as  $\sigma_\theta = mp$ , where  $m$  is the ratio of mean liner radius,  $a$ , to thickness,  $w$ , as  $m \approx a/w$ . Substituting the ground reaction pressure,  $p$ , for tangential stress in equation (2) yields normalized linear displacements as,

$$\frac{u_r}{a} = \frac{mp}{E_L}(1 - \nu_L^2) - (1 + \nu_L)\alpha_L T_L \quad (3)$$

### Thermal Behavior of the Drift

Consider a circular drift of radius,  $a$ , within an infinite medium of material coefficients representing thermal expansion,  $\alpha_M$ , rock mass modulus,  $E_M$ , and rock mass Poisson ratio,  $\nu_M$ , as illustrated in Figure DE-4.

The Lamé coefficients representing bulk modulus,  $\lambda_M$ , and shear modulus,  $G_M$ , define the stress-strain relations in radial coordinates, where the tangential strain,  $\epsilon_\theta$  is defined as

$$\epsilon_\theta = \frac{u_r}{r} = \frac{1}{4G_M(\lambda_M + G_M)} [-\lambda_M \sigma_r + (\lambda_M + 2G_M) \sigma_\theta] - \alpha_M (1 + \nu_M) T_R(r, t) \quad (4)$$

where  $\sigma_r$  and  $\sigma_\theta$  are the radial and tangential stresses, and  $T_R(r, t)$  is the radial temperature distribution. At the drift wall, the temperature is given as  $T_R(a, t) = T_L(a, t)$ , enabling drift wall displacements to be evaluated by substituting for wall stress (Stephens and Voight, 1982) as

$$\sigma_r = 0; \quad \sigma_\theta \Big|_{r=a} = \frac{\alpha_M E_M T_L(a, t)}{(1 - \nu_M)} \quad (5)$$

Substituting equation (5) into equation (4) yields null tangential strain at the drift wall and, hence, null radial displacement, for all time, irrespective of the thermal history at the drift wall.

### Reaction Behavior of Drift with "Liner Pressure"

Reaction of the drift wall with the radial pressure supplied by the interior liner,  $p$ , as illustrated in Figure DE-4 enables radial strains to be defined as

$$\frac{u_r}{r} = \frac{p}{2G_M} \frac{a^2}{r^2} \quad (6)$$

where  $G_M$  is the shear modulus of the rock mass ( $G_M = \frac{E_M}{2(1+\nu_M)}$ ). At the drift wall,  $r = a$  and the radial displacement, inclusive of thermal loads in the rock mass, is  $u/a = p/2G_M$ .

### Liner-Drift Interaction

Assuming that the liner is installed in intimate contact with the drift wall, thermally induced liner and support stresses can be evaluated by equating interface displacements. Equating the displacements of equations (3) and (6) yields the magnitude of thermally induced support pressure,  $p$ , as

$$p = \frac{(1+\nu_L)\alpha_L T_L}{\frac{1}{2G_M} + \frac{(1-\nu_L)^2 m}{E_L}} = \frac{\frac{a_L}{a_R} E_R R_m T_L}{1 + m \frac{(1-\nu_L^2) E_R R_m}{(1+\nu_R) E_L}} \quad (7)$$

and liner stress,  $\sigma_\theta$ , as

$$\sigma_\theta = mp \quad (8)$$

where, for convenience, subscripts R and L represent parameters for the intact rock and liner. Mass moduli are related to intact moduli through a reduction coefficient,  $R_m$ , as  $R_m = E_M/E_R$ . Poisson ratios and thermal expansion coefficients for the intact and fractured systems are taken as sensibly equivalent, as  $\nu_R \approx \nu_M$  and  $\alpha_R \approx \alpha_M$ .

Where rock mass modulus,  $E_M$  (or corresponding shear modulus,  $G_M$ ), is of the same order as liner modulus,  $E_L$ , and ratio of drift diameter to liner thickness,  $m$ , is large, these relations may be approximated as

$$p \approx \frac{(1 + \nu_L) \alpha_L E_L}{m(1 - \nu_L^2)} T_L \quad (9)$$

$$\sigma_\theta = mp \approx \frac{(1 + \nu_L) \alpha_L E_L}{(1 - \nu_L^2)} T_L \quad (10)$$

These expressions yield the following important results, that:

1. Thermal liner stresses,  $\sigma_\theta$ , are controlled primarily by the composite liner properties of modulus,  $E_L$ , Poisson ratio,  $\nu_L$ , thermal expansion coefficient,  $\alpha_L$ , and liner thickness,  $w$ . These parameters are controllable, to some degree, during design and fabrication, by means that include providing compressible lagging or blocking, backfill, or compressible joints to control the indeterminate influence of liner creep and thereby the magnitude of thermally induced stresses.
2. There is only weak dependence on the rock mass parameters of modulus and Poisson ratio.
3. Liner thermal stresses are surprisingly independent of the coefficient of thermal expansion of the rock mass,  $\alpha_R$ , depending only on the instantaneous liner temperature differential above ambient,  $T_L$ .

These observations relate to the thermal behavior of a liner placed within a single circular-section drift in an infinite medium. Bending stresses that may develop in the liner are neglected, as is the influence of lateral convergence due to the presence of adjacent drifts. Despite these shortcomings, this analysis gives important insights into the expected response of the drift liner system.

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## ELICITATION SUMMARY

JOHN E. GALE

### OVERALL PROCESSES

The rock mass at the Yucca Mountain site is well fractured. Near some of the fault zones, the rock mass is intensely fractured. At least three fracture or joint sets have been mapped in the boreholes and tunnels at the Yucca Mountain site. These include a SE-NW trending, near-vertical, SW-dipping set; a SW-NE trending, near-vertical, NW-dipping set; and a NNW-SSE trending set with a near-horizontal NE dip. However, the fracture sampling lines were orientated primarily vertical or near horizontal, which introduced bias into the data sets because of the undersampling of fractures that have intermediate dips. Within this structural framework, it is clear that the impact of the fracture system on the near-field thermal-mechanical-hydraulic-chemical (TMHC) coupled processes and the impact of these processes on repository performance have not been evaluated properly. Given the sparse fundamental data on coupled behavior, it appears that the most significant effects on repository performance will be those that are introduced by the full TMHC processes, primarily the permanent or near-permanent changes that the dissolution and deposition of minerals will have on both the permeability of fractures during thermal loading and the ability of the rock mass to dissipate the thermal load. The impact of shear displacement on fracture permeability during both the thermal loading and cooldown will affect the development of heat pipes and provide the sub-horizontal pathways for long-term flow and transport through the repository. This will certainly be the case if the vertical fractures are effectively sealed by the migrating boiling front. The thermal-mechanical impacts, in terms of inducing roof migration, will be significant. However, an assessment of the significance of these impacts requires that agreement be reached on the stress and displacement boundary conditions that should be applied to the repository as a whole and to the immediate area of the drifts specifically, as well as at the

edges of the repository (see proposed stress conditions due to thermal loading in Witherspoon et al., 1977).

### THERMAL-MECHANICAL (TM) EFFECTS (DRIFT STABILITY)

If we consider a drift at ambient temperature as the reference case, the ratio of the maximum and minimum in situ stresses,  $\sigma_1/\sigma_3$ , determines the stress concentrations in the immediate rock mass around the drift. Assuming a drift at the repository level that was created by a tunnel-boring machine (TBM), where  $\sigma_1$  is vertical and approximately 7 Mega Pascals (MPa) and  $\sigma_2$  and  $\sigma_3$  are acting in the horizontal plane, with an average value of 3.5 to 4 MPa (Wilder, 1996), the tangential stress in the side wall (at the springline) should be approximately 14 to 18 MPa (Hoek and Brown, 1980). This result uses a simple model of a circular hole in a stressed elastic body. The tangential stress in the roof should be approximately half of the vertical stress.

If we now apply a thermal load and note that the coefficient of linear expansion for the intact rock is about  $7$  to  $10 \times 10^{-6} \text{ } ^\circ\text{C}^{-1}$  (from Wilder, 1996), the maximum compressive stresses around the drifts will change with increases in temperature and the volume of rock that is thermally loaded. As these thermally induced stresses change, they will produce a range of shear and normal stresses on existing fracture planes. One can visualize the proposed repository as having the shape of a thick penny in terms of both physical layout and in terms of the shape of the peak temperature field. Opinions vary on whether the analysis of the thermal-mechanical effects on vertical fractures and thermally induced stresses should assume plane stress (no confinement) or plane strain (complete confinement) boundary conditions, especially near the center of the repository. Given the shape and size of the repository, the most likely condition will reflect a combination of both boundary conditions, I assign a weight of about 70% to plane strain boundary conditions and about 30% to plane stress conditions.

At the maximum thermal load, temperatures are predicted to exceed 130°C or at least 100°C above ambient for a considerable distance from the repository drift level (from Wilder 1996). At the edge of the waste emplacement drifts, peak temperatures are expected to reach 200°C and will extend at least one or more radii into the rock mass. For the purposes of this discussion, I assume that the temperatures within the plane of the repository, including the pillars between the drifts, will reach a maximum of 200°C. The rock mass elastic modulus computed for the TSw2 Topopah unit as reported in Wilder (1996) is approximately 23 Giga Pascals (GPa). Similar values are reported and used by Nolting and Sun (NFEE Workshop 2) for a rock mass with a rock mass rating (RMR) of 65 or a rock quality of 5. The measured Young's modulus for intact rock is reported in Wilder (1996) to be approximately 33 GPa. I assume that the computed rock mass modulus takes into account the rock mass stiffening that occurs as the normal stress on the fracture planes increase, and that these higher rock mass values reflect rock mass moduli at higher temperatures. It would be difficult to justify a modulus reduction factor for the rock mass of 0.1 to 0.5, relative to the intact rock values, in light of this assumed "work-hardening" effect due to the stiffening of the joints.

At peak thermal loading, based on the above rock properties and assumed boundary conditions, vertical stresses will remain close to 7 MPa, but horizontal stresses will increase to about 20 to 40 MPa in the zone between the emplacement drifts at 200°C and the maximum extent of the 100°C isotherm. At these stress ratios, the tangential stresses at the drift wall in an elastic body would be very close to zero at the springline, approach about 80 to 100 MPa at the crown of the drift and decrease rapidly with decreasing temperature and increasing distance from the drift to about 20 MPa at the 100°C isotherm. Nolting and Sun (NFEE Workshop 2) report major principal stresses as high as 70 MPa at the drift crown for a fractured rock mass with a rock mass quality (RMQ) value of 5 (good rock) based on FLAC simulations using 100 MTU/acre thermal loading. The computed stresses are sensitive to the properties of the rock mass and movement in existing fracture planes. It is clear that the stresses at the drift crown will greatly exceed the computed rock mass strength of 18 to 19 MPa presented in Wilder (1996). Even taking into account the fractured nature of the host rock and the changes in properties that



will result from movement along joint planes, there will be failure at the crown of the drift.

Equally important are the changes that will take place on the fracture planes in the rock mass adjacent to the drifts, but within the thermally loaded zone, as the principal stresses change from 7 MPa vertically and 3.5 to 4 MPa horizontally to about 7 MPa vertically and between 20 and 40 MPa horizontally. Initially, the near-vertical fractures that are located more than two drift diameters from the drift wall will be subjected to 3.5 to 4 MPa of normal stress. Close to the drift wall, in the zone of stress concentration, the normal stresses on the vertical fracture planes will range from close to zero to about 3.5 MPa. The normal stress on near-horizontal fractures will range from near zero at the crown to 14 to 18 MPa at the springline. Outside the zone of stress concentration, the normal stresses on the near-horizontal fracture planes will average about 7 MPa. Given the range of possible fracture orientations, the shear stress on both the sub-vertical and sub-horizontal fracture planes will range from zero to a maximum of 7 to 9 MPa. With these low normal stresses, some of the rough fractures will be dilatant under the given shear stresses. If we now impose a thermal load that ranges from 200°C at the drift wall to 100°C farther back in the rock mass, the normal stresses on the fracture planes will rotate through a full 90 degrees (the major principal stress will now be horizontal rather than vertical) and will range up to about 40 MPa for fractures that are outside of the zone of stress concentration, and the shear stresses will range from zero up to 15 or 20 MPa. Based on the expected combination of normal and shear stress on the fracture planes, one can expect both dilatant and contractant behavior in the perturbed rock mass during shear displacement. An analysis should be conducted using a three-dimensional (3-D) discrete fracture/rock mechanics code such as 3DEC (Itasca Consulting Group, Inc., personal communication, 1998) with representative 3-D fracture geometry, site-specific fracture properties, rock moduli, in situ stresses, and equivalent thermal loading to examine the range of normal and shear displacements that will occur in a multiple drift environment, subject to an acceptable set of boundary conditions (primarily confinement) and simulating the rotation of the stress field due to thermal loading.

The instructive analyses presented by Morrison-Knudsen (R. Nolting et al., presentations at NFEE Workshop 2) show millimeters of movement in terms of drift closure. In fractured rock masses, much of this closure will be accommodated as slip on or closure of fractures. Based on the measured rock properties and computed rock mass properties, strains of 2 mm/m seem reasonable at 200°C. The compressive strength of the rock mass is relatively low at 18 to 23 MPa; local failure of the rock mass should occur with strains of 1.5 mm/m, even though the intact rock has a compressive strength of up to 100 to 150 MPa. Local failures that result in movement of rock blocks would produce failure of the concrete liner due to point loading at the contacts with the rock. Grouting the space between the liner and the rock would integrate the liner and the rock mass and increase the area of the liner in contact with the rock. The point load stresses would then be spread over a larger surface area, increasing the stability of the liner.

In its current design, the liner is expected to fail, which will lead to drift failure. When the drift fails, the crown will migrate with a bulking factor of about 30 percent (range of 15 to 45 percent), based on the blocky nature of the rock mass. This is equivalent to a porosity of 13 to 31 percent. For a 5-m drift opening, one would expect the crown to migrate 10 to 12 m vertically. There may be some peaking of the ceiling depending on the orientation of local fractures. The crown migration eventually will stop as the back-pressure develops in the caved material. There may also be some relatively minor heaving of the floor. Certainly, the rate of temperature increase is important. The more rapid the temperature rise, the greater the possibility of early collapse of the liner and the roof of the drift.

Rock block size is a function of the fracture distributions, as shown by the modeling being conducted by Nolting et al. (WFEE Workshop 2). To help assess the effects of the bulking factor, the work completed by Duncan et al. (1972), on rubble piles in drifts from blasts at the Nevada Test Site should be reviewed. The thermal conductivity of the rubble may be important to temperatures of the waste packages, because the rubble will act as backfill in the drift. A reasonable range of permeabilities to use in the modeling is 1000 to 100,000 darcies, based on the low fragmentation one would expect with caving of

these blocky rock masses. If backfill is placed in the drift, it will have only about 20 to 25 percent of the compressive strength of the rock, but should limit crown migration to about one meter, depending on how the backfill is placed.

### **THERMAL-HYDROLOGIC-MECHANICAL (THM) EFFECTS**

As noted above, in considering the impact of thermal loading on fracture porosity and permeability, we assume that at Yucca Mountain there is a well-developed fracture system having variable spacing, variable aperture (Vickers et al., 1992), and variable fracture lengths. All scales of fractures are present, from microfissures to major fault/fracture zones. The fractures are well interconnected and provide continuous pathways for flow on the drift and repository scale. The fracture surfaces are in intimate contact under current stress conditions, producing a high degree of variability in the fracture apertures or fracture pore space within each fracture.

It is also important to consider the time periods involved, ranging from a few hundred years during the thermal perturbation to many thousands of years, in which geologic processes may be operative. Most of the data and modeling have related to the shorter period. During the thermal period, the temperature-time history will determine the relative significance of THM effects. During maximum thermal loading, the tangential stresses are expected to increase to about 70 to 80 MPa in the first meter of the drift wall. Modeling shows zones of compression, extension, and rock mass failure developing around the drifts. Significant deformation should be expected at the edges of the repository or in the outside repository abutment pillar, i.e., on the edge of the penny-shaped zone. Under thermal loading, all three modes of fracture displacement are expected: normal dilation and closure due to changes in normal stress, and dilation and contraction due to shear displacement. When assessing the magnitude of these effects, an important consideration is the boundary conditions of either plane strain or plane stress.

In developing a conceptual fracture/matrix model, the nature of the fracture pore space is important. The structure of the fracture pore space will be different in extensional fractures than in shear fractures. Also, fracture pore space develops in response to both offset of the fracture walls and dissolution and deposition of material in the fracture plane over geologic times. This process produces a non-random distribution of contact points or asperities in the fracture plane, or what is best described as a structured distribution of small and large apertures. The structured nature of the pore space and contact areas will control the fracture stiffness and saturation levels within the fracture system, especially in the fractures that are near-vertical.

The impact of thermal expansion on the hydraulic properties of the fracture system is related to the stress or displacement boundary conditions that are applied at both the drift and repository scale. Thermal expansivity measurements on intact rock appear to give consistent and reliable results. Experimental data (Wilder, 1996) for plane stress boundary conditions show little to no change in the permeability of the fracture plane because the rock is free to expand away from the fracture, and the stress on the fracture asperities remain the same. Although I am not aware of any experimental data on plane strain coupled stress-flow effects from this project, under plane strain boundary conditions the intact rock is not free to expand outward. Thus the rock is forced to expand into the available fracture pore space so that the stress on the asperities or contact areas increases, the asperities are crushed and the apertures are reduced, plus the fracture walls adjacent to the open pore space expand into the open fracture pore space.

Assuming plane strain boundary conditions, the magnitude of normal fracture closure on a particular fracture is bounded by:

$$\delta = \alpha \Delta T E / K_n$$

where  $\alpha$  is the thermal expansion coefficient,  $E$  is the bulk modulus, and  $K_n$  is the fracture normal stiffness, which increases with increasing fracture closure.

The average permanent closure for these fractures should be about 0.1 to 0.3 mm, depending on the fracture roughness and the magnitude of the initial aperture. This closure is analogous to the permanent closure recorded from first-cycle data developed in laboratory tests. Because the fractures, outside the immediate zone that is impacted by excavation activities, are in a state of metastable equilibrium in terms of contact areas, the first-cycle of loading model with the well-noted hysteresis on unloading is the most appropriate model for the response of the fractures to the thermal load on intact rock. The overall change in fracture porosity, which is a function of fracture aperture and spacing, will be on the order of 0.0001 to 0.003. If we assume a range of initial apertures for the existing fractures, and use a Navier Stokes equation for a rough fracture having walls that are in intimate contact, these aperture changes will result in fracture permeability changes of 1.5 to 3 orders of magnitude.

As the load increases due to thermal-mechanical effects, the contact stress remains fairly constant. However, the contact area increases as asperities are crushed and material is dissolved and precipitated. Note that mechanical closure or mechanical apertures are not the same as computed hydraulic apertures. The pore space in the fracture plane evolves with time in response to stress and fluid dissolution effects, and a metastable equilibrium of the asperities is established. One would expect this process to accelerate in the presence of a high thermal load and hot fluids or vapor. The gradual change in aperture over time, or creep (see Reda and Hadley, 1986) that is occurring as a result of pressure dissolution at the contacts (Wilder, 1996) is not recoverable during cooldown of the rock, except perhaps over very long geologic times as the normal fluid circulation dissolves material at the contacts. We see no rebound effect after fractures have been permanently deformed in the laboratory (Reda and Hadley, 1986); hence we expect to see no rebound from the thermally induced fracture deformation in the rock mass surrounding the drifts.

Assuming plane strain conditions, shear stresses and shear strains will occur as the principal stress orientation evolves or rotates, changing the normal and shear stresses on fractures with different orientations with respect to the global coordinates. These changes in normal and shear stress would significantly increase horizontal permeability and

significantly decrease vertical permeability at distances of two to five drift diameters from the drifts. These changes likely would occur within localized zones and will be controlled largely by the fracture geometry. Shear displacements of only a few millimeters on fractures can induce significant changes in fracture permeability. Increases in local fracture porosity could be 0.0001 to 0.001, and increases in local fracture permeability could be by factors of 10 to 1000, depending on fracture roughness and the level of normal stress. Changes in bulk rock permeabilities would lie within the existing permeability ranges—that is, the magnitude of the THM coupling effect on bulk permeability is expected to be less than the ambient spatial variability of this property, if the fault zones are included.

These changes in fracture porosity and permeability likely will be similar within and over the entire horizontal plane of the repository but will vary at the edge of the repository where the lateral extent of thermal loading is dissipated. The Single Heater Test (SHT) or the Drift-Scale Test (DST) provides an opportunity is a way to determine the initial fracture apertures, calculate the change in mechanical aperture, and relate these changes to the hydraulic aperture change. The most effective approach to collecting the essential data on the structure of the fracture pore space is to inject a self-curing resin into a selected group of fractures. After this resin has cured, large samples of the fracture planes can be recovered by overcoring, the spatial structure of the fracture pore space can be mapped, and the interaction between the fracture pore space and the matrix pore space can be quantified. This approach preserves the in situ fracture versus matrix structure and allows one to rebuild the local fracture network and scale up from the small-scale aperture measurements so that the numerical model parameters for the discrete fracture planes provide compatible flow and transport properties for the fracture system.

In looking at the overall effects of thermal-mechanical changes in fracture porosity and permeability, it is possible that these TMH changes will have a significant impact on the potential of the fractured rock mass to develop heat pipes. Fracture permeability should be the primary control on whether heat pipes will develop within the fracture system by controlling the amount of vapor that rises or water that returns. The cubic law relating

fracture permeability to fracture aperture is valid in the pore space segments once relative roughness is taken into account. But when used as an equivalent hydraulic aperture or as a univariate statistic to describe the flow and transport properties of discrete fractures, the cubic law does not provide a good match between experimental measurements and numerical results. In addition, there are few data to support the scale-up of the flow and transport parameters from discrete fractures to flow and transport properties of the bulk rock mass. The approach that has been used to compute effective apertures at Yucca Mountain appears to have been based on the basic cubic law for smooth fracture planes, and the calculations of directional fracture permeabilities appears to have been based on an analytical or numerical approach that assumes that the fractures are continuous within their own planes to some finite boundary. Both of these approaches appear to be neither valid nor well based in current understanding of fractured rock hydrogeology. As a result, it is unlikely that current hydrogeologic models of the Yucca Mountain site reflect the real fracture porosity or the real directional permeabilities of the fractured rock mass.

Given the measured values of bulk permeability in the host rock, it is possible for liquid water to flow against the thermal gradient. If sufficient recharge is available, liquid water may flow, under the impetus of gravity, at rates sufficient to accommodate the repository heat output as latent heat transport. When the bulk permeability is less than about 50 md, the process becomes "throttled" so that the total pressure varies by as much as several bars along the thermal gradient, and gas-liquid phase interference prevents liquid counterflow. In this case a heat pipe does not form, and the dryout zone expands at a boiling front. The required bulk permeability is known from numerical and analytical models, and we seem to exceed that value at most locations in the host rock.

If we assume that the dryout zone will migrate as the 100°C isotherm migrates from the edge of the drift into the rock mass, then the zones of vaporization and condensation will migrate as well. In the condensation zone, the walls of the fractures will be eroded during heating because of dissolution of fracture minerals, especially those that form the contact points or asperities. This erosion will allow for mechanical closure of the fracture. There probably will be a high degree of hysteresis or permanent fracture closure. In the

vaporization/precipitation zone, the permeabilities are reduced as solutes are precipitated. Thermal-mechanical loading also will decrease the fracture permeability in this migrating zone, but contact area is being added due to mineral precipitation. Because of this increase in contact area, the stresses on the asperities should not increase very much, limiting the amount of mechanical aperture closing that will occur. This increase in contact area will minimize the development of heat pipes because the fractures will be filled, especially if the boiling front is stationary as the system reaches its peak or near steady-state temperature. The fracture permeabilities may be reduced enough (to less than  $\sim 0.05$  darcies) that the fractures would be choked and the transport of vapor or liquid impeded. In most fractures, where the pore space is highly variable and has a well-developed spatial structure, it takes only a slight change in the small apertures within the pore space to change the transmissivity or connectedness of fractures.

If the boiling zone is not stationary, since it must migrate as the temperature builds up in the drift initially, it is unclear how the combined advance and retreat of the boiling front and the condensation front would affect fracture permeability. The reduction in fracture permeability due to the combined effect of dissolution at the contact points and fracture closure in the condensation zone followed by precipitation of solutes in the vaporization zone, which is expected to be associated with the advance of the front, will not be reversed as the front retreats. Once fractures have closed, there is a strong hysteresis effect, and the fractures will open only slightly as the normal stress is decreased.

As stresses return to ambient levels during cooldown, shear displacements would be expected, primarily on those fractures having dips between 0 and 60 degrees. These fractures would then become the most active hydraulic conduits because small shear displacements can result in a large increase in fracture permeability if the normal stresses are low and the fracture surfaces are rough.



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## **THERMAL-HYDROLOGIC-CHEMICAL (THC) EFFECTS**

The pressure solution effects associated with crushing of asperities were discussed above in terms of THM effects.

Precipitation of secondary minerals along the walls of fractures can have a significant effect on fracture-matrix interaction. Fracture mineralization impedes the interaction between fluids in the fractures and fluids in the matrix and adds to the contact areas, thus increasing fracture stiffness. Moench (1984) showed that fracture skin in the form of a low-permeability mineral layer can act as a barrier to flow from the matrix to the fracture. The fracture type (extensional versus shear) and the nature of the fracture surface (coated versus clean) are important. Rough extensional fractures will experience less of a change in fracture-matrix interaction than shear fractures. However, mineral precipitation at the boiling front can change significantly the permeability of the fracture plane surface of even rough extensional fractures.

## **MULTIPLY COUPLED EFFECTS**

It is difficult to assess multiply coupled processes or effects. Certainly, TMH effects are enhanced by TMHC effects. Given the complexity of the system, the best approach is to identify the key processes and then characterize the linkages among these processes. For example, processes that include fracture displacement, fracture flow, aperture changes, pressure changes, and thermal expansivity terms are linked. Likewise, chemical processes such as liquid and vapor flow, dissolution and deposition, reactive chemistry and transport, all as a function of temperature, are linked. The only feasible approach to evaluating the coupling of these processes in a realistic time frame is to conduct computer simulations in which the processes are weakly coupled and the interaction loops are linked at appropriate time steps, temperatures, fluid/capillary pressures, and rock mass stresses. Obviously, as with any computer simulation, the logic, linkages, and model scales are critical. A model that simulates processes that are controlled or impacted by

discrete fractures must itself incorporate discrete fractures. Similarly, the displacement and other spatial boundary conditions must be defined, preferably using a nested model approach, so that the small-scale and drift-scale models reflect the boundary conditions of flux, displacement, stress, and temperature. It is not necessary, and it would be unproductive, to attempt to develop a fully coupled model at this stage of the Yucca Mountain project.

Computer simulations of THMC effects will need precise data sets for calibration and to provide constraints on coupled processes. Some of these data sets are being collected from the SHT and DST thermal experiments. However, key data on the fracture pore structure and the fracture versus matrix interaction are not being collected. In addition, the project lacks key data on the response of the coupling of flow and changes in mechanical aperture due to thermal loading under plane strain boundary conditions. In addition, the project lacks a database on the response of fractures to changes in both normal and shear stresses over the expected range of stress changes and temperatures.

## **DURABILITY OF EFFECTS**

Normal stress effects are partly reversible except for the hysteresis effect of fracture closure, which is essentially permanent. There will be little opening of the fractures due to changes in normal stress during cooldown. However, the shear stresses and shear displacements that will be induced by rotation of the stress field during the thermal loading will produce similar changes during both the thermal loading and cooldown parts of the repository lifecycle. The final changes in fracture permeability that will result from the shear stresses produced by the rotation of the principal stresses during cooldown will be permanent.

The TMHC effects can be considered permanent or very nearly so, except where a fracture is subject to high shear stresses at low normal stresses. It will take thousands of years with normal unsaturated flow for the pore space within the fracture plane to

redevelop to anything that approaches its original porosity or permeability. It is unlikely that the minerals formed in the boiling zone will redissolve as the boiling front retreats.

## RECOMMENDED ACTIVITIES TO REDUCE UNCERTAINTIES

The uncertainties in determining the significance of the near-field coupled processes exist because the THMC processes in the fractured rock mass have been considered relatively unimportant. Experimental work on coupled processes that involve large blocks of both intact rock and fractures at in situ stresses are limited to the SHT and the current DST. The large surface-block experiment had no controls on the load or displacement boundary conditions and was essentially a plane stress thermal-mechanical-hydraulic experiment. The laboratory tests conducted under plane stress boundary conditions did not provide the data needed to cover those fractures within the thermally loaded rock mass that will be subjected to what is essentially plane strain or close to displacement-controlled boundary conditions. The SHT tests did not provide direct data on the structure of the pore space in the fractures that were impacted by thermal loading. Nor did the SHT experiment provide the necessary post-experiment data on the nature of the fracture versus matrix interaction.

To reduce selected uncertainties regarding the impact of coupled processes on repository performance, several immediate and short-term steps can be taken.

1. Conduct a suite of laboratory TMH experiments on discrete fractures from the Yucca Mountain site that extend the fracture closure into the linear part of the curve describing normal stress versus fracture closure. These experiments should be designed to measure the response of the fractures to both normal and shear stresses. In addition, either the samples should be thermally loaded, or the experiment should be run under displacement-controlled boundary conditions that incorporate the computed response of the rock to the thermal load. Pore space changes and contact areas should be established by fixing the pore space at specified stresses.

2. Develop and incorporate a suite of resin injection experiments at the SHT site, and later at the DST site, to establish the geometry of the discrete fractures and the nature of the fracture pore space as well as the interaction between the matrix pore space and the fracture pore space.
3. Use a series of weakly coupled numerical codes to evaluate the linkages and impacts produced by the near-field coupled processes. These models must be 3-D and must incorporate realistic stress and displacement boundary conditions as well as discrete fractures.
4. Change the proposed operational mode of the proposed repository to include ventilation to keep the drifts below 100°C.

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## **ELICITATION SUMMARY**

### **ROGER D. HART**

#### **OVERALL PROCESSES**

The thermal perturbation of the near-field/altered zone environment produces a coupled response among thermal, hydrologic, chemical, and mechanical processes. Resolving technical issues related to these processes requires analytical methods that account for the coupling effects. A method that incorporates the full coupling of these processes would be very difficult to develop; the alternative is to develop methods that partially couple processes, assuming that certain processes are more important than others. This approach may be reasonable if it can be demonstrated that the processes neglected have an insignificant influence on the coupled response.

The partially saturated thermal-hydrologic response may be considered the predominant coupled process affecting the near-field environment. The effect of the thermal pulse on the unsaturated flow regime and the influence of the partially saturated flow on the temperature profile in the host rock may be an important coupled process. Thermal-hydrologic testing at Yucca Mountain appears to demonstrate this coupling (Wilder, 1996). Complicating the understanding of this process, however, are the coupled effects of the geochemical behavior and the geomechanical behavior resulting from the thermal perturbation.

Of all the processes identified, geomechanical behavior appears to have received the least attention. In my view, however, evidence from field-scale testing at Yucca Mountain suggests that geomechanical behavior may have an important influence on the near-field environment. Specifically, thermally induced slip along joints within the host rock may strongly influence both the thermal-hydrologic response of the near-field environment (by

affecting the intrinsic permeability of the joint structure) and the mechanical response of the host rock around the emplacement drifts (by affecting the mechanical stability of the drifts). I believe that evidence from the Single Heater Test performed at Yucca Mountain may be interpreted to suggest this coupled effect, as discussed later in this summary. First, an overview is provided of the potential coupling effects from joint displacement.

### **Coupling Effect of Joint Displacement**

As the rock mass heats, thermally induced mechanical stresses will develop and induce both normal and shear displacements along joints within the rock mass. The orientation of the joint structure relative to the thermally induced stress field is the predominant factor affecting the type and magnitude of the joint displacement. If the magnitude of the stress acting in the normal direction to the joint trace is high relative to that acting in the shear direction, then joint-normal displacement (closure and opening) likely will predominate. If the magnitude of the normal stress is low relative to that of the shear stress, then shear displacement may predominate. In addition, as the joint shears it can also dilate (open). Joint dilation, as a result of joint shearing, is a function of the magnitude of the normal stress acting along the joint and the roughness of the joint: the lower the normal stress and the greater the roughness, the greater the dilation. The rate of dilation generally decreases as shearing continues. This typically is related to the reduction in roughness as the joint is sheared. The joint dilation may be proportional to the amount of slip—the proportionality factor is defined as the tangent of the dilation angle (see Figure RH-1). The dilation angle can also decrease as joint asperities progressively shear off with increasing slip.

As the rock mass cools, it is expected that the thermally induced stresses will also decrease. This process may reduce the normal stress acting along a joint, which in turn will cause the joint to open. If the magnitude of the normal stress is reduced such that shear stress predominates, then shear displacement also may occur, accompanied by further dilation. The shear displacement may also change direction upon cooling; depending on the direction of the shear stresses upon cooling.

Whether the rock mass is heating or cooling, both normal and shear joint displacements can occur in a multiply jointed rock mass; both may occur concurrently, and one type of displacement may be influenced by the other. For example, the stress field around a joint will be redistributed if the joint slips. This redistribution may decrease or increase normal stress acting on other joints, resulting in separation or closure of these joints. Alternatively, if the normal stress across a joint is reduced, in addition to opening, the joint may also shear and dilate, further opening the joint.

Joint displacements in both the normal and shear direction are predominantly nonlinear and irreversible. The response of joint closure/opening to normal loading and unloading generally is hyperbolic, with permanent deformation remaining after the loading is removed. The magnitude of irreversible displacement is affected by several conditions of the joint, including the initial area of contact, the relative roughness, and the strength and deformability of the asperities. As the joint is subjected to repeated cycling of loading/unloading, the irreversibility may decrease; however, this decrease generally requires several cycles of loading/unloading at relatively high normal stress. Bandis et al. (1983) describe an extensive study of a variety of joints that illustrates this response to normal loading.

The joint response to shear loading also is primarily nonlinear and irreversible. Once the peak shear resistance of the joint has been reached, the joint will undergo a shear displacement that is almost entirely irreversible upon unloading. The dilation that occurs after the peak shear resistance is reached also is predominantly irreversible. The irreversibility in the shear and normal directions is principally due to the damage that occurs to the joint asperities as the joint is sheared. Several investigators (e.g., Huang et al., 1993) have studied this effect.

The thermal-mechanical response of the joints may also affect the hydrologic behavior of the rock mass. Fluid flow through the space between joint surfaces is expected to be a function of the joint aperture. Opening and closing of the joint as a result of thermally and mechanically induced normal and shear displacements may be expected to have a



strong influence on the intrinsic permeability of the joint. This effect may also be expected to be primarily nonlinear and irreversible as a function of the joint normal and shear displacement. The magnitude of the effect of thermal loading on joint permeability is difficult to quantify. However, it may be expected that if thermally induced joint dilation is significant, then the effect on the intrinsic permeability of the joint may also be significant.

The coupling effects of joint displacements on the thermal-mechanical response and the thermal-hydrologic-mechanical response of the near-field environment are discussed separately below.

### **THERMAL-MECHANICAL (TM) EFFECTS (DRIFT STABILITY)**

Mechanical stability of the near-field environment at Yucca Mountain concerns the long-term behavior of the host rock and the repository liner in response to time-dependent processes. The repository drift may be stable during the initial emplacement operation, but may become unstable later during the peak heating period or during cooldown periods. Time-dependent processes that occur during the thermal evolution of the repository may produce the unstable conditions.

Two processes are considered to have a dominant effect on mechanical stability: thermally driven stress change, and strength degradation of the host rock and liner materials. Mechanical instability can occur as a result of (1) changes in the stress state and deformation in the host rock and liner as a result of the transient thermal load, and/or (2) reduction in strength of the host rock and liner, due to the stress level, moisture content, and temperature, which eventually may result in failure and collapse of the liner and possibly fall of rock blocks into the drift. Thermally driven stress changes can occur solely from thermal and thermomechanical causes. Strength degradation can occur from various coupled effects involving thermal, thermo-mechanical, and chemical processes.

Other time-dependent processes also may affect stability. For example, change in

groundwater flow in the rock matrix or fractures can change effective stresses, whereby the apparent material strengths may be reduced or increased. Time-dependent strains may also be introduced by groundwater changes, as fluid is expelled from or introduced into void spaces or fractures. The material may exhibit true creep behavior in which material deformation takes place under deviatoric stresses until the deviatoric stresses fall below some threshold. These processes, however, are considered to have less influence on the mechanical stability than thermally driven stress change and strength degradation.

## **THERMALLY DRIVEN STRESS CHANGE**

### **Process Description**

To evaluate mechanical stability as a function of thermally driven stress change, it is important to consider the types of failure modes that can result from thermal and thermomechanical causes. Instability in an unsupported jointed rock mass may result from either failure within the intact rock blocks or failure along the discontinuities. For example, the change in temperature field can induce deviatoric stresses within the intact rock that eventually produce an unstable shear stress state. Also, the increase in temperature can induce expansion within the rock that may result in tensile failure of the rock. Alternatively, thermal heating can induce shear and normal displacements along discontinuities in the rock mass that eventually result in slip or separation failure on the discontinuities. If the rock mass is supported by a thick concrete liner, an increase in temperature also may induce deviatoric stresses in the liner that produce shear failure, or tensile stresses that induce tensile failure.

Both the strength and deformation properties of the intact rock, rock joint structure, and liner material should be characterized when evaluating mechanical stability.

When defining properties, the conventional approach is to assume that the intact rock behaves as an isotropic elastoplastic material that has a continuum failure mode described by a Mohr-Coulomb failure envelope and tensile strength limit. The rock joint typically is characterized by a normal stiffness, a shear stiffness, and a

discontinuum failure mode described by a Coulomb slip criterion and tension cutoff. Failure of a concrete liner also is conventionally described by a Mohr-Coulomb criterion and tensile strength limit.

The thermal and mechanical properties associated with the failure modes of a jointed rock mass are summarized as below.

- thermal and index properties
  - mass density
  - thermal conductivity
  - specific heat
  - linear thermal expansion coefficient
- rock mass deformability properties
  - rock mass modulus
  - Poisson's ratio
- rock mass strength properties
  - cohesion
  - angle of internal friction
  - dilation angle
  - tensile strength
- rock joint-structure properties
  - rock joint geometry (dip angle, dip direction, spacing, persistence)
  - joint normal and shear stiffness
  - joint friction angle
  - joint cohesion
  - joint dilation
  - joint tensile strength

It can be difficult to define all of these properties at a reasonable level of certainty.

However, it may not be necessary to do so, if certain failure modes have a more

pronounced effect on mechanical stability than others. For example, if the continuum failure of the rock blocks dominates the mechanical response of a jointed rock mass, then emphasis should be placed on characterizing the rock mass strength. If the discontinuum failure of the rock joint structure dominates the response, then the emphasis should be placed on characterizing the rock joint parameters.

#### **Assessment of the Dominant Failure Mode**

The field-testing program at Yucca Mountain's Exploratory Studies Facility should help determine which failure process will be dominant during the thermal evolution of the repository. From my assessment of the field-testing programs completed to date, the Single Heater Test appears to provide the best information on failure processes that can affect mechanical stability.

The Single Heater Test measures the mechanical response of a large block (13m x 10m x 5m) of the welded tuff rock mass when subjected to thermal loading. The test is essentially an unconfined test, because three of the six sides of the block are unconstrained. The horizontal 5m-long heat source located in the center of the block provides the thermal load (approximately 4000 W). The mechanical response of the rock mass is monitored primarily by extensometers aligned both parallel and perpendicular to the axis of the heat source. In addition, wire and tape extensometers located along the free faces of the block monitor the response at the block walls.

The measurements and observations recorded from these extensometers during thermal loading provide insight into the mechanical response and potential failure modes of the rock mass. The rock mass properties derived from the Single Heater Test (as reported in TRW, 1997) are summarized in Table RH-1.

**TABLE RH-1**  
**ESTIMATES OF THERMAL AND MECHANICAL PROPERTIES**  
**FROM THE SINGLE HEATER TEST**  
**(from TRW, 1997)**

thermal conductivity	(2.0 W/(m °K))		
specific heat	(953.0 J/(kg °K))		
thermal expansion coefficient	$(5 \times 10^{-6} / ^\circ\text{C})$		
rock mass modulus	(3 – 23 Gpa)		
joint spacing	30 cm		
joint set	1	2	3
dip direction	40°	130°	300°
dip angle	70° - 85°	70° - 90°	15° - 40°

The following observations were reported.

1. The thermal expansion coefficient for the rock mass was lower than that measured in the laboratory. A value of approximately  $5 \times 10^{-6} / ^\circ\text{C}$  was estimated from the final thermal measurements. The laboratory measurements indicate a value of approximately  $10 \times 10^{-6} / ^\circ\text{C}$ . The laboratory testing also suggests that the thermal expansion coefficient increases with increasing temperature, an effect that was not evident from the field test.
2. The rock mass modulus was lower than that measured in the laboratory. The field-scale modulus was measured to range from approximately 3 Giga Pascals (Gpa) to 23 GPa. The laboratory modulus is estimated to be 34.5 GPa. The field test measurements suggested that the modulus increased as a function of increasing temperature, which may imply that thermally induced stresses cause the rock mass to stiffen.

3. The extensometers parallel and perpendicular to the heater displayed both expansion and contraction during the heating period. The extensometer measurements parallel to the heater (BX-1 and BX-3) indicated a general expansion for roughly the first 50 days of heating. Then, the rate of expansion generally decreased, and for some of the measurements the relative displacement changed from expansion to contraction. The extensometer perpendicular to the heater (BX-4) indicated a general contraction behavior during early heating (for roughly the first 20 days), then expansion. However, some contraction was observed at late heating times for selected points.
4. A "gross surface displacement" was indicated to occur along the south side of the block near the wire and tape extensometers (WX-3 and WXM-3) after roughly 50 to 150 days. The displacement was suggested to be due to loosening of a block of rock.
5. Water was observed to flow from boreholes 16 and 18, which are in the vicinity of WX-3 and WXM-3, during the heating period.

The reported assessment of the mechanical response, based on the observations and measurements, was that thermally driven fracture closure was primarily responsible for the observed behavior. Both the lower thermal expansion coefficient for the rock mass and the changing expansion/contraction behavior observed from the extensometers were suggested to be a result of closing fractures. The conceptual model for the behavior is illustrated in Figure 6-37 from the Single Heater Test Status Report, August 29, 1997 (TRW, 1997).

The report considered only an adjustment of the rock mass deformability and strength properties to account for closure of joints. This decision implies that the mechanical response to thermal loading may be simulated by degrading the continuum properties to account for the influence of joint closure. Mechanical stability then would be evaluated in terms of an equivalent continuum representation of the jointed rock mass.

### **An Alternative Assessment of the Dominant Failure Mode**

The above assessment neglects slip along joints as an influence on the mechanical response. I suggest an alternative assessment that the reported measurements and observed behavior of the test block exhibit the effect of thermally induced slip along rock joints.

I will present a two-phase analysis to test this alternative assessment. In the first phase, a three-dimensional (3D), linear thermoelastic analysis is performed to provide a base case for comparing the reported measurements. In the second phase, a simple conceptual model is proposed to explain qualitatively the observed behavior. The conceptual model is tested using a two-dimensional (2D) distinct element analysis.

The 3D thermoelastic analysis was performed with FLAC3D. Figure RH-2 shows the model grid of the heated block region. Four parameter cases were evaluated for their thermoelastic properties. The properties for each case are listed in Table RH-2. The four cases study the effect on the mechanical response of three values for the linear thermal expansion coefficient:  $5 \times 10^{-6} / ^\circ\text{C}$ ,  $10 \times 10^{-6} / ^\circ\text{C}$ , and  $20 \times 10^{-6} / ^\circ\text{C}$ , and two values for the rock mass modulus: 15 GPa and 32.4 GPa. In the model, relative displacements were monitored at locations corresponding to extensometers MPBX-3 and MPBX-4. The model simulated a thermal heating period of 270 days.

Figures RH-3 and RH-4 compare the results for case 2 to the MPBX-3 and MPBX-4 measurements. (The results for all four cases were presented at NFEE Workshop 3.) The results indicate that the displacements monitored at MPBX-3 and MPBX-4 in the FLAC3D model generally are of the same order of magnitude as the measured values. Also, the contraction/expansion behavior measured in MPBX-4 is generally reproduced in the FLAC3D results. However, the FLAC3D results indicate a monotonic expansion in the MPBX-3 direction and do not display the expansion/contraction behavior measured along MPBX-3.

The results are sensitive to changes in the linear thermal expansion coefficient. At early times (within approximately the first 50 days), the value of  $20 \times 10^{-6} / ^\circ\text{C}$  provides the closest agreement with the measured response for MPBX-3. At late times (150 to 270 days), the value of  $5 \times 10^{-6} / ^\circ\text{C}$  provides the closest match to the MPBX-3 displacement/time slope. The value of  $10 \times 10^{-6} / ^\circ\text{C}$  appears to provide the closest agreement with the MPBX-4 measurement.

The results are not sensitive to changes in rock mass modulus. The calculated displacements for MPBX-3 and MPBX-4 are the same for the two different modulus values (cases 2 and 3). I consider this result to be an effect of the boundary conditions imposed for the Single Heater Test (SHT). The experiment is essentially unconfined on the sidewalls. As the rock heats, the displacements developed primarily as a function of thermal expansion.

**TABLE RH-2**  
**SINGLE HEATER TEST PROPERTIES**

	Case 1	Case 2	Case 3	Case 4
<b>elastic properties</b>				
mass density (kg/m <sup>3</sup> )	2500	2500	2500	2500
Young's modulus (Pa)	1.50E+10	1.50E+10	3.24E+10	3.24E+10
Poisson's ratio	0.15	0.15	0.15	0.15
bulk modulus (Pa)	7.14E+09	7.14E+09	1.54E+10	1.54E+10
shear modulus (Pa)	6.52E+09	6.52E+09	1.41E+10	1.41E+10
<b>thermal properties</b>				
conductivity (W/m-K)	2.0	2.0	2.0	2.0
specific heat (J/kg-K)	953	953	953	953
heat capacity (J/m <sup>3</sup> -K)	2.38E+06	2.38E+06	2.38E+06	2.38E+06
linear thermal expansion (/°C)	5.00E-06	1.00E-05	1.00E-05	2.00E-05



The results suggest that linear thermal expansion coefficient for the rock mass decreases with increasing temperature. This is opposite to the behavior reported from laboratory-scale tests. The change in rock mass thermal expansion coefficient is also indicated from the changing expansion and contraction behaviors observed in the extensometer data.

My alternative assessment for the observed behavior is that localized slip on favorably oriented joints within the rock block is primarily responsible for the changing thermal expansion behavior. A conceptual model to explain this changing behavior is illustrated in Figure RH-5. For example, if two extensometer measurement points are located on opposite sides of a slipping joint (e.g., points A and B in Figure RH-5), it may be possible for one measurement to indicate a monotonic extension (B-O), while the other indicates extension followed by contraction as the joint slips (A-O).

This conceptual model was tested with a 2D distinct element model using UDEC. A model was created with one through-going joint oriented at the approximate dip direction of joint set 2 (see Table RH-1). The joint was positioned so that it intersects two positions corresponding to extensometer measurement locations. Points A, B, and O in the UDEC model correspond to the same positions in Figure RH-5. If the joint is "glued," it will not influence the thermally induced stress state and extensometer measurements.

However, if the joint is allowed to slip, a stress concentration localizes along one side of the joint. Also, the relative displacement measured between points on opposite sides of the joint can be made to change from extension to contraction (see Figure RH-6). Note that at approximately 50 days of heating, the bottom boundary of the UDEC model is prevented from moving. When this is done, the A-O measurement changes from extension to contraction. Note, however, that the B-O measurement, located below the joint, continues to show extension.

Although it was necessary to fix the bottom boundary in the 2D model to produce the

extension/contraction response, this should not be necessary in a 3D model. The 3D confinement may be sufficient to produce a similar response.

Also, the apparent rate of change of displacement of A-O during the first 50 days is greater for the slipping joint model than for the glued-joint model. This effect implies that joint slip may contribute to an increase in the rock mass thermal expansion, as was observed in the measurements.

The slipping joint also produces a discontinuity in movement at the right boundary of the model. This discontinuity in movement is qualitatively similar to that observed along the south side of the SHT block, suggesting that joint slip may have been responsible for the gross surface displacement recorded at WX-3 and WXM-3. Further, if joint slip does occur and the joint dilates, fracture permeability can increase, explaining the observed water flow at boreholes 16 and 18.

The preliminary conclusion of this assessment is that mechanical instability may be initiated by localized joint slip. The observed displacements from the SHT appear to be affected strongly by slip along individual joints. If this finding is further supported by the Drift Scale Test, then it may be reasonable to assume that localized joint slip may have a significant influence on the deformation of the rock mass around emplacement drifts and the initiation of a mechanically unstable condition.

The possible role of localized joint slip also implies that the orientation of rock joints relative to the emplacement drift may be an important property for the assessment of mechanical instability. For example, it appears that joint set 2 in the SHT may have been more favorably oriented to slip during heating than were the other two joint sets.

#### **Evaluation of Mechanical Instability due to Thermally Driven Stress Change**

The assessment of mechanical stability may require an analytical approach that accounts for the effect of localized joint slip. The distinct element method, as embodied in codes such as UDEC (in 2D) and 3DEC (in 3D), is such an approach.

A simple UDEC model of an emplacement drift is shown in Figure RH-7. Two joint sets are represented in this model: one corresponds to a vertical set (joint set 1 or 2), and the other to a horizontal set (joint set 3). By assuming that one set is vertical and the other horizontal, it is possible to impose a vertical plane of symmetry through the center of the drift and reduce the model in half. The joint spacing in this model is 30 cm.

A heat source can be applied to the model to represent the thermal loading from the waste package. For example, in the simple UDEC model, a heat source is located at the base of the drift. For demonstration purposes, a constant heat strength is applied to reach a temperature of approximately 200°C in about 40 days. Thermally induced stresses within the model loosen a wedge of blocks near the base of the drift. This wedge moves into the excavation, as illustrated in Figure RH-8. Note that this analysis is only to demonstrate that localized instability may occur from thermally driven stress change.

A liner could prevent this movement. A liner can be simulated by introducing liner elements in the UDEC model. The liner could be allowed to fail and/or be removed later in an analysis to simulate the time-dependent collapse of the liner. For example, at the peak heating period or during the cooldown period, the thermally induced stress change may cause different joints to slip and blocks to loosen around the drift when the liner is removed.

## **STRENGTH DEGRADATION**

### **Process Description**

Material degradation implies that the long-term strength of a material is significantly lower than the short-term strength. Degradation can result from progressive micro-fracturing due to the change in stress experienced by the material. For example, the mechanism of stress corrosion is related to stress level, moisture content, and temperature. Strengths and moduli are reduced as a function of these variables and time. Brittle rock and concrete may exhibit stress corrosion.

Alternatively, strength may change as a result of crystallization of the material at elevated

temperatures. This is another a time-dependent process that can produce strength degradation.

Concrete and rock are brittle heterogeneous materials that exhibit inelastic deformation because of the existence and formation of numerous microcracks. Under increased load, these microcracks coalesce into macrocracks, or fractures. For example, thermal-chemical processes may cause the formation of microcracking in concrete; these cracks may coalesce into fractures as the temperature increases. This process may affect the long-term mechanical stability of the concrete liner. If cracking coalesces to form notches in the liner surface, stress concentrations may develop near the notch and ultimately trigger localized failure. The failure may then progress until the liner collapses. It is important, then, to understand the process that causes this notch to form.

#### **Evaluation Approach**

Concrete at ambient temperatures may exhibit an insignificant decrease in strength for long periods. It has been demonstrated that concrete structures can last for hundreds of years. However, few data exist on the long-term strength of concrete structures at elevated temperature. This information is critical in order to evaluate strength degradation effects on a lined drift. The first step in evaluating strength degradation should be to collect data on the temperature dependency of concrete's strength.

Once this information is available, the next step is to develop a modeling approach that can represent the mechanism producing the time-dependent behavior. The modeling approach can then be used to estimate long-term mechanical stability.

Two approaches may be taken to simulate time-dependent strength degradation. One is an indirect approach in which the material is idealized as a continuum, and average measures of material degradation are used in constitutive models to represent the irreversible microstructural damage. The other is a direct approach in which the material is idealized as a collection of particles bonded together at contact points; the breakage of the bonds is used to simulate progressive damage of the material.

The difficulty with the indirect approach is that it assumes a uniform reduction in strength and cannot adequately represent the strong dependence of the rate of degradation on localization (i.e., the development of shear bands). Local cracking can cause load transfer, which thereby can degrade strength at an increased rate.

The direct approach can adequately simulate this localization if a sufficient number of particles can be prescribed to represent the microcracking process. Increases in computing power have made it feasible to model large boundary-value problems with direct approaches. An example is the Particle Flow Code (PFC), which currently is being used to simulate the development of excavation damage around the Test Tunnel of the Mine-by Experiment at the Underground Research Laboratory (URL) in Canada (Potyondy and Cundall, 1998). PFC is simulating the time-dependent development of notches in the regions of compressive stress concentration in the roof and floor of the circular test tunnel at URL. A micromechanical stress-corrosion model (i.e., a time-dependent cracking model that depends on load, temperature, and moisture) is being developed in PFC to reproduce the strength degradation. The model reproduces the behavior of rock specimens subjected to static-fatigue tests and also produces notches when applied to tunnel excavation conditions.

I believe that a similar approach could be followed to evaluate strength degradation of the concrete liner for the emplacement drifts. It should be possible to simulate the liner material using a direct method such as PFC. The time-dependent strength degradation could then be reproduced in the model so that mechanical stability could be evaluated.

### **THERMAL-HYDROLOGIC-MECHANICAL (THM) EFFECTS**

To evaluate the impact of thermal loading on fracture permeability throughout the host rock, it is useful to define this permeability for the Yucca Mountain setting. In this case, the host rock is considered to be unsaturated, and two-phase (gas-liquid) flow may occur defined by an effective fracture permeability for the gas and for the liquid. The effective

permeability may be defined as

$$k_g = k k_{r,g} \quad \text{for the gas}$$

$$k_l = k k_{r,l} \quad \text{for the liquid}$$

The intrinsic permeability of the fracture typically is defined as

$$k = a^2 / 12$$

based on the assumption of parallel-plate flow, where  $a$  is the fracture aperture. If the intrinsic permeability is normalized to a unit thickness perpendicular to the fracture, the cubic flow law is obtained. The relative permeabilities of the gas and liquid, respectively, are strong and nonlinear functions of phase saturation. If  $k_{r,l} = 1$ , then the fracture is completely saturated with liquid, and if  $k_{r,g} = 1$ , then the fracture is completely saturated with gas. However, the sum  $k_{r,l} + k_{r,g}$  typically is much less than 1, indicating that each phase interferes strongly with the flow of the other.

Thermal loading will affect both the intrinsic and relative permeability. Most of the studies at Yucca Mountain have focused on understanding the effects of thermal loading on relative permeability. Little information is available on the effect on intrinsic permeability.

#### Effect of Thermal Loading on Intrinsic Permeability

As noted above, intrinsic permeability is a function of fracture aperture. The change in aperture is a function of the normal displacement (i.e., opening and closing) of the fracture. Typically, closure of a dry rock joint varies hyperbolically with compressive stress. At high compressive stresses, a large increase in compressive stress results in a small increase in closure. At low compressive stresses, a small increase in compressive stress results in a large increase in closure. When a joint contains a fluid or gas, the joint closure is determined, in part, by the fluid compressibility.

Joint apertures are affected by changes in shear and normal displacements of the joint. Because of the strong dependency of intrinsic permeability on aperture, the effective permeability for the gas and the liquid also may be strongly influenced by aperture change. When assessing the impact of thermal loading on fracture permeability, it is important to know how strongly thermal loading affects the intrinsic permeability versus the relative permeability. The effect of thermal loading on intrinsic permeability typically is neglected. However, computational methods are available to evaluate this effect.

One approach is to use a continuum model and determine regions of slip based on a slip condition such as

$$F_s = (\sigma_n \tan \phi + c) / \tau_n$$

where  $\sigma_n$  is the normal component of the stress tensor on the plane with normal  $n_i$ ,  $\tau_n$  is the magnitude of the shear component of the stress tensor on the plane with normal  $n_i$ , and  $\phi$  and  $c$  are the friction angle and cohesion associated with the plane. Thus,  $F_s < 1.0$  indicates slipping in the rock along the the plane with normal  $n_i$ . An extension to this approach is to use a ubiquitous joint model, which represents the effect of rock joints by a continuum elasto-plastic model with anisotropic strength, i.e., predefined planes of weakness. Both of these models can predict slip regions, but it is difficult to assess the change in intrinsic permeability because we lack a relation linking deformation to change in permeability.

An alternative approach is the distinct element method, which can explicitly simulate the effect of joints and the effects of aperture change on intrinsic permeability. In the distinct element codes UDEC (in 2D) and 3DEC (in 3D), normal displacement of a joint is a direct function of normal stress, via joint normal stiffness, and joint shear stress, via joint dilation angle. The codes define the dilation component as depicted in Figure RH-1. The effect of joint opening and closing can also be coupled to a cubic-law fracture flow relation, or to other flow relations.

Studies are ongoing to evaluate the effects of thermal loading on fracture permeability during the Drift Scale Test, using both the continuum and distinct element methods described above (e.g., see Damjanac and Fairhurst [1998]). The results of these analyses identify dilation as a critical parameter in assessing the impact of thermal loading on fracture permeability. The analyses also suggest that fracture permeabilities may increase (as a result of joint slip and dilation) along the sub-vertical joint structure and decrease (due to joint closure) along the sub-horizontal joint structure. (This response may be missed in a continuum analysis.)

A natural extension of the fracture permeability model in the distinct element method would be to incorporate relative permeability with intrinsic permeability by adding a two-phase flow algorithm to the fracture flow model. Such a model would make it possible to assess the relative effects of thermal loading on phase saturation versus aperture change.

## **DURABILITY OF EFFECTS**

Displacements of joints within the host rock are primarily nonlinear and irreversible. If thermally driven shear displacement of the joints occurs, I believe it is reasonable to expect an associated dilation that may also be primarily irreversible. I also expect that if the joints dilate, the intrinsic permeability of the joints will increase. It is difficult to assess the relation between the joint opening/closing and the change in intrinsic permeability. However, I believe this information is important for evaluating the significance of coupling the geomechanical behavior of the host rock with the thermal-hydrologic response.



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## RECOMMENDED ACTIVITIES TO REDUCE UNCERTAINTIES

- **Evaluate Alternative Design Measures**

I believe that the most viable approach to reduce uncertainties related to the thermal perturbation of the near-field environment is to consider alternative design measures for the emplacement drifts. Practical alterations of the design may be shown to reduce the uncertainties related to both the mechanical stability in the near field and the magnitude of the effect of thermal loading on joint permeability. There are several components of the drift design that might be altered to minimize the adverse effects of the thermally driven stress change and strength degradation processes. Figure RH-9 illustrates some of the components that may be considered. (This figure was provided by Professor Charles Fairhurst [Itasca Consulting Group] after discussions concerning the drift design issues.) For example, it may be possible to alter the size and shape of the drift to increase its stability. The size should be as small as convenient. Alternative shapes should be evaluated; e.g., a slight increase in height of the excavated roof could be considered to increase dynamic stability. A lightweight fill designed to deflect water to the sides of the tunnel could be placed in the gap between the liner and the roof. A combination of support measures may be appropriate, such as noncorrosive bolts and thermally resistant liner materials, or materials that can withstand long-term deterioration. The study by Potyondy and Cundall (1998) demonstrates a relatively new analytical approach to evaluating long-term deterioration of materials, such as concrete and rock joints, under various environments (elevated temperatures, induced stresses, etc.). Other long-term considerations may be self-shielding canisters and ventilation cooling.

- **Assess the Importance of Joint Shear and Normal Displacement**

I believe it is important to determine whether thermally induced joint displacement, and specifically slip along joints, has a strong influence on the behavior of the near field during the thermal perturbation. It should be possible to evaluate this influence based on field testing. For example, acoustic emission (AE) monitoring can be utilized to ascertain locations of rock damage during the thermal loading/unloading

cycle. It may then be possible to correlate this information to locations of specific joint structure in the host rock. In addition, it may be possible to compare the field AE distributions (in magnitude, location, and time) to results of discrete element numerical analyses and thus provide a quantitative link between the AE data and thermally induced joint slip. Similar field testing is being conducted for the Tunnel Sealing Experiment at the URL in Canada. This testing is being performed by Dr. Paul Young and his research group at Keele University, United Kingdom (e.g., see Talebi and Young, 1990, and Martino et al., 1993, for a description of AE monitoring). I recommend that his methods be reviewed for possible application to the Drift Scale Test.

- **Analyze the Coupling Effect of the Joint Displacement**

*Need for Discontinuum Analyses.* I recommend discontinuum analyses to evaluate the influence of joint orientation and spacing on the drift stability and the extent of joint shear and normal displacements throughout the host rock during the heating period. It should be possible to validate these analyses by comparison to field test measurements and observations. Specifically, locations of localized failure, identified by distinct block movements and localized inflows of water, should be identified for comparison to discrete element models. These comparisons also should help confirm whether thermally induced joint slip is significant.

Discontinuum analysis should be viewed primarily as a numerical testing approach to help understand the influence of joint structure on the thermal-hydrologic response. These analyses may compliment continuum calculations and help identify limitations in the continuum models. (A possible limitation in applying a continuum approach to represent the observed mechanical behavior in the Single Heater Test is noted above.) It may be feasible to adapt modified continuum models, such as the ubiquitous joint model, to apply to drift-scale analyses. However, it may prove difficult to represent thermally induced normal and shear joint displacements and their coupling influence in a continuum model.

For sub-horizontal and sub-vertical orientations of joint sets, a full two-dimensional model of the emplacement drift will be required, and a three-dimensional analysis may be necessary to represent the combined influence of the three joint sets. These models would require fairly substantial amounts of computer RAM. However, it should be possible to perform a series of model runs for a reasonable variation of conditions in order to define joint orientations that are more susceptible to slip during early, peak temperature, and cooldown periods. It is not necessary to include the joint structure in absolute detail in the model; the influence of joint structure on the behavior of the host rock can be evaluated even if the joint spacing in the model does not coincide with that measured in the field. Validating the model with field test data should help assess the level of detail required in the model.

It may be appropriate to create at least two near-field models: one that represents the behavior at the center of the repository, and one that represents the behavior at the repository edge. Joint shear effects are expected to be greater at the edge, because heating from adjacent drifts may increase the normal stress and thus decrease shear effects on joints in the center of the repository.

*Defining an Adequate Data Base for Analyses.* Discontinuum analyses require specific parameters to represent the behavior of the joints as well as the intact rock mass. I believe that the most important data for these analyses are those that identify the rock joint geometry (dip angle, dip direction, spacing, etc.). These data appear to be fairly well characterized within the vicinity of the Single Heater Test and Drift Scale Test. By comparing discontinuum models to field test results, it should be possible to evaluate whether the joint geometry is sufficiently defined for drift-scale analyses.

Of the data related to the mechanical behavior of the joints at Yucca Mountain, information on joint dilation appears to be the least characterized. The data reported by Olsson and Brown (1997) describe a fairly large dispersion in measured dilation

angles for the rock joints. I recommend that additional data be obtained under thermal and mechanical loading conditions representative of those at the drift scale.

A significant uncertainty is the effect of changes in the joint aperture on the intrinsic permeability of the joint. In rock mechanics one commonly assumes a cubic relation between flow and aperture. However, there apparently are few data to confirm this relation for joints subjected to the thermal-mechanical loading conditions at Yucca Mountain. Further, there appears to be a higher uncertainty regarding the relative influence of changes in intrinsic permeability as a function of aperture change, than of changes in effective permeability for unsaturated and two-phase flow.

*Selection of Model Boundary Conditions.* The analysis of mechanical stability in the near field is complicated by both the spatial scale of the repository and the temporal scale of the thermal loading. A numerical model of the near-field environment should contain a fairly detailed representation of the emplacement drift geometry and rock structure; however, the repository covers several thousand square meters. Also, the time frame for thermal heating and cooling may extend for several hundred years. The large areal extent of the repository and the long thermal loading period make it difficult to develop a numerical model of the near-field, because these conditions will affect both the thermal and mechanical behavior over a considerable volume surrounding the repository. Consequently, it will be difficult to determine where to locate artificial boundaries for the numerical model so that the boundaries do not significantly influence the behavior of the area of interest.

The location of artificial boundaries to minimize effects on mechanical response can be different from that to minimize thermal effects. Generally, the boundary should be located roughly 10 times the dimension of the object of interest (e.g., the emplacement drift) from the object so that the effect on stress and displacement is not significant (say less than 5 percent). The location of the artificial boundary to minimize the effect on temperature in the model will depend on the time frame of heating and cooling. These requirements may necessitate the creation of a model

grid that is too extensive to operate in terms of computer memory and computational time.

One way to address this difficulty is to utilize a coarse global (repository-scale) model to determine boundary conditions to apply to the near-field (drift-scale) model. With this approach, temperature and traction profiles are calculated at specified time intervals (say every 20 or 40 years) at a distance of approximately 5 to 10 boundary-to-drift-size ratios above and below the repository. These profiles are then applied as boundary conditions to the near-field model, and the equilibrium state is calculated for each time period. This approach should provide a better representation for actual temperature and traction conditions at the specified time.

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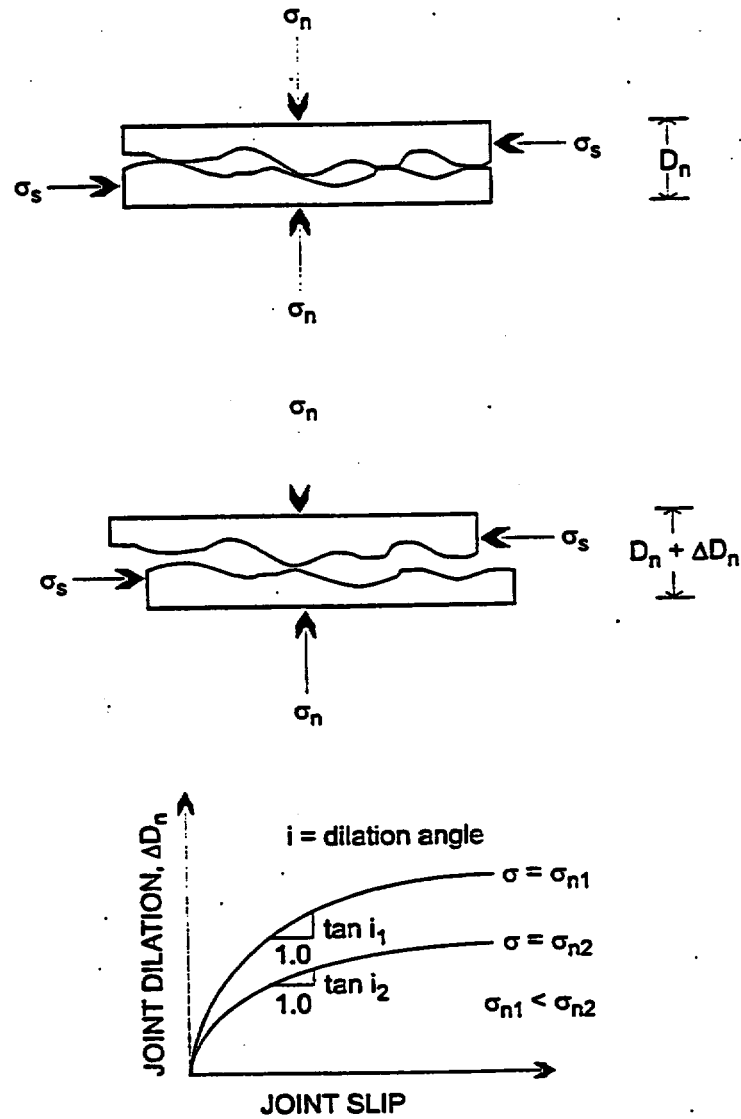


Figure RH-1 Aperture Change as a Function of Joint Slip

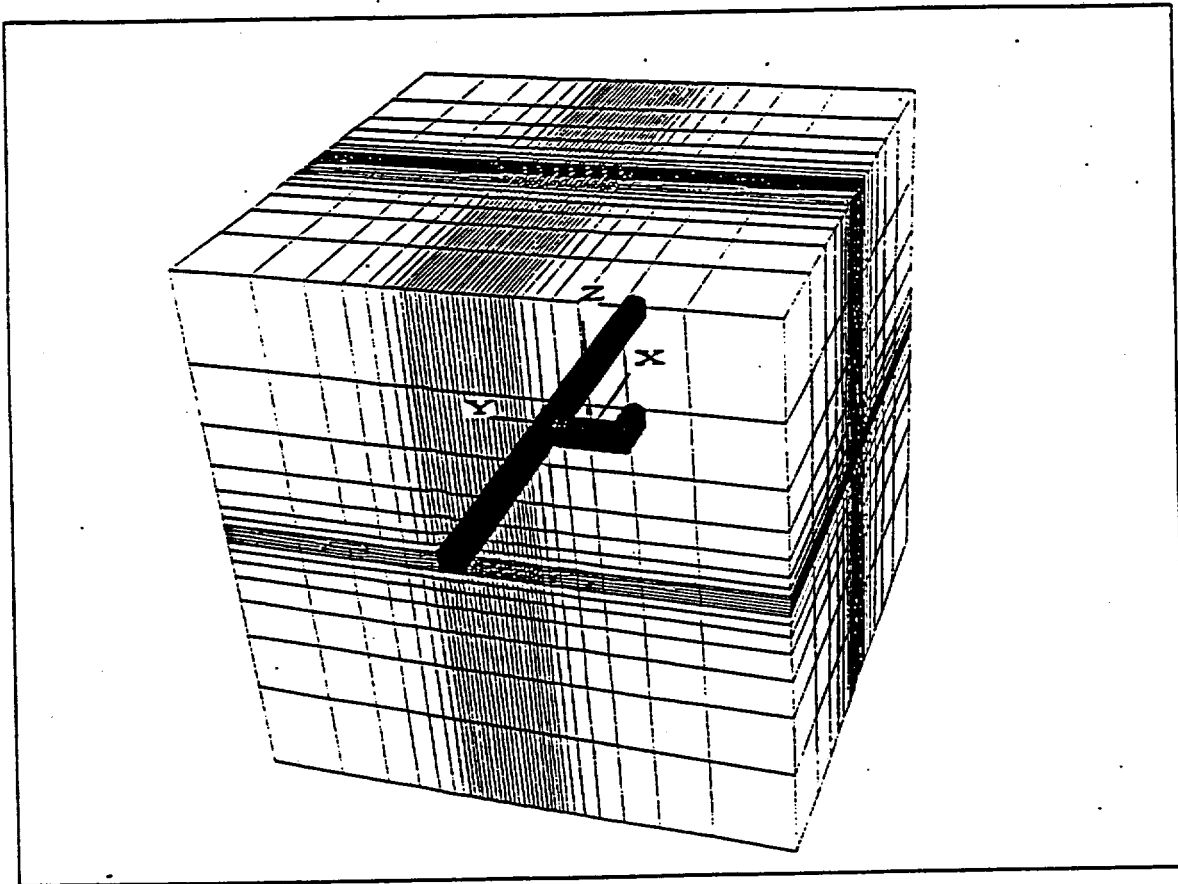


Figure RH-2 FLAC 3D Model Grid



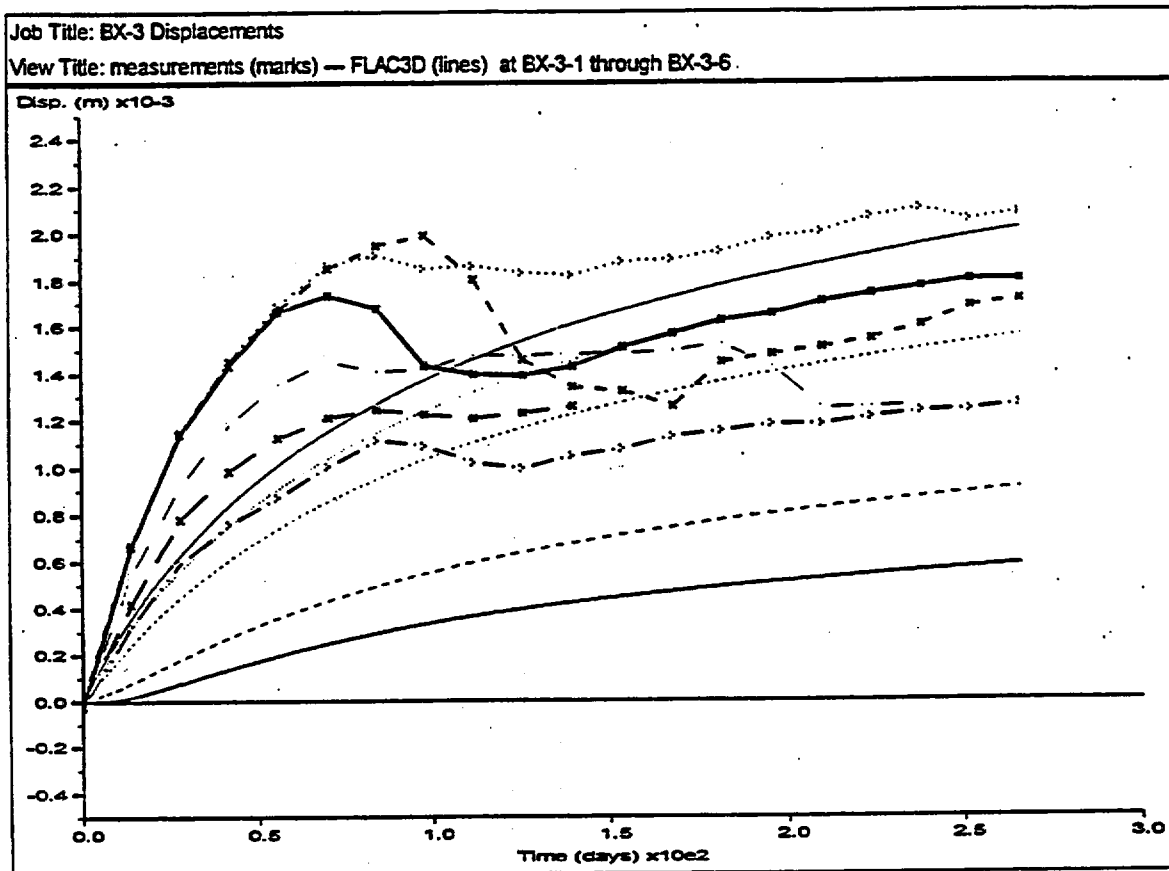


Figure RH-3 Comparison of FLAC 3D Results to MPBX-3 Measurements (Case 2)

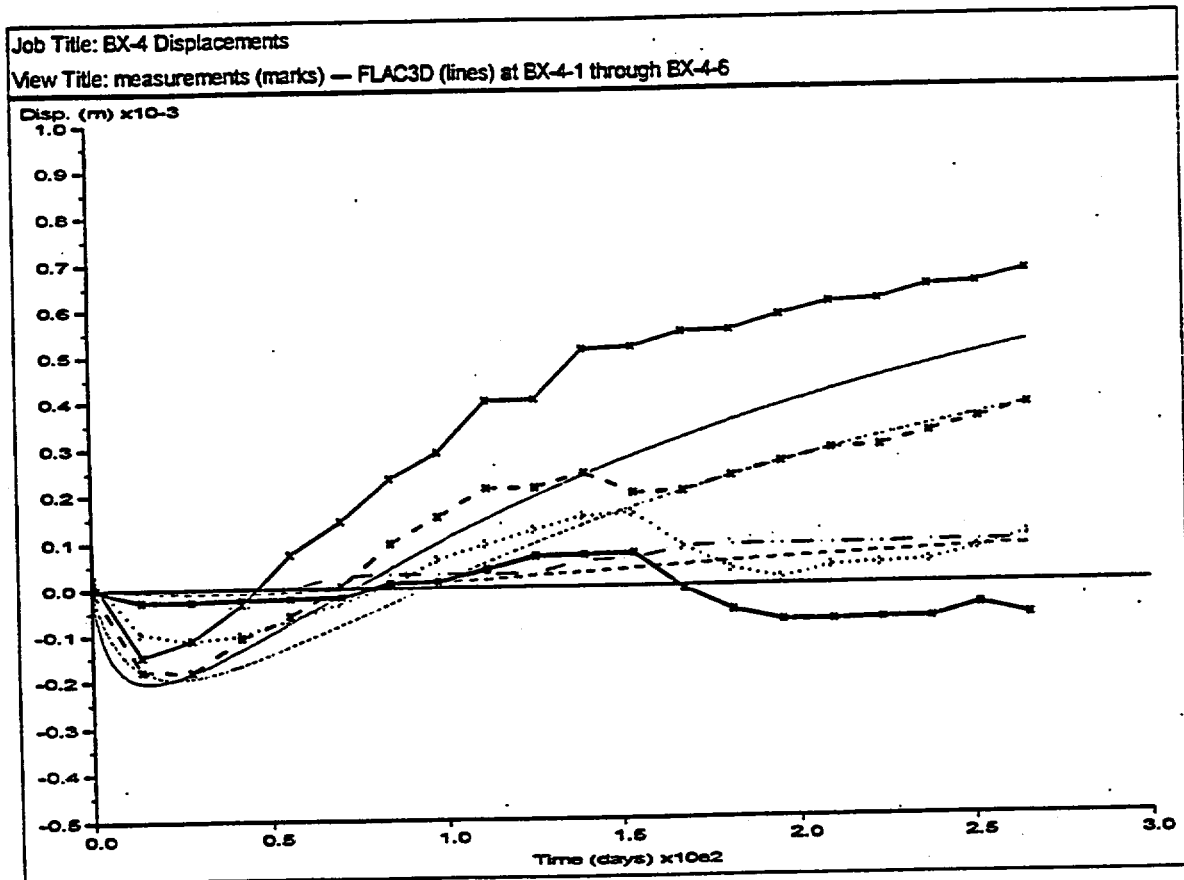


Figure RH-4 Comparison of FLAC 3D Results to MPBX-4 Measurements (Case 2)

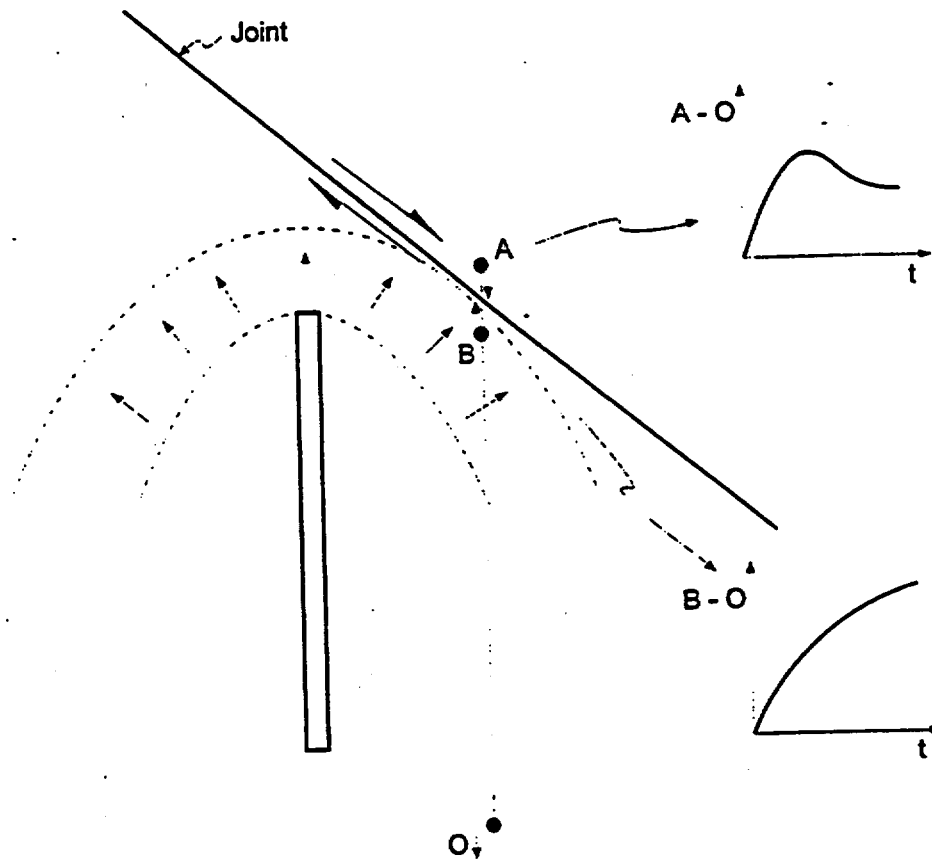


Figure RH-5 Mechanism for Extension/Contraction Behavior of MPBX-3

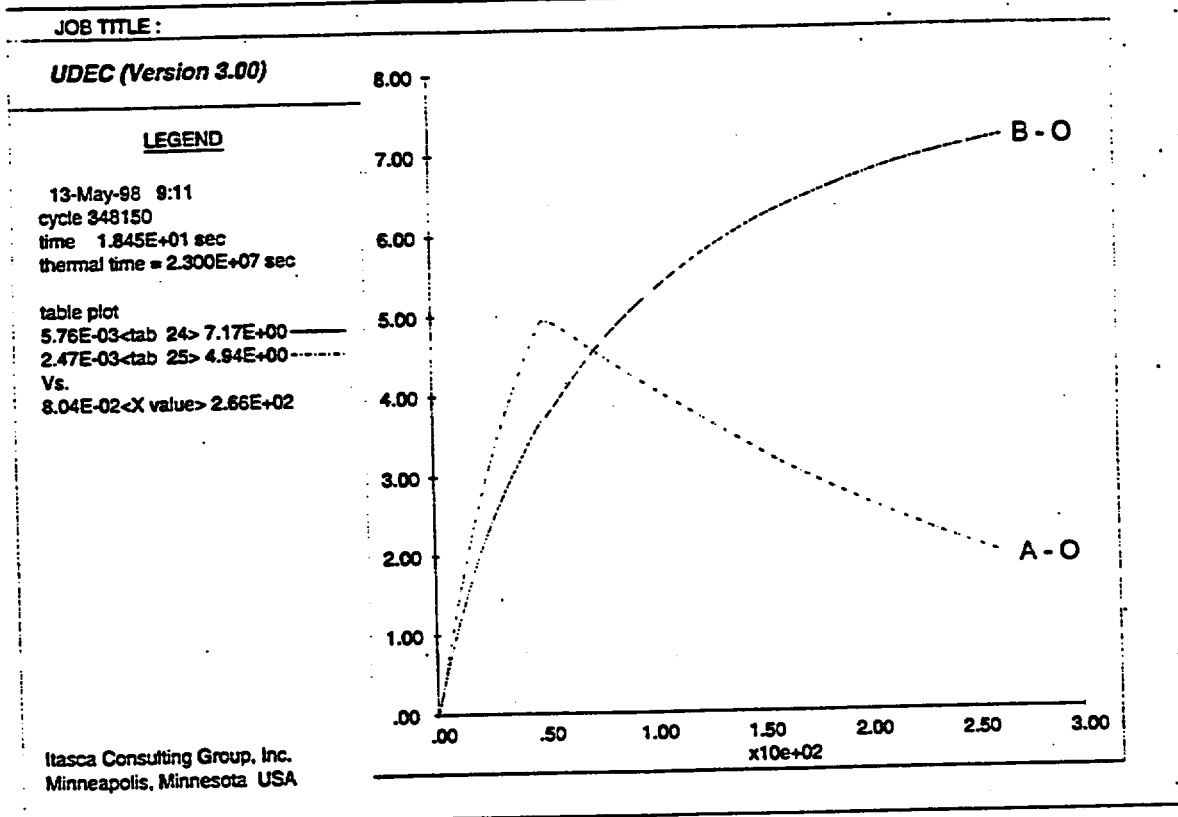


Figure RH-6 A-O and B-O Displacements for Slipping Joint

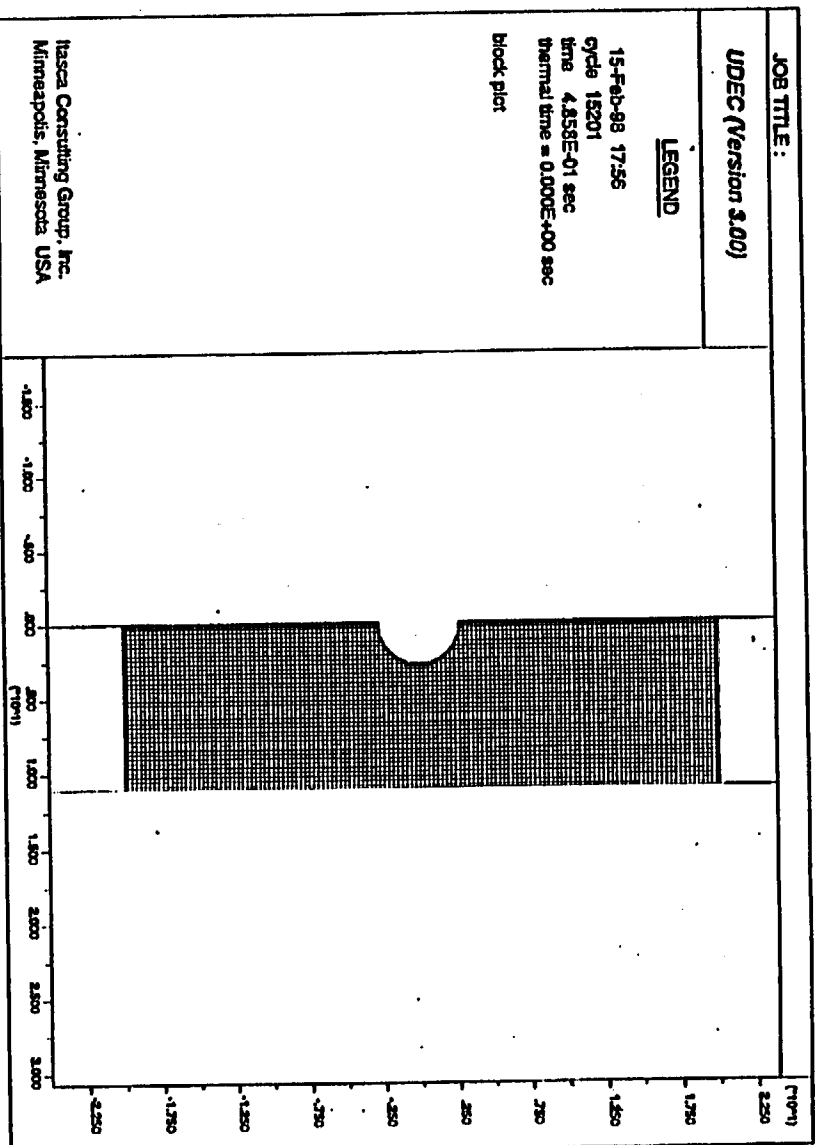


Figure RH-7 Simple UDEC Model for Single Emplacement Drift

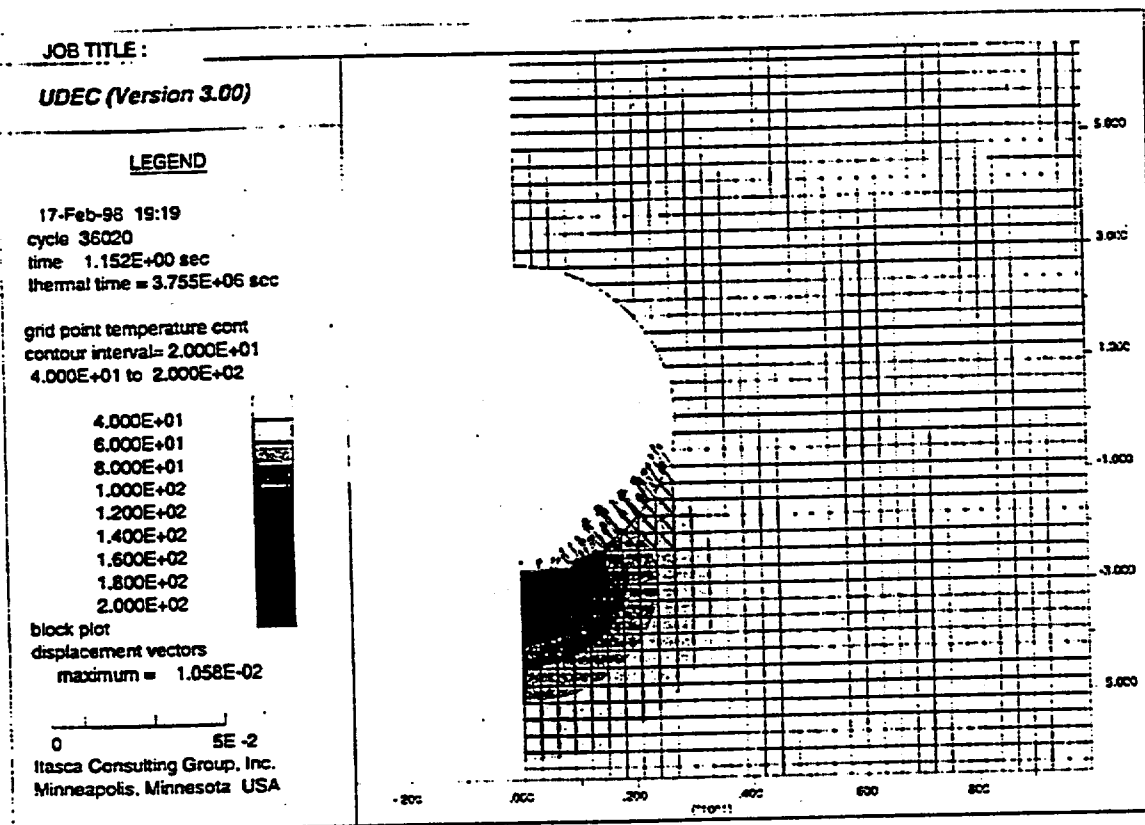


Figure RH-8 Thermally Induced Displacement of Wedge of Blocks into Drift

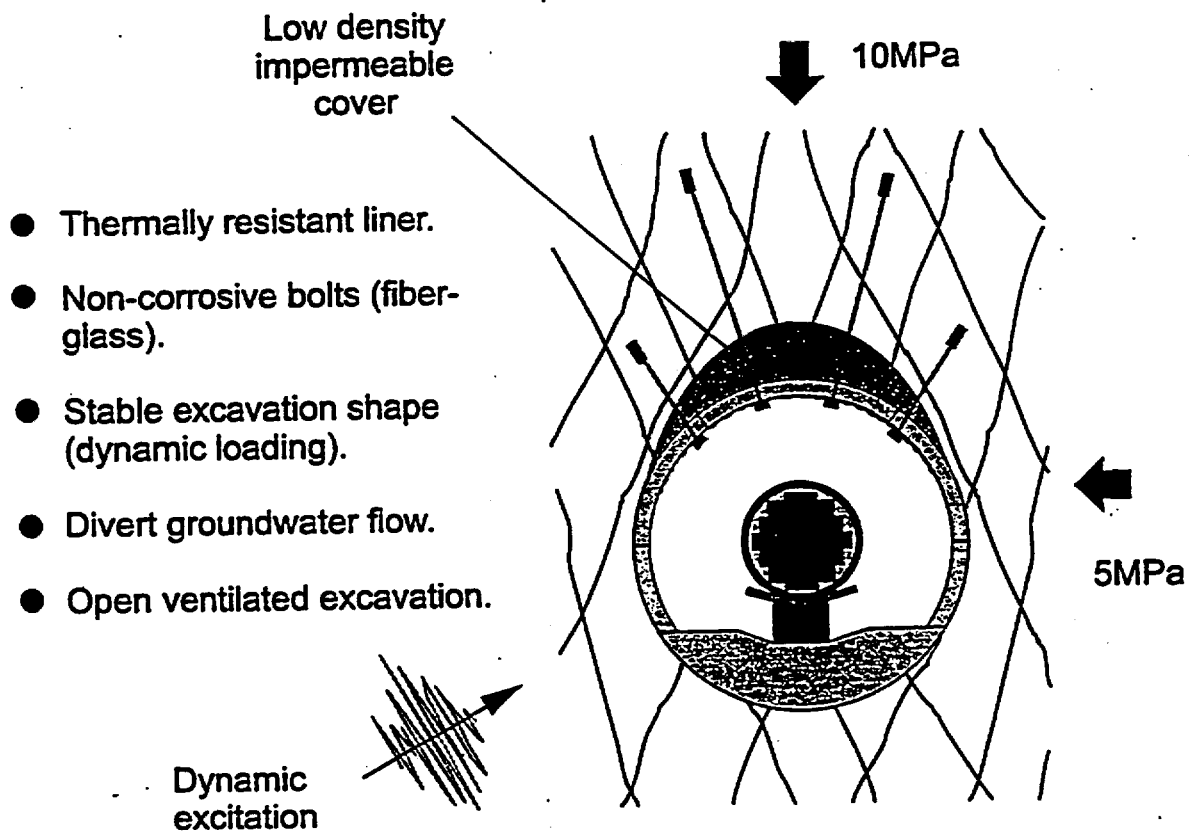


Figure RH-9 Design Components of the Emplacement Drift

## **ELICITATION SUMMARY**

### **BENJAMIN ROSS**

#### **OVERALL PROCESSES**

The combination of heat transfer and fluid flow is the most important coupled process related to the thermal perturbation of Yucca Mountain. Mechanical and chemical changes may have large quantitative consequences, but they are less likely to move the system into a qualitatively different regime. Two patterns of thermally driven liquid flow potentially could transfer significant amounts of heat: countercurrent gas-liquid flow, and mountain-scale convective flow.

The most critical unknown about mountain-scale convection is whether it will make a significant contribution to heat transfer. Hot gas will flow upward in the repository, and it will carry significant amounts of water vapor with it; the question is whether the convective heat transfer will be significant compared to conduction. The answer to this question depends on only one parameter that is not well known: the bulk permeability of the rock mass. Strong mountain-scale convection would increase the temperature difference between the center and rim of the repository, move heat from below to above the repository, and move more water above the repository. Above the repository, convective flow could enhance heat pipe effects; below the repository, heat pipes and convective flow are antagonistic mechanisms.

Countercurrent gas-liquid flow in some form is almost certain to occur at Yucca Mountain; the details are less clear. Water near the heat source will vaporize and move outward (due to pressure effects) or, more likely, upward (due to buoyancy). As the gas enters cooler regions, water will condense; the question is what will happen next. There are several possibilities: (1) the condensate will be drawn into the tuff matrix by suction effects; (2) capillary effects will draw water uniformly back toward the heat source;



(3) water condensing above the repository will flow uniformly downward under the influence of gravity; and (4) the water-steam system will flow in chaotic "chugs." The results of Yucca Mountain project's Large Block Test and Single Heater Test suggest that the fourth alternative is most likely.

### **THERMAL-MECHANICAL (TM) EFFECTS (DRIFT STABILITY)**

TM effects and implications to drift stability are not my area of expertise. It is possible that thermal-mechanical effects could increase gas permeabilities around the rim of the repository, which would increase the strength of buoyant gas flow. Under ambient conditions, vertical gas permeability is greater than horizontal, based on barometric studies. If the thermal load enhances vertical permeabilities at some distance from the repository, this effect could reinforce mountain-scale convection. If the natural ventilation alternative is selected for the repository, drift stability becomes important because if rockfalls blocked air flow through the drifts, the ventilation air flow would be greatly reduced.

### **THERMAL-HYDROLOGIC (TH) EFFECTS**

There are three plausible heat-transfer regimes: a conduction-dominated system, mixed convection and conduction, and a regime in which countercurrent flow is a major heat-transfer mechanism.

Whether convection is important to heat transfer depends only on the thermal loading and the bulk permeability of the rock mass. Several numerical models (T. Buscheck's work presented at the NFEE Workshops and our own unpublished modeling for Sandia) and an analytical stability analysis (Zhang et al., 1994) all point to a threshold of about 10 to 30 darcies for mountain-scale convection to be significant. Convection is a scale-dependent process and, with smaller scales, the threshold is higher. Dry-out will suppress convective heat transfer. Most measurements suggest that the average permeability of the welded tuff is below this threshold (vertical  $K_v \sim 10$  darcy). However, the gas

permeability of fault zones seems to exceed the threshold. These permeabilities are among the most reliable numbers we have, since they are measured (via barometric fluctuations) on the mountain scale.

Convection has not been addressed well by modeling to date. Recent modeling efforts have emphasized the smaller drift scale. (Remember convection is scale-dependent.) Conduction dominates convection around a drift-scale-sized heat source. Mountain-scale modeling conducted earlier mostly used permeabilities smaller than now seem likely from measurements of gas permeability. In addition, the assumption of local thermodynamic equilibrium artificially suppresses convective gas flow when a dry-out zone develops. While the dry-out zone is growing, the rock is moist right up to the boiling isotherm. The partial pressure of water vapor at the boiling isotherm is equal to the total gas pressure, so the gas in the dry-out zone is 100 percent water vapor. As a result, dry-air constituents ( $N_2$ ,  $O_2$ , etc.) cannot move from below to above the repository, so convective circulation is impossible. In reality, macroscopic mixing processes (and to a lesser extent molecular diffusion) will carry air into the dry-out zone. But how much air is carried will depend on the scale of the mixing process and thickness of the zone where the temperature is near boiling, both of which are difficult to predict. Also, upward pressure of stagnant air beneath the dry-out zone would represent an unstable situation, leading to development of small circulating cells where air and water vapor would mix. It is difficult to model instability-driven flows of this type.

In summary, mountain-scale convection is one of the most important processes affecting heat transfer and fluid flow. I am sure that it is important to water flow and think there is a good chance (more than 10% but less than 50%) that it is important to temperature.

In deciding whether countercurrent flow will alter the heat transfer established by conduction, the key question is whether liquid water will flow back toward the heat source. Above the heat source, both suction and gravity can drive return flow; below the source, only suction will be operative. Some key uncertainties about heat pipes are the following: whether condensate will remain in the fractures or be absorbed into the

matrix; whether suction-driven flow occurs in fractures; whether water will remain in the system to recirculate many times or will drain out the bottom; whether return flow will be uniform through the fracture network or whether condensate will collect in fingers; and whether return flux will be steady or episodic.

Models must be used cautiously to predict fracture-matrix interactions under thermal conditions. Several conceptual models are available to explain the apparent discrepancy between incomplete saturation of the matrix and fast flow in fractures (as has been observed with chlorine-36 in the Exploratory Studies Facility [ESF]). These models lead to different predictions about fracture/fracture-matrix interactions in the period when condensate drains into the dry-out zone. One alternative is a generalized equivalent continuum model (G-ECM) in which the fractures and matrix are at pressure equilibrium, but material properties are such that fractures can flow when the matrix is not saturated. In this model, condensate that enters dried-out rock is quickly taken up into the matrix.

A second way of describing the interactions is a dual-permeability model (DK) in which fractures flow because the fractures are not in pressure equilibrium with the matrix. For a DK model, fracture matrix interactions are already small—a range from  $10^{-1}$  to  $10^{-5}$  is estimated for the interaction parameter. After heat begins to mobilize water and condensate drainage begins to occur, the assumption of a low value of interaction parameter will allow the water to flow from the condensate zone downward through the dry-out zone.

A third kind of model that reconciles fast flow with incomplete matrix saturation is based on variability of infiltration rate in time and space. Fast-flow paths develop only near the high-flux regions. This model is more like a discrete fracture model with transient flux boundary conditions. It again allows condensate to drain through the dry-out zone without resaturating the matrix after cooling begins.

Given these uncertainties in model extrapolation, one must pay close attention to field tests when predicting thermally driven fluid flow. The field tests show evidence of

countercurrent flow, but the small scale of the experiments limits their relevance. For example, in the Single-Heater Test, the condensate could shed around the edge, so the extent of the heat pipe could be underpredicted. The most interesting result is the presence of time instabilities in the Large Block Test. Numerical models are not good at identifying physical instabilities. Intuitively, one would expect that the scaled-up system should be less stable than a test system. In modeling countercurrent flow, the modeler must assume condensate behavior (not explicitly, but as incorporated in material properties). Because these are the primary unknowns, models are even less helpful than experiments in predicting the extent of countercurrent flow phenomena.

When an ECM model describes countercurrent flow, it tends to depict a uniform heat pipe, but I believe that an improved model would depict countercurrent flow occurring with irregular return flow of water, alongside mountain-scale convection and local zones of condensate shedding. I assign a weight of 80% to the irregular-flow model, and 20% to a model of uniform heat pipes and recycling. I would develop the unstable-flow model based on the assumption of mountain-scale convection drawing moisture from below to above the heated zone. Rather than forming a uniform condensate cap across the repository, it is likely that local wet zones—perhaps local zones of perched water above low-permeability intervals of the TSw—will form, concentrating downward flow into cooler zones where water will pass down and out of the system. The cooling effect as the water passes will cause additional condensation to flow and allow the process to reinforce itself. The evidence for fast paths in the ambient system makes the occurrence of these local zones more plausible. Any system having a more dense fluid above a less dense fluid will be inherently subject to instabilities, and such local shedding zones are the sort of phenomena that occur in an unstable system. The net effect of the shedding would be to remove both ambient infiltration and condensation from the countercurrent flow zone. I expect these local zones to more likely pass downward through a few pillars between the drifts, where the temperatures are lower, than into the drifts, but seepage into the drifts certainly is possible, especially where there are cooler waste packages.

This type of unstable system is difficult to model. Locally, it can be described as follows:

$Aq_h > m_f h_{fg}$ ; the water will not pass through

$Aq_h < m_f h_{fg}$ ; the water will pass through

where  $A$  is the area,  $q_h$  is the local heat flux,  $m_f$  is the mass flux rate in the flowing fracture, and  $h_{fg}$  is the latent heat of vaporization. However,  $m_f$  depends on the entire system, including feedbacks, and this equation cannot be used directly to make predictions.

Fluids heated from below are often unstable. Multiphase flow phenomena in fractured porous media are rich in instabilities (geysers are one example). Plus, more complex systems have more ways to become unstable. Perhaps the system can be modeled by assuming the matrix is saturated to the point of fracture flow, adding a heat source, and including some local shedding zones to see if they decay away or are reinforced. The presence of temporal instabilities and chaotic behavior observed in the Large Block Test suggest that this type of behavior is plausible.

The consequences of mountain-scale convection are a greater temperature difference between the center and rim of the repository; smeared temperature gradients at the edges of the repository; and more water above the repository, which will flow down either immediately or later. Convective gas flow is likely to profoundly modify countercurrent flow behavior. Convective flow can reinforce heat pipes above the repository by strengthening the upward flow of vapor away from the heat source and by moving water from below to above the repository, thus replacing the water that drains from the system. Below the repository, however, a uniform heat pipe zone cannot coexist with convective flow. In this case, buoyant convection eliminates the countercurrent gas flow, and gravity does not aid liquid flow back to the dry-out zone. Because convection is scale-dependent, the models and experiments to date have not addressed this interaction. The interaction can have an important effect on countercurrent flow, even if convection is not a significant heat transfer mechanism by itself, because gas flow is a major mechanism of moisture transport long before it becomes a major mechanism of heat transfer.

An important issue at the drift scale is the heat transfer mechanism and the presence or absence of backfill. With no backfill, the  $\Delta T$  between the waste package and the drift wall is  $< 5^{\circ}\text{C}$  (except soon after emplacement, when thermohydraulic processes have not fully come into play), and radiation and convection are the dominant heat transfer mechanisms, with radiation being much more important. With backfill, radiation is eliminated, but it is not clear whether convection is important. I am aware of no calculations of convective heat transfer for the geometry of containers in a backfilled tunnel. One can get a rough idea of what will happen by looking at another geometry, a rectangular tunnel with one hot vertical wall and one cold vertical wall, which has been studied (Bejan, 1984). For this geometry, with a Rayleigh number corresponding to a backfill permeability around the top of the range of natural gravels, the Nusselt number, which expresses the ratio of convection to conduction, is about 1 to 5. At the top of this range, a  $\Delta T$  of  $30^{\circ}\text{C}$  calculated by conduction-only analysis would be reduced by convection to  $\Delta T \sim 6^{\circ}\text{C}$ . In such a case, there would be little gain from using backfill to reduce relative humidity.

I like the idea of using passive ventilation to moderate the temperature and relative humidity. One needs to consider how long the passive system would have to be operable.

### **THERMAL-HYDROLOGIC-MECHANICAL (THM) EFFECTS**

Buoyant gas flow will depend on permeability, being strongest in high-permeability zones. I expect the PTn (Paintbrush Tuff) to act as a roof for gas flow, so that the buoyant gas flow goes through a loop. In such a case the volume of flux is controlled by the least permeable segment of the loop. Under current conditions, vertical permeability is several times greater than horizontal; therefore the gas flux would be much more sensitive to changes in horizontal than in vertical permeability.

Faults are likely to be important in creating more permeable zones, but so may zones of enhanced permeability from the thermomechanical changes. For example, if enhanced

horizontal permeabilities occurred near the drifts due to shear along horizontal fractures; they could have important effects. Because the measured permeability of the TSw unit seems to be just below the threshold where convection starts to affect temperature, a relatively small increase in gas permeability could move the system into a different heat transfer regime.

### **THERMAL-HYDROLOGIC-CHEMICAL (THC) EFFECTS**

At present the uncertainties about mechanisms of fluid flow are so great that even rather large possible changes in a flow parameter do not add significantly to the uncertainty. Therefore, the coupled processes of interest are limited to those that can cause very large changes in parameter values and processes that can change parameters to which the flow regime is highly sensitive. One example of a process that could make a large change in a parameter would be the formation of an impervious caprock by precipitation of dissolved minerals. An example of a process that changes a sensitive parameter would be the thermomechanical enhancement (or decrease) of gas permeability, which as discussed previously could move the system from a conduction-dominated to a conduction-and-convection heat transfer regime.

In discussing possible thermal-hydrologic-chemical effects, it is useful to distinguish among processes that affect flow within fractures, processes that affect flow within the porous matrix, and processes that affect fracture-matrix interactions.

#### **Flow in Fractures**

In the Yucca Mountain system, filling of fractures by chemical precipitates will have less effect on fluid flow than one might think. The effect of fracture filling on liquid water flow is limited because the permeability of the fractures far exceeds the amount of water available to flow through them. Even rather large reductions in absolute permeability of a fracture are compensated for by changes in relative permeability, with the effective hydraulic conductivity remaining nearly constant. On a microscopic scale, water moves through narrow channels within the fractures, and if one channel becomes blocked, the

water simply finds another. As a result, over a large range of permeability changes the permeability has little effect on water flow.

A parallel mechanism limits the effect of fracture filling on gas flow. Two mechanisms—the cubic relationship between transmissivity and fracture aperture, and the wetting behavior of water that fills narrow apertures while leaving wide ones open—concentrate gas flow in the widest fractures and in the widest-aperture channels within an individual fracture. Mineral precipitation can occur only in the wet portions of a fracture; therefore it will first fill the parts of fractures having narrowest apertures, which contribute least to gas flow.

Consequently, precipitation of minerals in a fracture will have a very limited effect on fluid flow through the fracture until the fracture is almost completely filled. Sealing of fractures is indeed observed in geothermal systems, where what is known as a caprock frequently is found. In the Yucca Mountain system, any caprock would form at the interface between the boiling zone and the condensate zone. The front would have to stay in one place long enough for fully a impervious zone to develop in this way. Although such an occurrence seems possible, I would assign it no more than 5% to 10% probability.

A second proposed mechanism for reducing of fracture permeability is "healing" through dissolution of asperities that cause the fracture faces to move closer together. This mechanism would, like precipitation and for the same reasons, have little effect on liquid flow, but it would reduce gas flow. I give this mechanism a relatively low probability of occurrence in the unsaturated zone. Because the flow of unsaturated-zone water seems to concentrate in localized pathways more than in the saturated zone, the systematic dissolution of asperities that is required for this kind of healing seems less likely in the unsaturated zone. Indeed, it seems unlikely that the permeability of the welded tuff at Yucca Mountain would be as high as it appears to be, were it not that fractures heal more slowly in the unsaturated zone than in the saturated zone.



**Fracture-matrix interactions**

The primary chemical effect on fracture-matrix interactions is likely to be the "armoring" of fracture surfaces by coatings of precipitate that hinder exchange of fluids between fractures and matrix. How important this would be depends on the mechanisms that control the rate of fluid exchange in and out of the matrix and on how much effect the matrix has on fluid flow overall.

It seems clear that the matrix permeability is high enough that gases will quickly (on repository time scales) equilibrate between fractures and matrix. Thus the primary issue is whether fracture armoring will impede exchange of liquids between fractures and matrix.

As discussed above, several conceptual models are consistent with available data about the relationship between water flowing in the fractures and water in the matrix. In the dual-permeability model, fracture-matrix interactions are already so slow that water flows from ground surface to repository level without equilibrating with the matrix. Further reduction in these interactions as a result of fracture armoring will almost certainly make little difference.

In the generalized equivalent continuum model, the matrix saturation determines whether fast flow occurs. This model predicts that when condensate drains into the dry-out zone, capillary pressure equilibrium is still in force so that water will move back into the matrix, thus shutting off the condensate drainage through fractures. In this model, fracture-matrix interaction kinetics play little role in determining fluid behavior. As long as this remains the case, reduction in fracture-matrix interaction due to precipitation of dissolved solids on the fracture walls would have little effect on fluid behavior. But if the walls were coated in a way that cut off interchange completely, behavior would change significantly.

Although these models give widely varying predictions about whether fracture armoring could affect uptake of condensate into the matrix, there seems to be little practical

difference. In models in which kinetics of fracture-matrix flow are important, the data drive one to conclude that the fractures exchange little water with the matrix even under current conditions, so additional barriers to this exchange would have limited effect. On the other hand, in models based on fracture-matrix equilibrium, moderate amounts of fracture armoring has little effect because the model is not sensitive to the rate of exchange between the two continua. Only a nearly impermeable coating that effectively cuts off the fractures from the matrix would affect fluid flow. Even this extreme case only brings us from one hypothesis about current conditions to the other.

Thus it seems probable that fracture armoring will have little effect on flow. Even in the unlikely event that armoring causes a major change in fracture-matrix interactions, the change is within the range of uncertainty resulting from lack of knowledge about mechanisms of flow under present conditions.

#### **Flow within matrix**

It seems likely that more water will evaporate on the fracture walls than at locations within the matrix. Therefore, more precipitation will occur there. Because fluid flow within the matrix is essentially limited to transfer in and out of the fractures, chemical effects on flow within the matrix can be subsumed within the effects on fracture-matrix interactions.

### **MULTIPLY COUPLED EFFECTS**

Constructing a fully coupled THCM model that is deductive is too large an effort to be feasible. In practice, the effort to develop a comprehensive model often is so distracting that inadequate effort is made to correctly model the really important processes. Success is much more likely if one tries first to identify important phenomena (e.g., fracture-matrix interaction, formation of a caprock) and then to develop the linkages that appear important.

Figure BR-1 shows the linkages that I believe are important and those that, because of a lack of feedback, apparently can be treated individually, using the results of the coupled-processes model as input. The figure shows that chemical and mechanical changes in permeability have limited influence on either gas flow or water flow in the fractures, unless a caprock develops. Overall, I think that chemical processes could potentially be important if a caprock can develop, and are more likely to be important than mechanical influences.

### **DURABILITY OF EFFECTS**

Redistribution of water will, in the long term, be reversed. Recent research showing a higher infiltration rate than previously thought suggests that the moisture distribution will return to ambient fairly quickly after the thermal perturbation ends (at about 50,000 years).

I do not expect the THC changes to be reversible. Caprocks are observed to persist in geothermal systems. At Yucca Mountain, caprock precipitation would occur in the heat pipe zone; subsequent drainage would occur at lower temperatures. There is a large volume of rock and only small fractures. Furthermore, the precipitates would be silicates, not carbonates, making them much less likely to dissolve at lower temperatures. The chemical changes to the fracture-matrix interaction also seem likely to be largely irreversible and long-lasting.

I don't have an opinion on whether TM changes are reversible.

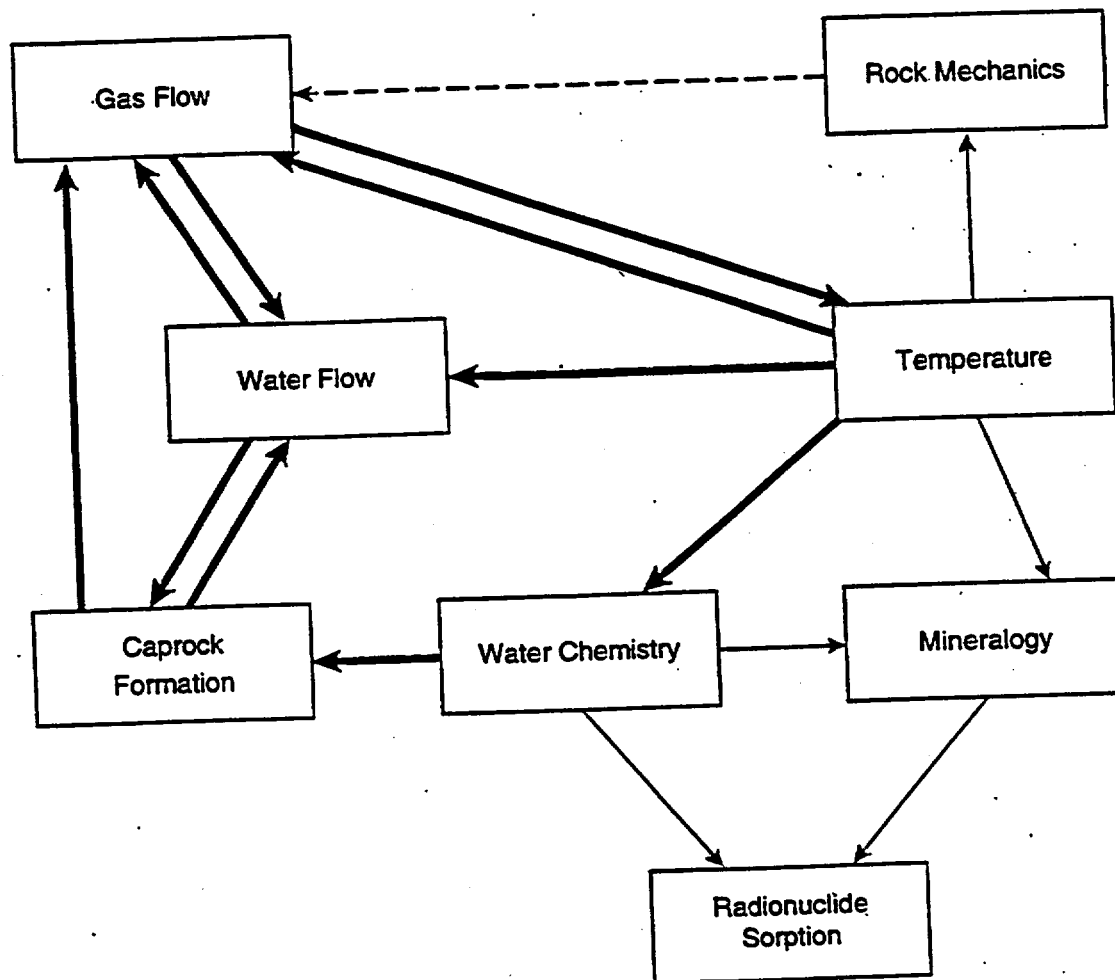
### **RECOMMENDED ACTIVITIES TO REDUCE UNCERTAINTIES**

1. Run numerical models in which instabilities are present in initial conditions and see whether they grow or are damped out.

2. Use skepticism in relying on models in which the qualitative behavior rests on assumptions of uniformity, such as models of gas flow in which convective flow is prevented because the mass fraction of dry air is extremely low in the dry-out zone.
3. Adopt conclusions about the behavior of refluxing condensate based on numerical models only after checking them against models based on several different conceptualizations of how to extrapolate from current to thermal conditions.
4. Complete the drift-scale test.
5. The natural ventilation alternative for repository design should be developed to the same extent as other alternatives, such as backfill and drip shields.
6. A mathematical analysis of convective heat transfer within the drift should be performed for the backfill alternative.

## REFERENCES

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- Zhang, Y., Lu, N., and Ross, B, 1994, Convective instability of moist gas in a porous medium: International Journal of Heat Mass Transfer, v. 37, p. 129-138.



**EXPLANATION**

- Feedback loops
- Influences with little feedback
- Possible influence

Figure BR-1 Diagram of significant influences for coupled effects.

## **ELICITATION SUMMARY**

### **ROBERT S. SCHECHTER**

#### **OVERALL PROCESSES**

The most relevant processes are those that impinge upon the integrity of the waste packages and/or accelerate the distribution of released radioactive materials into the environment. Factors that increase the rate of ambient water influx into the drift and those that alter the composition of the water influx to increase its corrosiveness are of primary concern. Of course the stability of the drift also is another primary concern, but I will not discuss this factor because to do so would involve complex mechanical considerations that are beyond the expertise of this respondent.

In the near field, the heat generated by decaying radioactive waste and the ambient flux are the primary engines driving potentially detrimental processes.

I note here that sufficient circulation of fresh air through the drift to remove both heat as it is generated and moisture as it arrives will greatly reduce many of the uncertainties. I recommend this mode of repository operation.

The dissipation of heat into the environment by conduction will result in an endless chain of vaporization/condensation steps. These processes likely will not achieve a steady state primarily because they continuously alter the rock permeability within the zones in which they occur. In fact, this alteration of permeability as a result of dissolution/precipitation processes represents one of the greatest uncertainties to be addressed. Because extremely long times are involved, it may not be possible to satisfactorily predict the outcome. Indeed, this respondent is not entirely reassured by the modeling or experimental evidence. One must anticipate the worst case—a greatly increased permeability in the rock surrounding the drift, extending beyond the point where substantial vaporization and

condensation have taken place. Permeability alteration within the condensation/vaporization region seems quite important, if not crucial, and I strongly recommend that this issue be given the highest priority for additional research if the drift is not ventilated.

The corrosion of the waste packages will be affected by the composition of the water that enters the repository. The corrosion rate will be a function of the  $\text{CO}_2$  and  $\text{O}_2$  concentrations in the influx. The  $\text{CO}_2$  (and the  $\text{O}_2$ ) concentration of the residual water contained within the pores surrounding the drift depends on the suction pressure, which is a function of the liquid saturation. Near the drift, the saturation is lowered by drying out, currently caused by the circulation of air, ultimately to be caused by the heat from decaying waste. At low water saturations, suction pressures higher than 1500 atm have been reported. At this suction pressure, the  $\text{CO}_2$  concentration in the pore water is many ( $\approx 80$ ) times higher than the concentration in aqueous systems in equilibrium with the atmosphere. The  $\text{O}_2$  concentration also will be greatly enhanced by the suction pressure. These increased concentrations may adversely affect the quality of the water entering the drift. During the heating phase, the reduction in the saturation of water in the region surrounding the drift increases the suction pressure of the water because the residual water will reside primarily in smaller pores.

### **THERMAL-HYDROLOGIC-CHEMICAL (THC) EFFECTS**

The assumptions underlying the thermal and chemical hydrologic phenomena are as follows.

- (1) Yucca Mountain is in capillary equilibrium.
- (2) The permeability of the matrix is orders of magnitude smaller than the permeability of the fracture system. The fracture system is extensive and well connected.
- (3) The temperature distribution is determined by thermal conduction within the rock matrix. Thus, the near-field temperatures are essentially symmetric with respect to the drift.

- (4) The results of the Single Heater Test (at the Yucca Mountain Exploratory Studies Facility) are valid and hence require attention. This test indicated a substantial accumulation of water below the heater chamber. It also indicated a considerable accumulation of water within the fractures above the heater chamber. Thus, one issue to be addressed is the behavior of the condensate within the fracture system.

If any of the underlying assumptions are discredited as a result of ongoing research, then assessments made here may require revision.

### **I. The Drying-Out Period**

During this initial phase, water contained within the pores of the matrix surrounding the drift is expected to be vaporized as the rock is heated. The water in the larger pores will be vaporized first (Kelvin effect). Vaporization will be gradual because of the distribution of pore sizes. Because the rock temperature is fixed by conduction, we may imagine the temperature of the rock matrix at a given time and radial position to be fixed and independent of the vaporization and condensation processes that are taking place. The vaporization of water from a region in the zone that is drying out is a complex, nonequilibrium process. At capillary equilibrium, all of the water-gas interfacial curvatures at a given elevation above the fully saturated zone (water table) are the same and hence exhibit the same initial vapor pressures. The vaporization process will cause vaporization from certain pores and perhaps condensation of water vapor into other pores. This complex redistribution among the matrix pores will depend on pore geometry and will not be considered here. A relevant aspect of the process appears to be the residual minerals that are precipitated as the pore waters are evaporated. The volume of residual minerals will depend on the  $\text{CO}_2$  concentration within the matrix pores (corrected for curvature effects). The precipitation attending the evaporation of pore fluids likely will result in a reduction of matrix permeability. Because this permeability is orders of magnitude smaller than the fracture permeability, this reduction will be difficult to demonstrate either by field experiments or by modeling.



Entering the fractures during this early stage will be moist air. The partial pressure of the water in this moist air will equal the vapor pressure of water at the temperature of the matrix at that point corrected for the Kelvin effect. It will, therefore, be somewhat less than the vapor pressure at the local temperature of the matrix.

The moist air flowing in the fracture system ultimately will be transported through the system of fractures into regions of lower temperature. Water will adsorb onto the fracture surfaces and perhaps even condense in small crevices along a fracture surface. The effect of this adsorption or condensation on fracture permeability hinges on the formation of liquid lenses or droplets. A lens or droplet is defined as a liquid entity that spans the entire fracture aperture in some region. This can be visualized as a mist condensing on the fracture surfaces but increasing in extent until water drops from one surface merge with drops from the adjacent surface.

This process is complicated by the fact that the two fracture surfaces are not entirely distinct. They touch at certain discrete points, or contacts that support the stresses that tend to close the fracture. Droplets may tend to form around the contacts and, therefore, initially appear as pendular rings. Very small openings between the asperities are also likely sites for droplet formation. The rationale supporting this assertion is provided in Appendix I. Once liquid drops form, they will tend to grow because of capillary condensation and will become full-scale lenses.

The lenses will not, in general, occupy the full cross-section of a fracture, thereby blocking the local flow of the gaseous phase. In crude terms, even though blocking of gaseous flow is possible, there is a self-regulating feature that mitigates against this possibility. If gas flow is blocked entirely by liquid condensate lenses, then the supply of water transferring from the air to isolated lenses will be disrupted, and lenses will no longer be sustained. Capillary forces are continually drawing condensate into the formation (imbibition). The lifetime of a lens that is cut off from its source of water is finite (see Appendix II). Thus, portions of a fracture isolated from moist air by a system of condensate lenses will not be permanently isolated. Once lenses blocking the air flow

have been removed or reduced in size by capillary forces, gas entry will again be possible.

In the fractured system during the drying-out regime, condensate will form as lenses at discrete points in fractures because the flow of vapor-laden gas occurs primarily in the fractures. The size of a lens will increase by condensation until gravitational forces cause it to move downward or until the rate of imbibition balances the rate of condensation. As a lens moves downward in a fracture above the drift, it moves into hotter regions and will tend to disappear because of both evaporation and imbibition. Lenses formed below the drift will tend to have a longer lifetime, because the downward flow will be into cooler, not hotter, regions and because the liquid saturation in the matrix is on the average higher, reducing the capillary forces that tend to draw liquid from the lens into the rock matrix. From this viewpoint lenses tend to form, flow, and then disappear. New lenses will not necessarily re-form at the same points as the previous ones, because the morphology of the porous medium is continually altered by the dissolution and precipitation of minerals. We must visualize the TH regime as a dynamic one in which mineral is being continuously redistributed and the flow in the fractures is sporadic. Furthermore, because of the mechanisms involved, there appears to be a net downward flow of condensate, as observed in the Single Heater Test (SHT). Thus, I do not expect a true steady state to develop during the TH period. This is one of the great uncertainties engendered by allowing the heat generated to be dissipated into the environment.

To address the effect of thermal-chemical modifications on fracture permeability, it seems reasonable to imagine that mineral dissolution will be most active at those sites where condensate drops first form. In Appendix I, it is suggested that the most likely sites are the small fracture apertures. This being the case, the narrow openings in the fracture will be enlarged. It would, therefore, seem to follow that condensation and dissolution will increase fracture permeability. This trend is contrary to results in the Wilder report. To rationalize these results, it has been suggested that the dissolution of fracture-lining minerals may smooth the fracture face. The proposed mechanism is that the contacts (points of zero aperture) that support the fracture dissolve more rapidly than

other minerals lining the fracture surfaces because of the stresses applied to these contacts. Thus, once these contacts are removed, the surface tends to become smoothed and the fracture aperture decreases. One other possibility is clogging of the fracture permeability by colloidal particles, in the presence of condensate water. This explanation is plausible because of the expanded double layer surrounding charged colloidal particles. Thus, several hypotheses have been offered to account for the observed trends.

The clogging of pores as fresh water flows through sandstones is a phenomenon much investigated by the oil industry. Even rock samples that have little clay may exhibit a large sensitivity to fresh water. Apparently porous rocks always contain small colloidal particles. Clays are not the only source of suspended colloidal particles; plugging in fresh water may be caused by small silica particles. I believe that a part if not all of the observed permeability reduction was due to clogging by colloidal particles. The permeability reduction observed in sandstones in response to fresh water invasion is often on the order of 100X. The reduction of fracture permeabilities will be significant in fractures with apertures that are less than 5 to 10 times the diameter of the suspended colloidal particles. Clogging in fractures having very large apertures probably is not significant.

Another factor is the difference in the rate at which the various fracture-lining minerals react with condensate. Certain minerals, such as clay with a layered structure, are expected to dissolve at rates far slower than crystalline materials, such as feldspar or quartz. Thus, the effect of dissolution on fracture conductivity may also depend on the morphology of the mineral deposits on the fracture face as well as the condensation sites.

During the elicitation interview, the question of mineral supersaturation and its potential impact was raised. This is a complex issue that has never been systematically researched. It will likely yield some interesting and relevant phenomena when fully addressed. It is possible that mineral precipitation will occur in distinct bands of high crystal concentration (Liesegang rings) thereby increasing the potential for pore or fracture clogging.

Another issue is the lifetime of a condensate lens compared to the reaction time. A condensate lens once formed tends to imbibe into the matrix (see Appendix I). If the lifetime is much less than the reaction time, the primary site of mineral dissolution will be at the condensation sites and within the matrix. The crude calculations shown in Appendix I suggest that the condensate will imbibe before reaction is complete. This result implies that the dissolution that takes place in the fractures will tend to increase the fracture permeability. There may, in fact, be little evaporation of condensate in the fractures. Therefore, the fracture-matrix interaction is an important, if not critical, feature of the process, and projections based on models that do not account for the minute details of this complex interaction will be unreliable.

## **II. The Cooling Period**

Even as the rate of heat generation decreases, the matrix temperatures will continue to increase. However, at some moment, the boundaries of the dry zone will begin to recede toward the drift, primarily driven by water seepage and capillary forces. The seepage is thought to be primarily through the fractures, and the capillary-driven flows will be through the matrix, primarily from the saturated zone. The water flowing through the matrix will be relatively concentrated in carbon dioxide and oxygen (see Appendix IV on the relationship of Henry's Constant to curvature).

## **DURABILITY OF EFFECTS**

The processes that take place as a result of the dissipation of heat into the environment are not reversible.

## **RECOMMENDED ACTIVITIES TO REDUCE UNCERTAINTIES**

Assessing the long-term state of the drift and the release rates of radioactive materials into the environment requires a considerable faith in the efficacy of the computer models used for making the predictions. To gain confidence in models, field tests are most

useful. Another helpful approach is to measure the response of simple systems in the laboratory and then compare with model predictions.

1. A field test that can and should be performed is the confirmation of the ambient flux. An isolated cavity (large enough to intersect many fractures) should intercept fluxes that comport with those predicted by models.
2. A primary uncertainty is the matrix/fracture interaction and whether this interaction is properly represented by existing models. A research program that includes both laboratory studies and comprehensive computer simulations should produce responses useful for comparison with the model predictions.

## APPENDIX I: ON THE FORMATION OF LIQUID DROPS

When moist air flows through the connected fracture system, a thin layer of adsorbed water will form to coat the mineral surfaces. The thickness of this layer increases with the relative humidity, and at some point the film thickness attains macroscopic dimensions (a few hundred angstroms). The thickness of the layer is determined primarily by electrostatic forces (see "Surface Forces" by B. V. Derjaguin, N. V. Churaev, and V. M. Muller Consultants Bureau, New York, 1987). Because most mineral surfaces in contact with water at near neutral pH are negatively charged and the air/water interface is also negatively charged, thick water films will tend to form.

Because the adsorbed film is thick, it is reasonable to suppose that the film thickness on a fracture face is determined partly by capillarity. Where the curvature of the rough fracture surface is negative, the film will be thick; and where it is positive, the film will be thin. Thus, the water film has a complex geometry that depends on the geometry of the fracture surfaces. The nucleation of a drop will occur where the films on opposite fracture faces merge. Because the film thicknesses are a sensitive geometry, the merger sites are difficult to anticipate. It seems plausible to assert that the films will overlap at places where the fracture surfaces are in closest proximity. Such sites represent the small openings along the flow paths through the fracture.

Once the condensate drops form at these narrow sites spanning the fracture aperture, the drops will become further enlarged because their curvatures will promote further condensations. Thus, the formation of a lens is rather like nucleation. The existence of a drop promotes further condensation, and a drop will become a lens.

## APPENDIX II: IMBIBITION OF CONDENSATE

This analysis is intended to define a time scale for the lifetime of a condensate drop formed within a fracture. The calculation does not take into account motion of the drop nor the mass transfer of water vapor to the drop. Thus, the calculation is not of particular value in quantifying fracture/matrix interactions, but instead is intended to provide a comparison of imbibition times with reaction times when a condensate drop forms.

A drop of condensate spanning the fracture walls will exhibit a capillary pressure that depends on its shape. If the droplet capillary pressure is less than the capillary pressure of the water in the adjacent matrix, there will be a flux of water from the drop into the adjacent matrix. This water flux will at first be high; as the saturation builds up within the matrix immediately adjacent to the drop, the capillary forces will be diminished and the flux will decrease. We may capture the essence of this complex process by considering the saturation front created by the imbibition from the drop as it advances into the matrix to be a sharp one. We let  $S_i$  be the initial saturation (determined by capillary equilibrium) immediately adjacent to the condensate drop.  $S_i$  is, therefore, a function of the elevation of the matrix above the saturated zone. Furthermore, we let  $S_f$  be the saturation within the matrix evaluated at the droplet capillary pressure. We imagine imbibition to take place as a piston-like process so that if  $D(t)$  is the distance that the saturation front has progressed into the matrix, then by Darcy's law

$$u_N = \frac{k}{\mu} \left[ \frac{\Delta p(S_i) - \Delta p(S_f)}{D(t)} \right]$$

This equation shows the flux to be driven by a difference in capillary pressure. Because the capillary pressure in the matrix increases with elevation above the saturated zone, the driving force will be greater above the drift. Liquid condensate drops will have a slightly longer lifetime below the drift. Although this difference is not worthy of consideration,  $D(t)$  represents the distance of penetration of the saturation front; and  $u_N$  is the water flux

normal to the fracture surface.  $k$  is the permeability of the matrix to water. The water viscosity,  $\mu$ , is evaluated at the temperature of the matrix. Clearly, a volume balance yields

$$\frac{dD}{dt} = \frac{u_N}{\phi(S_f - S_i)}$$

Integrating, we obtain following expression for the flux of water from a condensate drop into the matrix

$$u_N = \left[ \frac{\phi k (S_f - S_i)}{2\mu} \right]^{1/2} \left[ \frac{\Delta p(S_i) - \Delta p(S_f)}{t} \right]^{1/2}$$

Thus, if a drop that spans the entire width  $w$  of the fracture has an initial cross-sectional area,  $A_0$ , then as the drop shrinks,  $A$  will decrease although surface energetics will dictate that the drop remain attached to both fracture walls. Therefore, imbibition into the matrix will continuously reduce the contact area between the drop and the fracture faces so that the volume change of the drop (or lens) is given by

$$w \frac{dA}{dt} = -2Au_N$$

or finally

$$w \ln \frac{A_0}{A_c} = \left[ \left( \frac{k\phi}{2\mu} \right) (S_f - S_i) \right]^{1/2} [\Delta p(S_i) - \Delta p(S_f)]^{1/2} T^{1/2}$$

where  $A_0$  is the initial condensate area and  $A_c$  is an area so small that a drop of height  $w$  becomes unstable and divides into two, forming individual drops that no longer span the



fracture aperture.  $A_c$  may be calculated by examining the stability of surfaces of constant curvature spanning the fracture width  $w$ . The critical area,  $A_c$ , is of the magnitude of  $w^2$ .

This equation shows the lifetime of a water droplet,  $T$ , as it relates to the saturation of the adjacent matrix and the width of the fracture. The temperature will enter through its effect on the viscosity and surface tension. We note that the capillary pressure in the water drop is approximately

$$\Delta p(S_f) \approx -\frac{2\gamma}{w}$$

where  $\gamma$  is the surface tension and  $S_f \approx 1$ . Data taken from the Wilder report are as follows:  $w \approx 40 \mu m$ ;  $\phi \approx 0.11$ ; and  $S_i \approx 0.4$  at a capillary pressure of 20.8 atm which corresponds to a height of 225 m above the saturated zone. From the literature, we find  $m = 0.8937$  cp and  $\gamma = 71.97$  dynes/cm all at  $25^\circ C$ . Based on these values

$$\frac{2k\phi}{2\mu} = 7.11 \times 10^{-12} \frac{m^2}{\text{sec} - \text{atm}}$$

We also have  $Dp(S_i) = 20.8$  atm and  $Dp(S_f) = -0.03$  atm.

This yields

$$w \ln \frac{A_0}{A_c} = (2.67 \times 10^{-6}) T^{1/2}$$

where  $T$  is in seconds. Thus, for a typical fracture and an initial drop-fracture contact area that is 10,000 times the critical area, the lifetime of a drop will only be about 350 minutes. Even if the initial area is  $10^6$  times the critical area, the time is increased to only about 720 minutes. These times appear to be comparable to the times required for complete chemical reaction of the condensate with the fracture lining minerals.

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Therefore, we conclude that much of the condensate will be imbibed into the matrix before the reaction with the fracture lining minerals is completed.

An implication of this calculation appears to be that laboratory experiments that begin with a fracture created in an unsaturated core will not be representative, because condensate will imbibe prior to the completion of the reaction. To study the influence of condensation on fracture permeability based on laboratory experiments is a complex problem—one that probably has not been satisfactorily resolved.

### APPENDIX III: LIQUID LENSES UNDER THE INFLUENCE OF GRAVITY

As condensation takes place, condensate droplets will form in the fracture and will grow in extent as moisture is transferred from the vapor. At some point, it may be expected that a condensate lens, having grown to a sufficient size, will begin to flow downward in the fracture under the influence of gravity. To determine the point of incipient motion, one must balance the gravitational forces against the capillary forces that will act to keep the lens from moving. Because the surfaces of the fracture wall are quite rough, we expect the contact angles at the trailing edge to be nearly zero (receding contact angle). Similarly, at the leading edge, the contact angle may be expected to be 180 degrees because of the surface roughness. Thus, if the fracture is inclined at an angle  $\alpha$  with respect to the horizontal, then a force balance equating the gravitational force to the surface tension forces gives the following equation for the critical length  $L_c$ ; that is, that length such that the lens will move downward under the influence of gravity. The critical length is found by the simple equation

$$w L_c \rho g \sin \alpha = 4 \gamma$$

where  $g$  is the acceleration due to gravity and  $\gamma$  is the surface tension.

Based on this equation, for fracture aperture  $w = 40 \mu\text{m}$ ,  $L_c = 72 \text{ cm}$  when the fracture is vertical. According to this simple equation, there will be little downward liquid flow in the fractures as long as the capillary forces are operative, and there may be significant holdup of condensate ( $L_c \sim 2 \text{ cm}$ ) even for fracture apertures as large as 1 mm.

The results of the Single Heater Test indicate that there are fractures having apertures on the order of 100  $\mu\text{m}$ ; it is through these fractures that gravity-driven flows occur.

#### APPENDIX IV: HENRY'S CONSTANT ENHANCED BY CAPILLARITY

During NFEE Workshop 2, there was considerable discussion that the pore water samples "squeezed" from the rock cores have a different composition than the readily sampled waters contained in the more permeable fractures. This discrepancy seemed to be a source of some difficulty because it was not predicted by geochemical models. I prepared this note to point out that water samples drawn from a partially saturated porous medium will not necessarily have the same composition as the water in the fractures, even though both types of water are in equilibrium with the same minerals. In this note I focus on the solubility of gases in both types of water. It should be emphasized that the same sort of thermodynamic analysis may be carried out to determine the effect of capillary pressure on mineral solubility.

In a partially saturated porous medium, such as a partially dried-out core sample (the usual case unless extreme precautions are taken at the time of coring), the wetting phase exists at pressures less than that of the nonwetting phase by an amount given by the Laplace equation. Thus, we may write

$$P_{\text{wetting}} - P_{\text{nonwetting}} = -\frac{2\gamma}{r} = - \text{capillary pressure}$$

where  $r$  is the radius of curvature of the gas-liquid interface, and  $\gamma$  is the surface tension. In this analysis we assume that the water in a partially saturated zone is the wetting phase and that the gas in equilibrium with it is the nonwetting phase. Further, we imagine the nonwetting gas phase to contain certain components that have limited solubility in the aqueous phase (i.e.,  $\text{CO}_2$  or  $\text{O}_2$ ). Furthermore, we take both the gas-phase mixture and the aqueous solution to be ideal in the thermodynamic sense (this may easily be corrected using activity coefficient corrections). Thus, the chemical potential of one of the solutes present in the gas phase may be written as follows:

$$\mu_g = \mu_g^0 + kT \ln p_1$$

where  $p_1$  is the partial pressure of the component in the gas phase. This equation assumes the gas phase to consist of a mixture of ideal gases; thus, the equation only applies at modest total gas pressures. It probably is, however, a good approximation under atmospheric conditions. The chemical potential of the solute dissolved in water may be represented by the equation

$$\mu_L = \mu_L^* + kT \ln x_1$$

where  $x_1$  is the mole fraction of the solute in the aqueous phase. (This may not be the most appropriate representation since it is not convenient in the limit as the mole fraction of the solute approaches unity [pure solute].) This equation takes the aqueous phase to be an ideal solution over the entire range of solute mole fractions. If the solution is not dilute, activity coefficient corrections will be required. The equilibrium between phases separated by a plane interface is given by

$$\mu_g^0 - \mu_L^* = kT \ln \frac{x_1}{p_1} = kT \ln H_1^\infty$$

where  $H_1^\infty$  is the Henry's constant  $= x_1/p_1$  for a plane interface; that is, an interface of zero curvature. If the interfaces are curved, the Henry's constant will differ. The purpose of this note is to determine the effect of partial saturation and hence capillary pressure on the Henry's constant and thereby to determine the enhanced solubility of the gas in a partially saturated medium. The standard chemical potential of solute in the wetting phase of a partially saturated rock will change because of the change in the pressure of the wetting phase assuming the pressure of the nonwetting phase to remain constant.

Since  $\frac{\partial \mu_L^*}{\partial p} = \bar{V}_1$

= partial molar volume of the liquid solute at the temperature and pressure of the system

(a hypothetical quantity), we may then correct the standard state chemical potential for the capillary pressure as follows:

$$\Delta\mu_L^* \approx -\bar{V}_1 \frac{2\gamma}{r}$$

so that the chemical potential of the solute in the wetting phase may be written as

$$\mu_L = \Delta\mu_L^* + \mu_L^* + kT \ln x_1$$

Equating this expression for the solute in the wetting phase, we find

$$\frac{x_1}{p_1} = H^\infty \exp \left[ \frac{2\gamma\bar{V}_1}{rkT} \right]$$

This equation shows that the Henry's constant in the wetting phase is larger, perhaps much larger than for a system with a plane interface. Thus, the concentrations or the mole fractions of  $\text{CO}_2$  and  $\text{O}_2$  in the aqueous phase of a partially saturated medium will depend on the capillary pressure at the saturation. The  $\text{CO}_2$  and  $\text{O}_2$  concentrations will be a function of saturation; at small saturations where  $r$  is small, these could greatly exceed the concentrations found in the wetting phase of a fully saturated medium.

A similar analysis may be applied to the saturation of the residual water with respect to the various minerals that may be in contact with the wetting phase. Thus, for example,  $\text{CaCO}_3$  solubility will be increased in the wetting phase of a partially saturated porous medium relative to the solubility in water in a fracture. Furthermore, because the  $\text{CO}_2$  content of the wetting phase depends on the wetting phase saturation, the pH will also depend on the saturation. Since the solubility of minerals is often sensitive to the pH, we would not expect water "squeezed" out of the core samples to have the same composition as water found in the fractures unless the core is initially fully saturated. Water retained

in the cores will have a different CO<sub>2</sub> content and hence a different pH and, therefore, would be expected to have different mineral concentrations than fracture water. This difference could explain the discrepancies between water samples noted during the NFEE Workshop 2. Also explained is the enhanced CO<sub>2</sub> concentrations that were mentioned during our tour of the Repository.

The modelers must, therefore, take into account the effects of capillary pressure and recognize the profound changes in water composition that may influence the corrosivity of the water seeping into the drift.

As an example of the magnitudes that may be expected, consider an idealized porous medium that is composed of an array of infinite cylindrical rods of radius, R, arranged on a cubic lattice. Collins gives the following relationship between the saturation of the porous medium and the radius of curvature, r, of the interfaces:

$$S = \frac{4}{3\pi} \left[ \sqrt{\left(\frac{r}{R}\right)^2 + 2\frac{r}{R}} - \cos^{-1} \frac{R}{r+R} - \left(\frac{r}{R}\right)^2 \sin^{-1} \frac{R}{r+R} \right]$$

Based on this idealized model we may calculate the results shown in Table 1.

r/R	S saturation	Enhancement of Henry's Constant
0.4	0.0328	1.09
0.3	0.0248	1.12
0.2	0.01623	1.19

NOTE: Data used in calculation are  $V_1 = 57.6 \text{ cm}^3/\text{gmole}$  (approximately liquid CO<sub>2</sub> at 20°C),  $R = 0.1 \text{ micrometer}$  (a small sand grain),  $g = 72.5 \text{ dynes/cm}$  (the surface tension of water at 20°C).

This table indicates that the CO<sub>2</sub> dissolved in the water contained in the capillaries may have a mole fraction as much as 20 percent more than in the fracture water. Although this seems to be a minor correction, the additional dissolved CO<sub>2</sub> will lower the pH and alter mineral solubility.



## ELICITATION SUMMARY

### YANIS YORTSOS

#### OVERALL PROCESSES

The thermal loading in Yucca Mountain will affect thermodynamic variables, such as density (expansion of solids and fluids) and solubility; liquid-vapor phase changes; and chemical transformations. The temperature effects come through: (1) higher than ambient temperatures (absolute effect), and (2) temperature gradients in space and time (relative effect). (Note that in linear thermoelasticity, temperature gradients,  $\beta \nabla T$ , are equivalent to a body force,  $\rho g$ ).

Thermomechanical effects are essentially changes of density and shape. Solid thermal expansion affects rock geometry through joint and aperture displacement. Expansion of fluids in the presence of gravity results in natural convection. Vapor-liquid phase change causes bulk fluid movement above the repository (gravity-driven heat pipes).

Thermochemical effects consist of solid phase transformation (negligible at the expected  $T$ ) and changes in the chemical compositions of solids, minerals, particulates, liquids, and gases through various physico-chemical processes that are temperature-dependent. The latter will have a kinetic dependence and, in addition to temperature, will be affected by liquid and gas flows and their compositions.

Predicting thermal-mechanical (TM) and thermal-chemical (TC) effects requires understanding and modeling near-field environment (NFE) processes, in particular: the overall heat transfer (including natural convection), the countercurrent liquid-vapor flows and the liquid-vapor phase change in a fracture-matrix system, and the matrix-fracture interaction. In particular, determining the flow path of water after its vaporization from the matrix, and its subsequent condensation, is a key to the thermal-hydrologic-chemical (THC) analysis. (Potentially more than 300 mm/yr of liquid water, a rate far exceeding the 7 mm/yr currently accepted as a percolation flux, will be mobilized during the thermal period.) This complex problem is influenced by phenomena occurring over disparate size scales (from

matrix block for liquid-vapor flows to mountain scale for heat transfer) and time scales (from an order of years for heat pipe flows to hundreds of years for chemical kinetics). A somewhat different version of coupled processes than that of Hardin and Chestnut (1997) emphasizing thermo-mechanical and flow effects is shown in Table YY-1

**TABLE YY-1**  
**COUPLED PROCESSES**

Conserved Quantity	Driving Force				
	$\nabla T$	$\frac{1}{2} (\nabla u + \nabla u)^T$	$\frac{1}{2} (\nabla v + \nabla v)^T$	$\nabla C$	$\nabla V$
Thermal Energy	Fourier's Law	Strain Energy	Viscous Dissipation	Dufour Effect	Peltier Effect
Momentum (Solid)	Thermal Stresses	Hooke's Law	Pore Pressure		
Momentum (Fluid)	Natural Convection, Heat Pipes	Geometry Change (Fracture Aperture)	Stoke's Law Darcy's Law	Osmosis (Membrane)	Electro-Osmosis
Mass	Soret Effect	Stress-induced Diffusion	Ultrafiltration	Fick's Law	Electrophoresis
Charge	Seebeck Effect		Streaming Current	Diffusion Current	Ohm's Law

The commonly accepted scenario for near-field/altered zone (NF/AZ) hydrology during the thermal period is as follows: vaporized water is expelled from the matrix toward the fractures (a back-of-the-envelope calculation predicts pressure drops from matrix blocks to fractures on the order of 1 atm); steam moves in fractures countercurrent to refluxing water, in buoyancy-driven heat pipes above the repository and in capillary-driven heat pipes below; part of the condensing liquid water flows countercurrent to steam, while another part sheds around the drifts or flows away from the drift, for heat pipes above or below the repository, respectively; at the vaporizing end of the heat pipes, refluxing liquid water vaporizes to steam, creating and sustaining a countercurrent flow. For the purpose of the NF/AZ elicitation, I will accept this scenario without significant loss, even though it is based on some restrictive assumptions of a homogeneous and symmetric system. For purposes of the

TSPA, however, the project must additionally demonstrate its robustness, given that: (1) boiling in porous media, to which the problem is related, includes regions of instability (Ramesh and Torrance, 1990; 1993); and (2) the Large Block Test at Yucca Mountain exhibited analogous instabilities after the inadvertent infiltration of rainwater for a short time period (D. Wilder, NFEE Workshop 1).

My assessment of the coupled effects can be summarized as follows. Important thermo-mechanical (TM) and thermal-hydrologic-mechanical (THM) effects should be expected following the onset of the thermal period, with qualitatively different behavior at the center and the edges of the repository, due to the different boundary conditions in the two regions. A reduction in the apertures of vertical fractures near the center of the repository is likely. Corresponding changes in fracture permeability will depend on the original fracture values, the relative effect being smaller for larger-aperture fractures. Expected changes can be in the range of one to two orders of magnitude. At drifts near the edge, fracture opening and slip are possible. At the expected (near 100°C) temperatures in the NFE, the kinetics of relevant chemical reactions are relatively slow (compared to typical geothermal reservoirs) to effect significant changes. Thus, significant TC and THC effects should be the result of: (1) mineral deposition in fractures at the vaporizing ends of heat pipes; and (2) possible fracture healing due to dissolution of fracture asperities (W. Lin, NFEE Workshop 1). The latter represents a coupled THMC effect, is attributed to pressure solution, but it is not well understood. Both these THC effects will act to reduce fracture permeabilities, by one to two orders of magnitude in the fracture-healing case, and perhaps by a greater degree for deposition. The latter may lead to the formation of a cap depending on the extent of heat pipes. With the exception of the latter case, I suspect that the overall effect of THM and THC falls within the range of natural variability. However, for a given initial permeability distribution, the anticipated reduction in permeability will create progressively shorter heat pipes, decrease natural convection, increase the temperature and extent of the dryout region, and will affect seepage fluxes in the drifts following the thermal period.

## **THERMAL-MECHANICAL (TM) EFFECTS (DRIFT STABILITY)**

Because this area is outside my expertise, I will not offer substantive comments. I expect slip of joints to be important in evaluating drift stability, and simulations should be conducted to evaluate this effect. The collapse of the drift is important in analyzing the viability of the project, given the effect of the granular medium to be created on increasing the heat transfer resistance (by conduction rather than radiation) and on the seepage fluxes in the drift. Of some interest is the possibility of a power-law distribution in block sizes (which is common in some fragmentation processes; for instance, see Turcotte, 1986). The flow properties (absolute and relative permeabilities) of the induced self-similar packings can be studied using an Apollonian packing model (e.g., see Adler, 1992).

## **THERMAL-HYDROLOGIC-MECHANICAL (THM) EFFECTS**

Thermomechanical effects are essentially changes of volume and shape. They follow instantly the temperature field (with the exception of kinetic-driven processes, such as crack growth, strength degradation, pressure solution, and creep, which actually are coupled THMC effects). Although a small effect per se, thermal expansion of solids is important for fractured systems. It may result in either a reduction or increase in fracture apertures in response to changes in normal and/or shear stresses across joints. Volume expansion may create some new cracks, but these will be less effective than major fractures in the hydrologic response. Because of symmetry and the almost planar heat source, I expect a reduction in the aperture of vertical fractures near the repository (except for edge drifts), due to increased normal (horizontal) stresses, as a result of confinement. Near the edges (or for an isolated drift), the behavior might be different, and opening of fractures is possible. High shear stresses could lead to slip on horizontal joints. The detailed response, which must be sought by numerical simulation, will be influenced by the system geometry and dimensionality (two-dimensional vs. three-dimensional), the heterogeneity in properties, and the applied boundary conditions.

The anticipated thermal stresses for laterally constrained boundaries can be roughly estimated from the following:

$$\Delta\sigma_{th} \approx \alpha E \Delta T / (1 - \nu) \quad (1)$$

where  $\alpha = O(10^{-5})^\circ\text{C}$ ,  $\nu$  is the Poisson ratio, and the (fractured rock) modulus  $E$  is on the order of 10 Giga Pascals (GPa). Stresses on the order of 10 to 20 Mega Pascals (MPa) are expected as a result of thermal loading ( $\Delta T \approx 75^\circ\text{C}$ ). The resulting effect on mechanical aperture is estimated as follows:

The change in fracture aperture  $d$  due to the change in normal stress can be described by the hyperbolic law

$$\Delta\sigma_{th} = \frac{d}{\alpha - \beta d} \quad (2)$$

for the case of mated joints, and by an exponential law for the case of uncorrelated joints.

Here  $d$  is the effected joint closure, and  $\alpha$  and  $\beta$  are constants such that  $\alpha/\beta = d_m$ , the maximum joint closure. At the above stress levels, changes in joint apertures in the range 10-100  $\mu\text{m}$  can be expected. The above relationship describes the loading part of the cycle. Upon unloading, the behavior is hysteretic, resulting in a smaller change in aperture.

At the expected thermal stresses, some horizontal fractures near the center of the repository and many joints near the edge of the repository may experience slip. But it is not clear whether the slip will crush asperities or override them and cause dilation. If dilation occurs, irreversible permeability increases of one to two orders of magnitude are possible. But if asperities break, then the permeability may decrease. This effect is in need of further study. In general, the geometry and orientation of joints are important parameters for determining slip. Because the thermal stress orientation will vary as a function of time during heat-up, the potential for change in fracture permeability on joints of various orientations will also be time-dependent.

Flow through fractures will affect the TM and THM assessment twofold: (1) by modifying the temperature field, and (2) by the development of pressure gradients. The first may affect

heat pipe development and lateral flow diversion and requires solving the full problem interactively. However, the effect of fluid pore pressure (expected to be about 0.1MPa) will be insignificant.

In vertical fractures away from the edge of the repository, the decrease in mechanical aperture will engender a concomitant decrease in hydraulic aperture and, hence, fracture permeability. The effect depends on the initial permeability. Assuming that the cubic law is valid, we expect

$$k = \frac{h^3}{12} \quad (3)$$

and

$$\frac{k_n}{k} = \left(1 - \frac{d}{h}\right)^2 \quad (4)$$

where  $k_n$  is the new permeability of a fracture of initial permeability  $k$  and aperture  $h$ , subject to aperture decrease by an amount  $d$ . For example, for  $d=50 \mu\text{m}$ , the permeability reduction would equal 1/4 for a larger fracture of  $h=100 \mu\text{m}$  and 1/36 for a smaller fracture with  $h=60 \mu\text{m}$ . The effect is therefore relative (greater for fractures of small aperture, and smaller for fractures of large aperture). Given the uncertainty in fracture permeabilities, the variation due to thermal loading is expected within the range of natural heterogeneity in the repository. For an initial distribution of fracture permeabilities  $f(k)$ , we can compute the new distribution  $f_n(k_n)$  from the following relation:

$$f_n(k_n) = \frac{(d + \sqrt{12k_n})}{\sqrt{12k_n}} f\left(\frac{(d + \sqrt{12k_n})^2}{12}\right) \quad (5)$$

assuming that  $d < \sqrt{12k}$ , and where we made use of relations (3) and (4). Thus, thermal effects will effectively skew an initial distribution toward smaller permeability values. The above expression can be used to assess the change in the distribution of fracture permeabilities in terms of thermal stresses (through the reduction in aperture  $d$  and expressions [1] and [2]) given an initial distribution  $f(k)$ . The fracture geometry (roughness

and aperture characteristics) will be affected by the thermal load. Fracture surface roughness has possible long-range correlations, which will influence transport and the fracture-matrix interaction. The effect of thermal load on two-phase flow parameters would be to increase the capillary pressure (decrease the van Genuchten  $\alpha$  parameter) of the fracture and decrease the effective diffusion coefficient as aperture decreases. Given a model for the reduction of aperture (for example as shown in Cook, 1992), in combination with the change in normal stresses, an approach similar to that of Katz and Thompson (1986) can be applied to estimate the variation in capillary pressure properties. This approach recognizes the existence of connected backbones of high conductance. Relative permeabilities and residual saturations will not be affected significantly. The expected reduction in the vertical permeabilities of fractures will lead to a reduction of the anisotropy of the fracture network and to a possible increase in lateral flow.

The effect of natural convection in single-phase flows can be evaluated using the Rayleigh number,

$$Ra = \frac{g \Delta T k L}{T_a \nu \alpha} \quad (6)$$

where  $L$  is the height of the zone across which the temperature difference  $\Delta T$  is applied,  $T_a$  is the mean temperature, and here  $\nu$  denotes kinematic viscosity and  $\alpha$  denotes thermal diffusivity. Analogous expressions apply for two-phase flow (for example, see Ramesh and Torrance, 1993). For single-phase flow in porous media, in which  $\Delta T$  is applied across a horizontal layer, natural convection is initiated when  $Ra \geq 4\pi^2$ , following which heat transfer is enhanced by increasing  $Ra$ . In other geometries (for example, in the saturated zone below the repository or at the edge of the repository), natural convection can be assessed by analyses of simpler problems, several of which are described in Gebhart et al. (1988). Equation (6) shows that decreasing values of  $k$  for instance by fracture aperture reduction would lead to suppressed natural convection.

## THERMAL-HYDROLOGIC-CHEMICAL (THC) EFFECTS

Solid-phase transformations are expected due to the transition from  $\alpha$  - to  $\beta$ -cristobalite, which occurs at 200° to 250°C. The accompanying volume expansion may produce some new cracks, but these will be not as effective as major fractures in fluid flow. The volume change will increase stresses, but probably not greatly.

The chemical composition of gases will change primarily through H<sub>2</sub>O and CO<sub>2</sub> content. The first is controlled through vaporization/condensation, the second through equilibria with liquid water, but also through natural convection and diffusion in the gas phase. Changes in the chemical composition of liquids will occur due to evaporation and condensation, and through transport and reaction with solid surfaces. We will estimate the processes of evaporation and condensation separately below.

Consider liquid evaporation. During heating, water evaporates in the matrix and at the boiling end of heat pipes (if they occur). We note that the effect of small pores (typically described as a Kelvin effect) should be considered vis-a-vis the lowering of vapor pressure (which in turn would require progressively higher  $T$  for progressively lower liquid saturation) and the thermodynamic partition coefficients. If the entire vaporization occurs at a single place, as suggested by the heat pipe scenario, the ensuing  $\Delta p$ , which is on the order of 1 atm, would imply temperatures as high as 120°C in the matrix. Evaporation in the matrix will produce liquids of progressively greater ionic strength, greater pH because of a lack of atmospheric CO<sub>2</sub>, and silica and carbonate precipitates. Silica precipitates will be controlling. A rough estimate of the volume of solids precipitated per 1 kg of H<sub>2</sub>O evaporated in the matrix is  $2 \times 10^{-2} \text{ cm}^3$ , which is hydraulically insignificant. However, precipitation in the fracture may not be, as discussed below. Evaporation of refluxing water in the fractures will lead to precipitation of calcite and silica from dissolution of calcite and silica minerals lining fracture and pore walls. This precipitation, which will occur at the repository ends of the heat pipe, can plug fractures locally. Potential effects on permeability are described below.

Vapor condensation will occur at the condensing end of heat pipes. The composition of water vapor initially will resemble that of distilled water; because of the chemical disequilibrium,



dissolution reactions of rock minerals will occur. If the ionic strength,  $I$ , is below a critical value (reported as 0.05 M for oil reservoirs, by Khilar and Fogler, 1983) clay mobilization may also occur. The latter effect is practically instantaneous and will lead to decreased permeabilities (e.g., see Sharma and Yortsos, 1987). Regardless of the path of return flow (through heat pipes or shedding around the drifts), dissolution reactions will occur, followed by precipitation somewhere else (at the vaporizing end of the heat pipes or at a location of lower temperatures for the case of liquid shedding and silica precipitates). However, the kinetics of reactions such as cristobalite dissolution are quite slow at expected repository temperatures (with reported kinetic constants of the order of  $k_{diss} = 10^{-12}$  mole/m<sup>2</sup> s although considerable uncertainty does exist). Indeed, Glassley (in Wilder, 1996) and Lichtner (NFEE Workshop 2) have shown that characteristic times for significant porosity changes are on the order of thousands of years. At first glance, this would suggest that THC effects are not important. However, this interpretation would be misleading as the following two processes may lead to non-trivial effects: (1) Fracture healing (W. Lin, NFEE Workshop 1), and (2) the continuous deposition of minerals at specific locations, for example at the vaporizing end of heat pipes.

According to Lin (NFEE Workshop 1), a significant and relatively fast reduction of fracture permeability may occur at high temperatures and in the presence of a convecting fluid, apparently because of the dissolution of asperities under increased normal stress. Significant permeability reduction (one to two orders of magnitude) has been reported from this mechanism. The postulated mechanism is pressure solution. Fracture asperities are prone to enhanced dissolution rates due to the higher chemical potential at points of contact, where local curvatures are higher. In addition, transport mechanism to move dissolving material away from the asperity is needed. In fracture healing, this will be provided by fluid flow. The only problem with this interpretation is that typical pressure solution mechanisms require much higher stress levels (see Dewers and Ortoleva, 1990 and related references) than those expected in the thermal period of the Repository. At present, fracture healing is a potentially significant but not well understood process.

Mineral deposition at the vaporizing end of a heat pipe (or elsewhere, provided that it occurs at approximately the same location and for an extended period) is another non-trivial THC

process. We can estimate its importance by proceeding as follows. Consider the refluxing liquid moving countercurrent to steam in a heat pipe and dissolving minerals lining the fracture. Assume, for simplicity, a constant dissolution rate. Then, the steady-state mass balance for a dissolving species of concentration  $C$  is

$$u \frac{\partial C}{\partial x} = r_{diss} = S_v k_{diss} \quad (7)$$

where  $u$  is the return liquid velocity along the return path of spatial coordinate  $x$ , and  $S_v$  is the specific surface area per unit bulk volume, where the dissolution reaction occurs. We assume that precipitation will not occur, due to small concentrations. According to the heat pipe scenario, complete evaporation occurs at  $x=L$  (where  $L$  denotes the length of the heat pipe). For constant dissolution rates, we obtain the simple result

$$C(L) = \frac{S_v k_{diss} L}{u} \quad (8)$$

Of course, a more complicated expression will result if we account for effects of concentration on the dissolution rates. Given the rather dilute solutions, however, equation (8) should be reasonably valid.

If the area where the mineral deposited by evaporation is denoted by  $A_m$ , the volume of minerals deposited per unit time is equal to  $\frac{\mu C(L) A_m M_w}{\rho_m} = S_v k_{diss} L A_m M_w / \rho_m$ , where  $M_w$  denotes molecular weight and  $\rho_m$  is density. Interestingly, this shows that the rate of deposition depends on the length of the heat pipe, which is implicitly determined from the solution of the overall problem. If we finally assume that such deposits will form a porous precipitate of porosity  $\phi_m$ , uniformly spread over the area  $A_m$ , the deposition zone will grow at a velocity given by

$$v_m = \frac{S_v k_{diss} M_w L}{\rho_m (1 - \phi_m)} \quad (8)$$

The simple result shows that the rate of growth of this zone is proportional to the length of the heat pipe length,  $L$ , and the dissolution rate product  $S_v k_{diss}$ . Furthermore, it is independent of the actual liquid velocity in the fracture (inasmuch as the latter does not affect the intrinsic dissolution rate or the effective specific surface area). A simple approach to estimate  $S_v$  would be to take a smooth planar fracture of aperture  $h$ . Then,  $S_v = 2/h$  and given the relationship (3) we further have  $S_v = 2/\sqrt{12k}$ . In this case, equation (10) further reads

$$v_m = \frac{0.57 k_{diss} M_w L}{\sqrt{k} \rho_m (1 - \phi_m)} \quad (10)$$

This expression gives a conservative result for the rate of growth, as the surface roughness of the fracture can be significant resulting into a larger specific surface area. We note that smaller permeability fractures fill-up faster, for otherwise identical conditions (although one should also recall that the length of the heat pipe zone will decrease as the fracture permeability decreases). For a quantitative estimate we take  $k_{diss} = 10^{-12}$  moles  $m^{-2} s^{-1}$ ,  $\rho_m = 2$  gr  $cm^{-3}$ ,  $\phi_m = 0.3$ ,  $M_w = 60$  gr  $mole^{-1}$  and  $L = 20$  m. Then, for a fracture permeability of 0.1 d, we find  $v_m = 4.68$  cm  $yr^{-1}$ , while for a permeability of 1 d, we have  $v_m = 1.48$  cm  $yr^{-1}$ . In the context of the present problem, this is a non-negligible rate of growth. We must point out that these predictions are based on a simple model, and under assumed parameter values for the specific surface area and the reaction kinetics. These parameters are subject to uncertainty, which needs to be further bounded by additional investigations. The mode of the return liquid flow (namely whether in terms of films, lenses, etc.) will also affect the specific surface area and should also be further examined.

The growing zone of mineral deposition would be characterized by a significantly reduced permeability, due to the small size of the deposited grains. As it is being formed, the permeability will start varying spatially. Heat pipe development under such conditions (including both capillary and gravity effects) was studied by Stubos et al. (1993). Eventually, this zone will become the equivalent of a "cap," similar to those observed in geothermal fields (although in the latter, the kinetics are much higher and precipitation may

occur at both ends of the heat pipe). The development of such a zone would affect significantly the seepage into the drifts, which is expected to occur sometime after the end of the thermal period. We believe that it must be considered in process assessment.

Because of the slow reaction rates, phenomena, such as fingering and formation of wormholes, common to acidizing processes in reservoir engineering, will be suppressed. For such chemically-induced flow instabilities to be important, the rate of dissolution (expressed in terms of a dissolution velocity  $\frac{k_{diss} M_w}{\rho_m}$ , which expresses the rate of the opening of the pore volume) must be comparable to the convective flow velocity  $u$ , namely the Damkohler number  $Da = \frac{k_{diss} M_w}{\rho_m u}$  must be of order 1. Using the above kinetic parameters, this would require the very small return liquid flow rate of the order of  $9 \times 10^{-8} \text{ cm yr}^{-1}$ , which is far below the one expected during the thermal period. For typical values, a Damkohler number of the order of  $10^{-7}$  is predicted, which would indicate insignificant dissolution-driven fingering.

In summary, in terms of precipitation and dissolution reactions, my inclination is that fracture healing and mineral deposition at the vaporizing end of heat pipes are the two key THC effects expected to have non-trivial effects on permeability. Fracture healing needs additional study to understand the underlying mechanisms. Additional work is also needed to narrow the range of uncertainty in the kinetic dissolution parameters.

## IMPLICATIONS

Reducing fracture permeabilities near the drift during heating will tend to diminish natural convection (reduced  $Ra$ ), thereby increasing local temperatures and gas pressure, to diminish the heat pipe effect, and to produce more symmetrical temperature profiles above and below the repository. The effect on natural convection was already discussed. The effect on heat pipes can be understood using the following simple analysis. The existence of gravity-driven, bottom-heating, steady-state heat pipes (like those above the repository) in

homogeneous media requires that the following condition is satisfied (Satik et al., 1991; Stubos et al., 1993).

$$\omega \equiv \frac{q_H \mu_v}{k L_v g \Delta \rho \rho_v} < \omega_{crit} \equiv \max \frac{k_l k_v}{k_l + \beta k_v} \quad (11)$$

where  $q_H$  is the heat flux (from the repository),  $L_v$  is the latent heat of vaporization,  $\beta$  is the ratio of kinematic viscosities (liquid to vapor), and subscript  $v$  refers to vapor. Parameters  $k_l$  and  $k_v$  are the relative permeabilities to liquid and vapor in steady-state countercurrent flow. These depend on saturation (and other factors, possibly). The value of  $\omega_{crit}$  depends on the relative permeabilities of liquid and vapor. The length of the heat pipe would be restricted (essentially the heat pipe would become capillary- rather than gravity-driven) when  $\omega$  exceeds the critical value. As shown in (11), this can happen at sufficiently low  $k$ . Under such conditions, the length of the heat pipe would scale with  $\sqrt{k}$  (just like the case of capillary-driven heat pipes—namely those below the repository, the length of which also scales with  $\sqrt{k}$ ) and they will not be effective in heat transfer any longer. A schematic of the  $\omega(S)$  curve denoting the possible steady-states developing in heat pipes and the maximum condition is shown in figure YY-1. The above analysis is based on the assumption of a relatively homogeneous porous medium and steady-state conditions. When heterogeneity in permeability is involved, the problem becomes more complex, as discussed in Stubos et al. (1993) and the termination of a heat pipe may occur earlier than indicated in (11). Furthermore, the analysis would need to be modified if there is substantial condensate return by imbibition in the matrix. This is a problem of fracture-matrix coupling that also needs further study, and it is briefly discussed below. However, we must note that the existing simulations using a variety of models (such as DKM) indicate that in the heat pipe zone, the matrix is almost fully saturated, thus limiting the potential for further imbibition. For the case of episodic flow of the refluxing liquid, the analysis is expected to hold, provided that time-averaged relative permeabilities are used.

## Fracture-Matrix Coupling

Of significance to the flow problems in the project is the fracture-matrix interaction. The first issue is the degree to which water will flow in fractures (advection) versus being imbibed into the matrix (diffusion). This is part of the general problem of fracture-matrix interaction and is common to heat, fluid, and mass transport. An extensive analysis was given by Yortsos (1997). In general, the ratio between advective and diffusive fluxes can be expressed in terms of a Peclet number

$$Pe = \frac{q_f L}{D_i} \quad (12)$$

where  $q_f$  is the flow velocity in the fracture,  $L$  is a characteristic matrix block scale, and  $D_i$  is diffusivity (thermal, capillary, and mass). High values of  $Pe$  imply a disequilibrium between fracture and matrix. For heat transfer,  $D_{th} \approx 10^{-6}$  to  $10^{-7}$  m<sup>2</sup>/sec, and under typical flow rates, the heat transfer may be assumed at equilibrium. For capillary imbibition, the capillary diffusivity depends on the permeability of the matrix, according to

$$D_{cap} \approx \frac{\gamma \phi_m^{3/2} \sqrt{k_m}}{\mu} \quad (13)$$

and, depending on the value of  $k_m$ , it may assume values of the order of  $10^{-9}$  to  $10^{-10}$  m<sup>2</sup>/sec, suggesting a much slower approach to equilibrium. Similar order of magnitudes pertain to mass diffusivity. The existence of mineral coatings on the fracture surface (which result in an effectively lower  $k_m$ ) will further reduce capillary diffusivity toward the matrix. For the case of heat pipes and return flow, which are of importance here, imbibition and heat transfer must be examined together.

A second issue is the pattern of liquid flow along fracture surfaces, namely whether it will occur in the form of fingers or channels, in terms of episodic movements or at steady-state. For downward liquid flow, the pattern will be a function of the relative roles of gravity

(which is destabilizing), capillarity (which is stabilizing), and viscous effects between water and gas (which is stabilizing). It will also depend on the correlation structure of the fracture aperture, and of course, on the imbibition capacity of the matrix. The competition between gravity and capillarity is expressed with the Bond number

$$N_B = \frac{g \Delta \rho k}{\gamma} \quad (14)$$

while that between viscous and capillary effects is expressed through the capillary number

$$Ca = \frac{q_f \mu}{\gamma} \quad (15)$$

Typically, in homogeneous porous media the transition between the different regimes (namely from capillary-controlled to gravity- or viscous-controlled) commences is obtained around values on the order  $10^{-5}$  to  $10^{-4}$ . Clearly, gravity will be favored in fractures of sufficiently high permeability, in which gravity fingers should be expected. On the other hand, for typical conditions,  $Ca$  is sufficiently small and capillarity should be controlling locally. In the latter case, the correlation structure of the aperture is expected to dictate the displacement patterns. More correlated fractures will lead to a higher potential for channeling. In such cases, the fracture-matrix interaction reduction factor (which is the amount of fracture area that is available for conductance into the matrix) should be less than 1. At present this reduction factor is assumed to be proportional to the relative permeability between different parts of the fracture, but this assumption needs to be carefully justified. The degree of fracture-matrix interaction has implications to the applicability of the ECM or DKM models as discussed in Yortsos (1997). Episodic flow events, particularly during the countercurrent flow in fractures, are also possible, as suggested in the study of Kneafsey and Pruess (NFEE Workshop 1). The relative permeabilities in such cases would express suitable time averages of these events and would involve an additional dependence on  $N_B$ . More study of this process would be useful.

## MULTIPLY COUPLED EFFECTS

Generic THMC effects include stress corrosion, creep, crack growth and rock degradation. These are described in standard references. For the particular project, here, fracture healing is expected to be the primary THMC effect. It was described above.

## DURABILITY OF EFFECTS

The TM response is in general hysteretic. If the joint surfaces are not well mated, there will be different and durable effects during the cooling period. If a fracture healing process occurs, the surfaces will be better mated. Assuming that due to past thermochemical alteration the joints in the repository area are reasonably well mated and that fracture healing will occur, changes in the permeability of vertical fractures can be reversible; however, the changes in vertical and horizontal fractures due to shear slip and the response to normal stress of fracture, with non-mated surfaces, would not. The TC and THC response is reversible as far as phase change and the effect on thermodynamic, mechanical, and transport variables (e.g., solubilities, enthalpies) is concerned. However, effects on kinetics and extent of heterogeneous (solid-liquid) reactions are irreversible. Dissolution-precipitation reactions are hysteretic due to the need for nucleation in the second case. Dissolution and precipitation reactions leading to fracture healing and the formation of a zone of precipitation at the vaporizing end of heat pipes would be irreversible.

## RECOMMENDED ACTIVITIES TO REDUCE UNCERTAINTIES

The reduction of uncertainties in the thermomechanical response will benefit from: (1) a numerical simulation of the thermomechanical response of the fracture-matrix system (discontinuum) in the two regions, near the center and near the edge of the repository; and (2) a further study (experimental and simulation) of the effect of joint slip on fracture permeability.



The reduction of uncertainties in the thermochemical response will benefit from: (1) further study and understanding of the process of fracture healing; and (2) a narrower bounding of the kinetic constants and specific surface areas of dissolution reactions in a matrix-fracture system.

Improvements in the modeling of heat pipes in a fracture-matrix continuum should be sought in the following two areas: (1) the understanding of the intrinsic flow mechanisms (for instance, along the lines of Kneafsey and Pruess, NFEE Workshop 1) and the effect of the matrix-fracture interaction; and (2) the scaling-up of these mechanisms to the numerical grid scale. For purposes of TSPA, the stability of heat pipes overlying a dry-out region in a fractured medium needs to be investigated, as pointed out above. Finally, the confidence to the TH modeling for predicting the mountain-scale response will be substantially enhanced by a successful matching of the TH response of the well-characterized Large Block Test (which is currently unsatisfactory with existing models, [Wilder, NFEE Workshop 1]).

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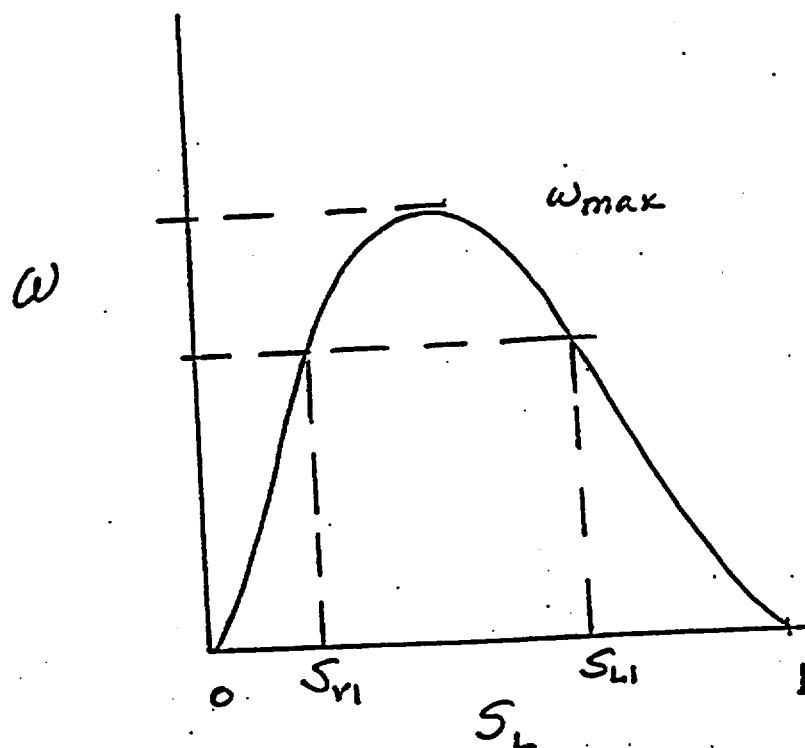


Figure YY-1 Schematic of steady-states ( $S_{v1}$  or  $S_{L1}$ ) developing in a gravity-driven heat pipe. When  $\omega$  exceeds  $\omega_{max} \approx 0.3$ , the heat pipe cannot be sustained by gravity and capillarity becomes an important factor.