YUCCA MOUNTAIN
SITE CHARACTERIZATION
PROJECT

THERMOHYDROLOGIC MODELING AND TESTING PROGRAM PEER REVIEW RECORD MEMORANDUM

January, 1995

Yucca Mountain Project

Thermohydrologic Modeling and Testing Program
Peer Review Record Memorandum

PRRM Approval

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PART I

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NOMENCLATURE

B - gravity number, $g\Delta\rho k/\gamma$, dimensionless
b - fracture aperture (L)
Ca - capillary number, $u\mu/\gamma$, dimensionless
D - capillary diffusivity (L^2/T)
g - acceleration of gravity (L/T^2)
k - permeability (L^2)
k_{rw} - effective water relative permeability, dimensionless
L - length (L)
P_c - capillary pressure (m/LT^2)
Pe - Peclet number, uL/D, dimensionless
q - volumetric flow rate (L^3/T)
q* - critical rate per unit width (L^2/T)
S - saturation, dimensionless
u - volumetric flow rate per unit area (L/T)
t_d - length of disturbance time (T)
v - variance, dimensionless
W - width (L)
γ - interfacial tension (M/T^2)
Δh - change in head, (L)
$\Delta\rho$ - change in density, (M/L^3)
λ - correlation length (L)
μ - dynamic viscosity (M/LT)
ρ - density (M/L^3)
ϕ - porosity, dimensionless

Subscripts

c - capillary
d - drift
e - mass
eff - effective
fa - fault
fr - fracture
i - initial
M - mountain
m - matrix
n - grid block
T - thermal

ACRONYMS

AML	- Areal Mass Loading
DOE	- Department of Energy
DSTFJ	- Drift Scale Test with Flat Jacks
EBSFT	- Engineered Barrier System Field Test
ECM	- Equivalent Continuum Model
ESF	- Exploratory Studies Facility
IFD	- Integrated Finite Difference
LANL	- Los Alamos National Laboratory
LBT	- Large Block Test
LBNL	- Lawrence Berkeley National Laboratory
LLNL	- Lawrence Livermore National Laboratory
LSLD	- Large Scale Long Duration
MINC	- Multiple Interacting Continua
MPC	- Multi-Purpose Canister
MTU	- Metric Tons Uranium
NAS	- National Academy of Science
NFE	- Near Field Environment
NRC	- National Research Council
NRC	- Nuclear Regulatory Commission
PESFT	- Prototype Engineered Barrier System Field Test
PI	- Principal investigator
PRRM	- Peer Review Record Memorandum
PRT	- Peer Review Team
PWR	- Power Water Reactor
RIB	- Reference Information Base
SANL	- Sandia National Laboratory
SCP	- Site Characterization Plan
SFT	- Spent Fuel Test
SNF	- Spent Nuclear Fuel
T	- Thermal
TH	- Thermo-hydrologic
THC	- Thermo-hydrologic-chemical
THMC	- Thermo-hydrologic-mechanical-chemical
TM	- Thermo-mechanical
TSPA	- Total System Performance Assessment
URL	- Underground Research Laboratory
USGS	- United States Geological Survey
UZ	- Unsaturated Zone
YM	- Yucca Mountain
YMSCP	- Yucca Mountain Site Characterization Project

GEOLOGICAL ABBREVIATIONS

BFn	- Bullfrog nonwelded hydrogeologic unit
BFw	- Bullfrog welded hydrogeologic unit
CFu	- Crater Flat undifferentiated hydrogeologic unit
CHn	- Calico Hills nonwelded hydrogeologic unit
CHnv	- Calico Hills nonwelded vitric hydrogeologic unit
CHnz	- Calico Hills nonwelded zeolitic hydrogeologic unit
PPw	- Prow Pass welded hydrogeologic unit (part of CHn)
PTn	- Paintbrush Tuff nonwelded hydrogeologic unit
QAL	- Quaternary and Tertiary alluvium and colluvium
TC	- Tiva Canyon Tuff
TCw	- Tiva Canyon welded hydrogeologic unit
TRw	- Tram welded hydrogeologic unit
TS	- Topopah Spring Tuff
TSv	- vitric zone within Topopah Spring Tuff
TSw	- Topopah Spring welded hydrogeologic unit
TSw1-3	- designated welded zone within the Topopah Spring Tuff

EXECUTIVE SUMMARY

Introduction

The Peer Review Team (PRT)[1] was established by the Yucca Mountain Site Characterization Office of DOE's Office of Civilian Radioactive Waste Management to conduct an external review of the Thermohydrologic Modeling and Testing Program of the Yucca Mountain Site Characterization Project (YMSCP). The objective of this review was to evaluate the YMSCP approach to understanding hydrothermal conditions at Yucca Mountain, Nevada that would be generated by repository heating.

The peer review process was initiated by Susan B. Jones, Assistant Manager for Scientific Programs, Yucca Mountain Site Characterization Office. She did so by releasing a Peer Review Notice, and by appointing a Chairperson (Paul A. Witherspoon), an Assistant Manager's representative (Ardyth M. Simmons, who served until October 13, 1995 and was succeeded by Robert A. Levich), and a Technical Secretary (Kathryn A. Mrotek). After a Peer Review Plan was set up to outline the general requirements of the review process, the following persons were appointed to serve on the PRT: Paul A. Witherspoon, R. Allan Freeze, Francis A. Kulacki, Joseph N. Moore, Franklin W. Schwartz, and Yanis C. Yortsos. The backgrounds and affiliations of this group are given in Appendix B.

The design and performance assesment of the proposed repository rely heavily on predictions from mathematical models that are based on the relevant physical and transport processes. In carrying out this assignment, it was therefore important for the PRT to recognize the need for an accurate process modeling of the behavior of the site under the hydrothermal conditions that would be generated by repository heating. Model predictions with reasonable assurances require the testing of various scenarios in a probabilistic framework using a reliable model. Reduction of uncertainties can only be accomplished by additional site characterization, improved understanding of the fundamental process components, and improved knowledge of the variation of time-dependent boundary conditions. A reliable model of the relevant physical and transport processes and their accurate representation in numerical codes are necessary. These issues are extensively addressed in this report.

Background

The potential horizon for a repository at Yucca Mountain (YM) is in the Topopah Spring Tuff (TS)[2] which is a heavily fractured tuff in the vadose zone some 325 m below the surface and about 250 m above the water table. A decision on technical site suitability is currently scheduled for 1998, with a license application for construction authorization in 2001. Under the new "Program Approach", it is necessary to achieve a "broad understanding of nearfield thermal-hydrologic-mechanical-chemical (THMC) processes such that defensible calculations of postclosure performance can be made." A successful license application will require an "understanding of coupled processes" and "substantially complete containment".

Yucca Mountain is a fault bounded volcanic plateau located in the arid, south-central part of the Great Basin. The Topopah Spring Tuff is enclosed in a series of ash-flow tuffs and has been disrupted by throughgoing faults that have the potential to act as paths of high permeability. The majority of the mapped faults are high angle, north- to northwest-trending normal structures, and there is extensive associated fracturing. Communication in the vadose zone, presumably through fast paths, is indicated by several factors, such as the pneumatic pressure communication between the volcanic units, and the presence of young water at depth. Because the matrix permeability in the TS is of the order of 10^{-18} m^2, it is apparent that the fast paths must be significantly more permeable.

The hydrologic system at Yucca Mountain depends on precipitation, infiltration and percolation. Mean annual precipitation at present is 170 mm/yr, but the amount of infiltration is an important issue that

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[1] See list of acronyms on Page vii.

[2] See list of geological abbreviations on Page viii.

has not been resolved. Model results have given values as low as 0.1 mm/yr; however, significantly higher values from field measurements have recently been reported. A major feature of the unsaturated system is the significant heterogeneity in flow and transport processes. An important consequence is the significant local variation in the moisture content of the geologic units. The average water saturation in the TS is 65%, whereas layers immediately above and below have much lower saturations. The matrix porosity of the TS is 0.08 to 0.12.

As the repository is subjected to a thermal load, all TH processes will be driven by a time-varying heat source due to decay heat from the SNF and the areal mass loading of the emplaced waste. The various processes and impacts will be carried out within a "thermal framework" that has a rather rapid temperature rise at first, followed by a long period in which TH processes in the near field environment and on the mountain scale are played out.

The principal conceptual model of the TH coupling involves an initial period in which heat is conducted into the rock on the repository scale. Temperatures in the vicinity of the repository rise above the boiling point (97°C) and vaporization of pore water takes place. This leads to a dried-out zone along fractures and the transport of water vapor through fractures to cooler regions where condensation takes place.

The overall system performance will mainly be influenced by the following fluid flow processes: (1) flow in a dryout region and the adjacent heat pipe around the repository during the early part of the project (~1000 years); (2) flow of condensed fluids and/or of surface infiltration in the rock formation, particularly in fast paths; and (3) the re-wetting of the dry region when boiling ceases at the later stages of the project (>1000 years). The establishment of a dryout region and delayed rewetting are the two key premises on which the concept of an "extended dry repository" is based. All these processes involve the simultaneous flow and/or displacement of two immiscible phases (gas, or vapor, and liquid water). Understanding and prediction of such flows requires adequate knowledge of the flow characteristics of formations comprising the site.

Heat transfer in the matrix is expected to be dominated by heat conduction. In the near field environment, this mode of heat transfer will be coupled with buoyant convection in the dry-out region, and with two-phase convection in the heat pipe region. The likely development of heat pipes is significant to heat transfer, due to their substantial capacity to transfer heat compared to simple conduction. At the mountain scale, we expect, in addition, convective heat transfer in the saturated zone below the repository, and buoyant gas-phase convection in the unsaturated zone.

As a result of the strong thermal disturbances that will occur in the repository, the following main classes of chemical processes are likely to occur: (1) dissolution-precipitation involving an aqueous phase and the enclosing rock matrix; (2) solid-solid phase transformations; and (3) mineral precipitation from an aqueous phase in response to changing temperatures or vaporization. Because many of these reactions involve a change in the volume of the solid phases and the release or uptake of water, they have the potential for altering the porosity, permeability and moisture budget of large volumes of rock.

The rock mass will also undergo thermally induced displacements and changes in stress that, in addition to the material properties, will depend on: (1) the frequency and orientation of the fractures that are present, and (2) the aperture distribution. As a result, apertures will generally tend to decrease as the matrix expands, and the net displacements for the rock mass will be less than what is predicted for a homogeneous rock. The corresponding implications on fluid permeability and flow paths are important.

These chemical and mechanical effects create the difficult problem of trying to predict the overall behavior of a rock mass that is being subjected to changes in temperature. Without data on the actual *in situ* behavior of the Topopah Spring Tuff as it is exposed to a changing thermal field, it will not be possible to develop a reliable procedure for predicting the magnitude, nor the degree of coupling, of the thermochemical and thermomechanical effects of this extensively fractured rock.

Critical Issues

The PRT has identified a set of critical issues that must be resolved by the testing and modeling program of the YMSCP. These have been classified as: (1) technical issues; (2) issues associated with the extended-dry-repository concept; (3) model calibration and validation issues; and (4) issues associated with uncertainty reduction. The technical issues include: (a) infiltration; (b) heterogeneities; (c) fracture-matrix interactions; (d) thermochemical effects; (e) thermomechanical effects; and (f) scale-up issues.

Infiltration rates are likely to have considerable impact on the extent and timing of the thermohydrologic response of the mountain to repository heating. It is conceivable that if infiltration rates are sufficiently high, they could overwhelm the dryout region. It will be difficult for the YMSCP to proceed to the necessary repository-design decisions without a significant reduction in uncertainty with respect to infiltration rates.

The tuffs of Yucca Mountain exhibit heterogeneity in their lithology, stratigraphy, structure, and thermohydrologic properties on a variety of scales. This heterogeneity has substantial impact on both the ambient hydrologic system and on the thermohydrologic system that will exist during repository heating. The dryout, condensation, and possible reflux of moisture during the period of thermal load are likely to be very sensitive to the heterogeneity of the fracture networks in the rocks. Fracture-matrix interactions are still poorly understood, even for single-phase fluid flow, and especially for two-phase flow of steam and water. The nature of these interactions will control, to a large degree, the nature of the heat pipes that may develop, and the potential for reflux of water that condenses above the repository.

The possibility that mineral dissolution and precipitation may effectively seal fractures or otherwise reduce their permeability in the nearfield environment of the repository is still an open, but important, question. Similarly, reductions in permeability due to mechanical changes in fracture apertures under a thermal load have been predicted but not confirmed. Some have suggested that such effects will be secondary, but as yet their overall importance in the proposed repository is uncertain.

Phenomena at different scales affect the physical processes in different ways. Implicit in the passage from one scale to another is an averaging process, the validity of which depends on the assumptions made. The numerical studies of the YMSCP have proceeded on the assumption of constant matrix and fracture properties over considerable distances. Such studies tend to underestimate the degree of channeling that may occur during infiltration or within heat pipes, and with respect to thermal and chemical transport. The ECM approach also relies on scale-up assumptions regarding the geometric representation of the fracture system and the assumed equilibrium between matrix and fractures.

The concepts associated with the extended-dry-repository continue to be issues of concern in the project. The extended-dry-repository concept is based on two key premises: (1) that a robust extended dryout region will prevail for a long time around the repository under high thermal loadings; and (2) that the rewetting of the dry region will lag significantly behind the thermal front. There are contrary scoping calculations, that cannot be easily dismissed, suggesting that fracture flows are not properly considered in the theoretical calculations, and that deleterious consequences could arise from high thermal loadings.

The relatively limited experience of the scientific community in modeling complex thermohydroloigc problems and the unique conditions at Yucca Mountain, impose a significant burden of proof to assure proper validation of the process models used in the project. This burden has yet to be met because appropriate field and laboratory experiments are not yet sufficiently far advanced. Consumers of the modeling studies in the repository-design and performance-assessment teams must be aware that until more-defensible validation data become available, there remains a strong possibility for surprises at the process level.

There is considerable uncertainty associated with thermohydrologic processes at Yucca Mountain. The three main types of uncertainty can be classified as process uncertainty, geologic uncertainty, and parameter uncertainty. Of these, it is the opinion of the PRT that reduction of process uncertainties should take the highest priority. This can be achieved by laboratory and field experimentation, and associated model validation and calibration.

Laboratory and Field Testing

The question of whether the laboratory and field testing programs are adequate to build confidence in the understanding and prediction of thermohydrologic processes at Yucca Mountain are examined. We have reviewed sequentially, activities related to site characterization, laboratory investigations, and field tests as they address the problems of boundary conditions, small scale processess, and large scale processes, respectively.

Site Characterization. Site characterization at YMSCP has been on going for over ten years, and is not yet fully complete. The site is geologically complex and obtaining thermal, physical, hydrologic and geochemical properties of the host rock has proven to be a challenging task. The characterization activities have reached the point where the physical geology of YM is sufficiently understood to support currently planned and future modeling and field test programs. However, the hydrogeology of the mountain, particularly in the Topopah Spring Tuff, where the potential site for a repository has been selected, is less well understood; and it is in this area where YMSCP needs to focus most of its future efforts.

One of the crucial items is the question concerning the existence of "fast paths". Measurements of the ^{36}Cl, ^{14}C, and ^{3}H levels in water samples collected from different geologic units have provided direct evidence of young waters, and, by extention, of fast paths within the unsaturated zone. Further evidence has been obtained from elevated levels of ^{14}C that were found in several wells in the Tiva Canyon Tuff at depths down to 125 m.

Another crucial item is the measurement of large-scale hydraulic properties. Air injection tests have provided air permeabilities in the regions probed, which range between 1×10^{-15} m^2 to about 5×10^{-11} m^2. Permeability values for the Topopah Spring Tuff varied between these two limits, with most in the range of 1×10^{-13} to 2×10^{-11} m^2. A new and novel technique, pneumatic testing, has been developed that is based on a model analysis of large frequency pressure variations, which reflect fluctuations in atmospheric pressure. With this new technique, the observed significant attenuation of pressure changes in the TS, compared to TC, has reinforced the belief that the intervening PTn layer acts as a "tin roof". The implications of this behavior in the TC are important regarding water infiltration. The characterization of fracture flow paths and air permeabilities remains a critical, high priority need of the YMSCP.

The PRT recommends that future activities must focus on: (1) updating the characterization of hydrostratigraphic units and fault zones; (2) determining saturation profiles and identifying perched water zones; (3) characterizing water movement especially with respect to infiltration; (4) continuing the application of pneumatic testing; and (5) continuing the fracture mapping in the access tunnel of the ESF.

Laboratory Investigations. A program of laboratory experimentation and testing has been supported by the YMSCP to determine properties and process-related quantities that bear on modeling and repository design. Extensive data have been compiled on the thermophysical and mechanical properties of the TS host rock, but there are much less data available on several potentially important geochemical, multi-phase flow and mass transfer processes.

From the existing thermophysical property and hydrological data (i.e., bulk permeabilities), the picture that emerges at this point is that the natural variation in properties is extensive within the mountain. This introduces some uncertainty into the results of predictive models which use volumetrically averaged properties. However, the PRT believes that no significant advantage to model development, model validation, and fundamental understanding of the relevant TH processes can be gained from additional laboratory programs of thermal property measurement in these areas.

The YMSCP in the White Paper (DOE, 1995a) has indicated that the following laboratory investigations will be undertaken: (1) thermally-driven fracture flow; (2) evaluation of heat pipe effects in fractured rock; (3) measurement of gas-phase buoyant convection; and (4) measurement of enhanced vapor diffusion. While each of these studies is believed to address several key issues related to model development and validation, the PRT suggests that experiments (3) and (4) should be of lower priority The PRT also suggests the addition of the following investigations to the laboratory program: (1) measurement of matrix water relative permeability at various infiltration rates; (2) studies of steam-water countercurrent flow in single fractures and in fracture networks; (3) experimental verification of the critical rate concept for infiltration of a matrix-fracture system, and (4) continuation of the fracture healing experiments of Lin and Daly (1989b) to test their relevance under repository conditions and build confidence in THC models.

Field Tests. Field experiments and tests carried out in G Tunnel at Rainier Mesa to address YMSCP needs in characterization and modeling have provided property data and measures of TH impacts on the host rock. In fact, many of the TH concepts and theories that have recently been developed in the project emerged in response to the observations of boiling, vaporization, condensation and reflux observed in the G-Tunnel experiments.

In an effort to expand the understanding of TH phenomena at YM, a series of five *in situ* thermal experiments has been planned that will start in 1996 and continue beyond 2006. They include: (1) Large Block Test (LBT); (2) Single Heater Test; (3) Drift Scale Test with Flatjacks (DSTFJ); (4) Spatially Distributed Single Heater Tests; and (5) Large-Scale Long-Duration Test (LSLD).

After a lengthy debate on the scientific and engineering merits of the LBT, the PRT concluded that this test addresses TH issues on length and time scales that lie in between the laboratory and *in situ* field tests. As such, the LBT should not be compared, or ranked, with other field activities. Five of the six members of the PRT believe the LBT is well suited to investigate a number of important hypotheses that are concerned with the TH behavior of the Topopah Spring Tuff. This test should be supported and continued to completion. The dissenting member believes that the desired program of investigations could be better carried out in a controlled drift-scale program of testing.

In the opinion of the PRT, the different Single Heater Tests and the Drift Scale Test with Flat Jacks (DSTFJ) can be considered intermediate scale underground tests, because of the similarities in objectives and overall testing plans. As will be discussed below in connection with the LSLD test, there are a number of critical problems facing the YMSCP that need to be addressed by thermally perturbing an appropriate volume of rock under conditions approximating that of the near field environment. The PRT does not believe it will be possible, using either single heater tests or the DSTFJ, to do this. In the opinion of the PRT, the heater tests are not needed. Five of the six members of the PRT recommend dropping the DSTFJ. The same dissenting member believes that, again with reference to the LBT, additonal testing is not warranted on this block and that an accelerated schedule of intermediate-scale underground testing would better serve the objectives of the YMSCP.

The PRT strongly supports the need for a large-scale, long-duration (LSLD) test. The process of increasing the temperature of a very large volume of the Topopah Spring Tuff, possibly up to maximum levels of about 200° C, raises some issues about rock system behavior, for which there is little or no field experience to serve as a guide to the expected response of the system. There are a significant number of critical issues that can only be addressed in an LSLD test. These include assessing: (1) whether the magnitude of infiltration will affect the whole thermohydrologic process; (2) whether the countercurrent heat pipe activity will actually develop; (3) whether condensation zones will actually coalesce; (4) whether dry-out zones will develop and coalesce; (5) whether the development of these various processes will be the same above the repository as they are below; (6) whether any of the above factors will be significantly affected by anisotropy of the fractured rock; and (7) whether the permeability of the Topopah Spring Tuff will be changed due to thermochemical and/or thermomechanical reactions.

The PRT believes that important results will be obtained from the LSLD, both from early and later results, and that subsequent analyses of the cumulative data will produce a picture that becomes increasingly more clear as those components of the controlling mechanisms are revealed. Therefore, the PRT favors a flexible schedule of testing and observation.

Modeling

The starting point for an analysis begins with a review of the past and present modeling activities, which focuses on: (1) the fundamental physics that are represented in the models; (2) the use of an effective continuum approach for upscaling basic properties to computational grid sizes of several tens of meters; (3)

the implementation of these concepts in a variety of THMC codes; and (4) decisions taken with regard to dimensionality and boundary conditions.

In terms of fundamental physics, most of the effort has been directed toward developing codes to represent thermal-only (T) and thermo-hydrologic (TH) processes. There has been some progress in thermo-mechanical (TM) and thermo-hydrologic-chemical modeling (THC), but essentially no progress on other types of complex coupling (e.g., THM and THMC). Codes developed for TH modeling are detailed and complete in terms of the coverage of the relevant processes.

One of the difficult steps in any modeling effort is to represent the heterogeneous nature of the hydrogeologic system at the scale of the computational grid. The main approach adopted for scaling up to the grid scale is based on the concept of an equivalent continuum (ECM). The ECM approach utilizes standard conservation and transport laws for a single continuum with coefficients that are designed to capture the geological and hydrogeological complexity. Inherent in this approach are assumptions about geometry of the fracture-matrix interactions, and the nature of fracture-matrix interactions. These assumptions provide the basis for defining an effective permeability, k_{eff}, an effective capillary pressure curve, $P_{c,eff}(S_{eff})$, an effective water relative permeability curve, $k_{rw}(S_{eff})$, and various transport coefficients.

The processes and scaling models are represented in various TH models (e.g., FEHM, NUFT, TOUGH2) that are used at the drift, repository, and mountain scales. The codes have been reviewed in detail and cross-verified in a variety of tests. However, work to date has not examined the efficacy of the ECM approach. There has been initial developmental work in THC modeling at LANL, and in TM modeling with the FLAC and ABAQUS codes at LLNL.

In evaluating the sufficiency of the modeling approach in the area of fundamental physics, the PRT finds the models to be largely comprehensive in their treatment of processes. There are details of the modeling approach such as: the estimation of capillary diffusivities, relative permeabilities in the tight TS matrix, the treatment of trapping and instabilities, the nature of counter current flow in heat pipes, the general treatment of two-phase flow, and THMC effects, which need to be studied in more detail. The PRT finds that the ECM model could be applied under some restrictive conditions at Yucca Mountain, and provides a useful qualitative approach to complex TH problems. However, the ECM is not general and is likely to be inadequate for many types of fracture-rock geometries as well as conditions where non-equilibrium fracture-matrix interactions develop. In the opinion of the PRT, the ECM quantitative predictions, particularly where they impact the design of underground projects, should be accepted with a great deal of caution.

The main computational codes (FEHM, NUFT and TOUGH2) have undergone extensive development and verification. The next step in their use, however, should involve investigations, primarily in underground tests, where the efficacy of ECM can be carefully examined. Given the apparent limitations of the ECM, further applications of these models would appear to be inappropriate without such confirmation. The THC and TM modeling is not sufficiently advanced, and the PRT believes it will be difficult to validate these codes in a timely manner. This situation, however, does not imply that THC and TM issues are not important, but that other alternatives (e.g., bounding calculations or field experiments) may simultaneously be required to meet program needs.

The PRT finds that the present use of 2D and 3D models is generally appropriate. Specific issues of experimental design and fast-fracture pathways will likely involve a more rigorous 3D treatment. Additional work in representing features of the upper and lower boundaries of the global system appears to be warranted.

Recommendations

On the basis of the detailed analyses in Sections 3, 4, and 5 of this review, the PRT has organized their main recommendations in four categories: site characterization, laboratory tests, field tests, and modeling. Details of the rationale for these recommendations are given in Section 6.

Site Characterization

The PRT believes that the following four programs, currently underway, must be continued without any significant reduction in effort:

(1). Measurement and interpretation of infiltration rates at the ground surface and in the shallow subsurface formations over Yucca Mountain.

(2). Analysis and interpretation of water samples using geochemical age dating techniques based on ^{36}Cl and ^{14}C.

(3). Air injection and pneumatic testing program to determine large-scale permeability distributions in the various lithographic units and fault zones in the mountain.

(4). Geological mapping, and borehole drilling program in the ESF, with special emphasis on assessing fracture and fault heterogeneity and connectivity.

In addition, the PRT has identified an additional site characterization program that we believe would have significant merit. We recommend initiation of the following program:

(5). Tracer tests, using vapor-phase tracers in ESF boreholes, to identify and asssess "fast paths", in the fractured repository host rocks.

Lastly, the PRT recognizes the value of the following program to site-characterization efforts, and recommends its continuation:

(6). Natural analogue studies of geothermal sites such as the Geysers, or those under study in New Zealand.

Laboratory Tests

The laboratory-testing effort within the YMSCP has two facets: (a) the testing of rock properties, and (b) the testing of processes related to TH, THC or TM coupling. We recommend continuation and enhancement of the following program:

(7). Measurement and interpretation of hydrologic rock-matrix properties, including relative-permeability functions and capillary-pressure vs saturation curves, with emphasis on differences between wetting and drying, and between primary and secondary imbibition, and on the appropriateness of the van Genuchten representation of the characteristic curves.

Of the four laboratory experiments proposed in the White Paper, the PRT believes that two have particular merit. These are described as experiments (1) and (2) in section 4.2.2 of this report. We therefore recommend that these experiments proceed:

(8). Thermally-driven fracture flow test (Figure 4.1a).

(9). Laboratory evaluation of heat pipes in fractured rock (Figures 4.1b and 4.1c).

The PRT recommends the following new process-oriented laboratory experiment:

(10). Experimental verification of the concept of a critical rate, q*, during infiltration of a fracture-matrix system.

On the THC front, the PRT was impressed with the experimental work of Lin et al (DOE,1995a) and recommends the following enhanced experimental program:

(11). Continuation of laboratory fracture-healing experiments, but with a stronger attempt to show relevance to Yucca Mountain conditions, and particularly the chemical processes associated with a heat pipe. In addition, the effects of mineral deposition at the fracture-matrix boundary should be investigated in the same experimental framework.

Field Tests

As mentioned above, there are a significant number of critical issues on the thermohydrologic behavior of the near field environment surrounding the repository that we believe can only be addressed in an LSLD test. Thus, the PRT is unanimous in its primary recommendation, which gives the highest priority, in terms of all TH activities, to the following *in situ* field test:

(12). Carry out the large-scale, long-duration (LSLD) *in situ* field test in the ESF.

The possibilities for what the PRT considered as intermediate-scale tests include: (1) Single-heater test; (2) Two spatially-distributed single-heater tests; (3) Large-block test; and (4) Drift-scale test with flatjacks. The PRT discards the first two of these as being of insufficient scope to insure the full development of all the relevant TH processes cited earlier. Of the two remaining, five of us prefer the large-block test, and one of us, the drift-scale test. On this basis, then, we recommend:

(13). Reinstatement of the large-block test into the TH program at Yucca Mountain.

The LBT has the advantage that it is almost ready to go and would provide timely results. It is suitable for equipment and model testing. It suffers in comparison with the drift-scale test, in terms of representativeness. The minority opinion is that the lack of representativeness is sufficiently severe to disqualify the worth of the test. The majority are not particularly strong in their preference of the LBT over the drift scale experiment. The LBT is not held to be indispensible, but it is held to be valuable, and given the investment already made, cost effective.

The PRT is firm in their position that in no way can either the large-block test or the drift-scale test be considered as a suitable substitute for the LSLD test.

Modeling

Our recommendations on modeling are as follows:

(14). The PRT concurs with the findings of Reeves et al (1994) that current TH computer codes address program requirements sufficiently well that they should be used as host structures for future development. Available resources should be focussed on enhancing existing codes, rather than developing new stand-alone codes.

(15). Enhancements in existing TH codes are needed to improve their representation of the fundamental physics, with respect to: (a) anisotropy of flow processes in matrix-fracture systems; (b) two-phase steam-water flow in matrix-fracture systems, with special emphasis on capillary effects and two-phase flow instabilities, and (c) representation of channeling and fast-path flow due to heterogeneities in the fracture network.

(16). The conditions under which the ECM approximation is valid must be investigated and identified. Under those conditions where it is not valid, alternative modeling approaches must be developed that do not rely on the ECM assumptions with respect to geometry, averaging of coefficients across grid blocks, and equilibrium between fractures and matrix.

(17) The PRT encourages continued TH modeling both at mountain scale (Bodvarsson, 1995), for support of performance assessment, and at repository scale (Buscheck and Nitao, 1995), for design support.

(18) Improvements may be needed in the representation of infiltration on the upper boundary of TH models to properly reflect the spatial and temporal distribution of infiltration rates. Similarly, the appropriateness of using the water table as the lower boundary condition on TH simulations needs further investigation.

(19) Three dimensional TH simulations will be needed at the *in situ* testing scale, but will not be feasible at mountain scale, where 2D simulations should suffice. Quasi-3D, and other hybrid modeling approaches, deserve attention.

(20) Improved validation of TH models is required in connection with the next round of laboratory and field testing. A convincing demonstration is needed, using rigorous comparison of observations with prior predictions, rather than retroactive calibration and fitting.

(21). Uncertainty analysis of TH behaviour using traditional geostatistical analysis to analyse parameter uncertainty is neither feasible nor warranted. The PRT espouses an alternative approach involving hypothesis testing in a decision framework. Reductions in process uncertainty, should have highest priority, followed by geological uncertainty, and then parameter uncertainty.

(22). THC modeling should move forward, but at a lower priority, and at a different scale than the current mountain-scale studies. The PRT would prefer to see simple scoping calculations first (the geochemical equivalent of Preuss and Tsang's TH scoping calculations), followed by numerical simulations at a scale that can be validated and calibrated by proposed laboratory and field tests. Another possible approach would be to try to apply thermochemical models such as EQ3/EQ6 to conditions anticipated to occur at the boiling front, rather than trying to fully couple TH flow models and HC transport models.

(23). THM modeling should also move forward, but at a lower priority, and at a scale suitable to validation and calibration testing with the LBT and LSLD tests.

The most important of the above recommendations is the one associated with the ECM (16). The question remains unresolved as to whether the ECM can continue to form the basis for ongoing analyses.

Programmatic Issues

In our deliberations, the PRT identified and discussed at length a major concern as to whether or not critical thermal testing could be accelerated to meet the needs of the YMSCP. For the schedule implied by the Program Approach, the most significant field-based thermal-testing data that might be available for the determination of technical site suitability in 1998 would have been the Large Block Test. With this test apparently canceled, the next potential test will take place in the ESF. A minimum-scale test has been proposed (the winged heater test) that attempts to optimize the acquisition of thermohydrologic data in relation to the fast-track schedule implied by the Program Approach. The winged heater test will probably yield results that could provide input to licensing activities. However, the PRT is concerned that the test may not yield sufficient technical data required to resolve fully uncertainties about post-closure performance.

We recognize that the technically more superior test (the LSLD test) likely cannot be executed and interpreted on a schedule that is appropriate to the Program Approach, and we suspect that our recommendation for reinstatement of the LBT, followed by the LSLD test, may strain management's ability to accept our recommendations. If forced to choose one test, and one test only, the PRT comes down in favor of the LSLD test. In other words, scientific defensibility must overrule management-mandated scheduling and cost constraints.

1. INTRODUCTION

1.1 Objective of the Peer Review

The Peer Review Team (PRT) was established by the Yucca Mountain Site Characterization Office of DOE's Office of Civilian Radioactive Waste Management to conduct an external review of the Thermohydrologic Modeling and Testing Program of the Yucca Mountain Site Characterization Project (YMSCP). The objective of this review was to evaluate the YMSCP approach to understanding hydrothermal conditions at Yucca Mountain, Nevada that would be generated by repository heating.

The design and performance assesment of the proposed repository rely heavily on predictions from mathematical models that are based on the relevant physical and transport processes. In carrying out this assignment, it was therefore important for the PRT to recognize the need for an accurate process modeling of the behavior of the site under the hydrothermal conditions that would be generated by repository heating. Model predictions with reasonable assurances require the testing of various scenarios in a probabilistic framework using a reliable model. Reduction of uncertainties can only be accomplished by additional site characterization, improved understanding of the fundamental process components, and improved knowledge of the variation of time-dependent boundary conditions. A reliable model of the relevant physical and transport process and their accurate representation in numerical codes are therefore necessary. These issues are extensively addressed in this report.

The DOE provided a list of general questions as shown in Table 1.1 for the PRT to keep in mind during their deliberations. The White Paper referenced in this table was prepared by the Principal Investigators (PIs) and provided to the PRT with a synthesis of relevant analyses and supporting information regarding possible thermohydrologic conditions which may occur at Yucca Mountain in the presence of a repository.

1.2 The Peer Review Process

The peer review process was initiated by Susan B. Jones, Assistant Manager for Scientific Programs, Yucca Mountain Site Characterization Office. She did so by releasing a Peer Review Notice, and by appointing a Chairperson (Paul A. Witherspoon), an Assistant Manager's representative (Ardyth M. Simmons, who served until October 13, 1995 and was succeeded by Robert A. Levich), and a Technical Secretary (Kathryn A. Mrotek).

In the second step of the process, this group prepared a more detailed Peer Review Plan and selected the members of the Peer Review Team. Appendix A is a copy of the Peer Review Plan and Appendix B is a list of the members of the PRT. In the next step, a considerable amount of background reading was provided to the PRT members so that they could become familiar with the hydrogeological setting at Yucca Mountain and investigations that addressed the various aspects of the thermohydrologic processes and conditions present in a potential repository at Yucca Mountain. A list of the documents reviewed by the PRT is given in Appendix C.

The first meeting of the PRT was held in Las Vegas, Nevada, on July 13 -14, 1995. A representative of each of the participating agencies in the Yucca Mountain Project YMP was invited to sit in as an observer and to act as a resource person on behalf of their agencies. Prior to this meeting, the Principal Investigators (PIs) of YMSCP prepared a White Paper (DOE, 1995a) entitled, "Modeling and Testing Thermohydrologic Processes in the Yucca Mountain Site haracterization Project." It was given to the PRT on July 13, 1995. The White Paper provides a synthesis of analyses and supporting information regarding thermohydrologic conditions that may occur at the Site in the presence of a repository. This report also summarizes analyses which have been performed to predict long-term conditions as well as information from laboratory and field experiments to support the reasonableness of these predictions.

Table 1.1. General questions regarding thermohydrologic modeling and testing program

1. *Is the framework presented in the White Paper adequate for understanding thermohydrologic processes and conditions that may be present in a potential repository at Yucca Mountain?*
2. *Will testing described in the White Paper be adequate to support the development of conceptual models for thermohydrologic behavior of the site?*
3. *Does the White Paper cover the range of alternate conceptual models that must be considered for understanding the thermohydrologic behavior of the site?*
    - *a Are there parameters that have not been addressed that have greater sensitivity and should be addressed?*
    - *b. What is the impact of not considering these process interactions?*
4. *Do the number, types, and spatial and temporal scales of proposed tests represent the range of conditions needed to build confidence in the thermohydrologic behavior of the site?*
5. *Do the coupled processes described in the White Paper reasonably encompass the range of effects associated with the influence of repository heat on the mountain?*
6. *Are there additional tests or analyses that would feasibly build additional confidence into understanding thermohydrologic behavior of the mountain?*

7a. *Is it reasonable to decouple thermohydrologic processes from thermomechanical and thermochemical processes in modeling behavior at the site?*

7b. *If it is not reasonable to decouple these processes, how might the coupling best be accomplished?*

On the first day of the first meeting, the PRT met in an open session with the PIs and observers to discuss the White Paper and the kinds of questions that the PRT was considering to elicit further information on YMSCP. On the second day, the PRT met in an executive session to organize a List of Questions to be addressed by the PIs at a second meeting of the PRT. A finalized List of Questions was delivered to DOE on July 20, 1995, and a copy of this list is given in Appendix D.

The second meeting of the PRT was held in Las Vegas on August 21-24, 1995 with a field trip to YM on August 25, 1995. There were a large number of PIs and agency observers in attendance at the four days of open meetings. All presentations were followed by lengthy discussions with considerable technical interaction between the PIs and the PRT. Appendix E provides a list of attendees at both PRT meetings.

The final step of the peer review process has been the preparation of this Peer Review Record Memorandum (PRRM). The outline of the PRRM was established by the PRT members shortly after the second meeting. All PRT members have contributed to the writing of the PRRM, and it has been coordinated and edited by the PRT Chairperson.

1.3 Scope of Peer Review

With the objectives of the peer review in mind and a list of some general questions that need to be considered by the PRT, it was important to define what the scope of the peer review should include. Table1.2 gives the scope of the peer review as defined by DOE.

Table 1.2. Scope of peer review of Thermohydrologic Modeling and Testing Program of the Yucca Mountain Site Characterization Project

1. *Evaluate the White Paper on thermohydrologic modeling and testing including key references cited within.*
2. *Evaluate adequacy of laboratory and field experimental program to build confidence in understanding and predicting thermohydrologic processes and development of models.*
3. *Evaluate sufficiency of models and modeling approaches to predict moisture redistribution and changes in water chemistry in response to heat.*

In pursuing the question of the adequacy of this site as a repository, a number of issues must be addressed. The key concern of the PRT is the ability to understand and predict adequately the complicated manner in which moisture migrates through the rock in response to the imposed thermal loading. Many components of this problem can only be resolved by an appropriate program of laboratory and field testing. Field studies show that relatively high water saturations occur throughout the Topopah Spring (TS) Tuff. It is in this unit that the potential repository is to be constructed. As a result of the thermal loading, temperatures exceeding the water boiling point (97°C at the TS location) will develop. The thermohydrologic laboratory and field program must be evaluated in terms of its adequacy to build confidence in the understanding and prediction of the movement of liquids and gases as temperatures exceed this boiling point.

Furthermore, because of the need to predict the behavior of a rock mass subjected to a variable thermal load over very long periods of time, the use of predictive mathematical models is necessary. There have been considerable efforts by various investigators in the development of an Equivalent Continuum Model (ECM). Therefore, one of the critical issues for the PRT is to evaluate the sufficiency of this model to predict the thermohydrologic response in view of the complex physics, chemistry and geology of the YMP. All these issues are extensively discussed in this report.

1.4 Organization of Report

The Peer Review Record Memorandum of the PRT is presented in six sections.

A program of investigations on the YMP has been developing over the past ten to fifteen years, and it is important to understand how the level of effort has expanded to meet programmatic needs. Section 2 provides background material on the general nature of the problem of characterizing a site for a radioactive waste repository. A review of the geology and hydrology of the site provides a description of a fault-bounded volcanic plateau and of the hydrogeologic conditions in the 600-m thick unsaturated zone in which a potential repository may be constructed at a depth about 350 m below the surface. A discussion of the conceptual models that have been proposed to understand the impact that the operation of the radioactive waste repository will have on the behavior of the rock mass is also included in Section 2. These models must reflect an understanding of the complex behavior of the total system, and a review is included of the thermal-hydrologic-mechanical-chemical processes that are involved.

Section 3 presents a discussion of the critical issues that must be addressed in the PRT review of the Thermohydrologic Modeling and Testing Program. Some of the technical issues to be addressed include: the impact of variability in infiltration, the impact of heterogeneities on the thermo-hydrologic behavior, the fracture/matrix interactions, the combined effects of the thermochemical and thermomechanical coupling, and the effects of analysis at different scales. One of the important components is the thermal loading strategy, which has a significant effect on the size and cost of construction, on the one hand, and the magnitude of the thermal impact on the rock mass, on the other. There are also issues concerned with the present state of validation of the various models developed, as well as the companion problem of their calibration from large-scale field tests. From the programmatic standpoint, a key issue is whether the proposed program is adequate to support efforts to license and operate the proposed waste repository at Yucca Mountain.

A review of the various laboratory and field tests that have already been carried out, or are planned, is presented in Section 4. One of the goals of this effort has been to gather data on the thermohydrologic parameters of the various rock formations. Before access to the interior of the mountain was provided by the ESF, it was only possible to characterize and perform laboratory measurements on surface and drill hole samples, map surface features, and conduct pneumatic tests within the boreholes. Carefully designed underground field tests are essential if the integrated thermal, hydrologic, chemical, and mechanical behavior of the unsaturated rock mass at Yucca Mountain, as it undergoes a significant change in temperature over a very long period of time, are to be understood. With the exception of the small diameter heater experiments and the heated block experiment, carried out in the G-Tunnel Underground Facility at Rainier Mesa (DOE, 1995a), there have been no large-scale experiments in the vadose zone of the magnitude envisioned for the potential repository at Yucca Mountain. Thus, an analysis of the appropriate site characterization and field activities hat should be carried out is a key issue in this section. Laboratory studies have documented many of the small scale physical properties of the rocks at Yucca Mountain. Studies are now required that will elucidate the hydrologic and chemical processes, particularly with respect to two phase flow in fractured rocks of low matrix porosity, as well as the complex fracture-matrix interactions This section describes the various field tests, currently in the planning stages, that are designed to address these problems.

The sufficiency of the modeling effort that has been undertaken over the past several years is discussed in Section 5. The emphasis is on models that have been developed to improve process understanding and optimize repository design. The complex behavior of the rock mass, as its temperature changes significantly, involves thermal-hydrologic-mechanical-chemical processes that are coupled in various ways. Among these couplings, the current emphasis is on models of the thermohydrologic (TH) coupling. In particular, the equivalent continuum model (ECM), which has been used extensively in developing concepts of repository behavior under various scenarios, is reviewed in some detail in this section. A relatively new three-dimensional Mountain Scale model is also discussed.

From this external review of the Thermohydrologic Modeling and Testing Program of the YMSCP, the PRT has developed a set of recommendations that are summarized in Section 6.

2. BACKGROUND

In conducting this external review, we assembled a wide range of background material that is presented in this section. This includes a brief introduction to the Yucca Mountain Site Characterization Project and the potential repository, a review of the geology and hydrology of the site, a discussion of the conceptual model of the hydrothermal environment, and the characteristics of the thermal, hydrologic, mechanical and chemical processes that result from the perturbation caused by the thermal environment.

2.1 Yucca Mountain Site Characterization Project

The potential horizon for a repository at Yucca Mountain is in the Topopah Spring Tuff, which is a fractured tuff in the vadose zone some 325 m below the surface. Depending on the areal loading of spent fuel canisters that is finally selected for emplacement of the radioactive waste, rock temperatures may reach maximum levels of 150° to 200° C. This design presents earth scientists with the unusual problem of characterizing the nature of a very large volume of partially saturated, fractured rock and developing new and novel methods of predicting its behavior over inordinately long periods of time under conditions of elevated temperatures above the boiling point.

The present YMSCP has been evolving over time from the basic plan and strategies set forth in the Site Characterization Plan (SCP) that was issued in 1988 (DOE, 1988). The SCP contains an extensive testing, design, and performance assessment program designed to produce a comprehensive understanding of Yucca Mountain under both ambient and perturbed conditions. The PRT is primarily concerned with one particular aspect of site investigations, the Thermohydrologic Modeling and Testing Program of the YMSCP.

Initial investigations at Yucca Mountain involved detailed geological field studies carried out by the USGS. One of their important findings was the identification in the fractured rock mass of "fast paths" for liquid and gaseous flow. These fast paths consist of connected pathways in the rock of high permeability created by faults and fracture networks.. In recent years, the site investigations at Yucca Mountain have been expanded to include theoretical and laboratory studies, field investigations, and underground testing. Until recently, this element of YMSCP has been well funded. Table 2.1 shows that funding for site investigations, and total costs at YMSCP, increased steadily from FY83 through FY95. However, both the total funding and the percentage for site investigations decreased sharply in FY96, and present forecasts indicate that total funding may decrease even further to $100 million by FY99.

Table 2.1. Fiscal year funding for Yucca Mountain Project (in million dollars)

Description	FY83	FY84	FY85	FY86	FY87	FY88	FY89	FY90	FY91	FY92	FY93	FY94	FY95	FY96
Total	50.4	65.3	63.5	90.0	103.2	140.9	180.2	180.6	181.1	189.4	229.1	279.7	325.0	250.0
Site Inves.	21.4	22.7	17.5	24.7	26.0	34.2	47.1	40.7	37.9	44.3	50.7	63.5	93.5	37.4
Percent	42	35	28	27	25	24	26	23	21	23	22	23	29	15

2.2 Programmatic Needs

Predictions of thermohydrologic conditions are required by several study teams within the YMSCP. These groups comprise the "customers" for the output from the thermohydrologic program. They include: (1) the repository-design team; (2) the waste-package design team; (3) the preclosure performance-assessment team; (4) the postclosure performance-assessment team; and (5) the team investigating site suitability and licensing issues. The requirements of these groups define a set of programmatic needs that must be met by the conceptualizations, laboratory experiments, field experiments, and modelling investigations of the thermohydrologic program.

Repository-design issues revolve around: (1) the thermal loading strategy; (2) the possible benefits of backfill as a component of drift closure; and (3) waste-package retrievability. The second and third items fall outside the mandate of this review and are not discussed further. Thermal loading strategy is discussed in a separate subsection below.

Waste-package design issues relate primarily to canister composition which is largely controlled by corrosion potential. The favoured waste-package design is a large multi-purpose canister (21 PWR MPC), with a loaded weight of 79,120 kg, consisting of an outer containment barrier 10-cm thick of A516 carbon steel and an inner containment barrier 2-cm thick of Alloy 825. This design is well-suited to the "extended-dry-repository" concept proposed by some members of the YMSCP. However, there is concern within the project that dry conditions may not be attainable for all canisters at all times.

The present concept for the placement of the multi-purpose canister in the drift is shown in Figure 2.1. If some canisters are expected to encounter wet conditions, much more expensive alloys may be required to deliver acceptable protection against corrosion. The presence of water in contact with the canisters during the period of the thermal pulse would require redesign using corrosion-resistant alloys that would be much more expensive, perhaps prohibitively so.

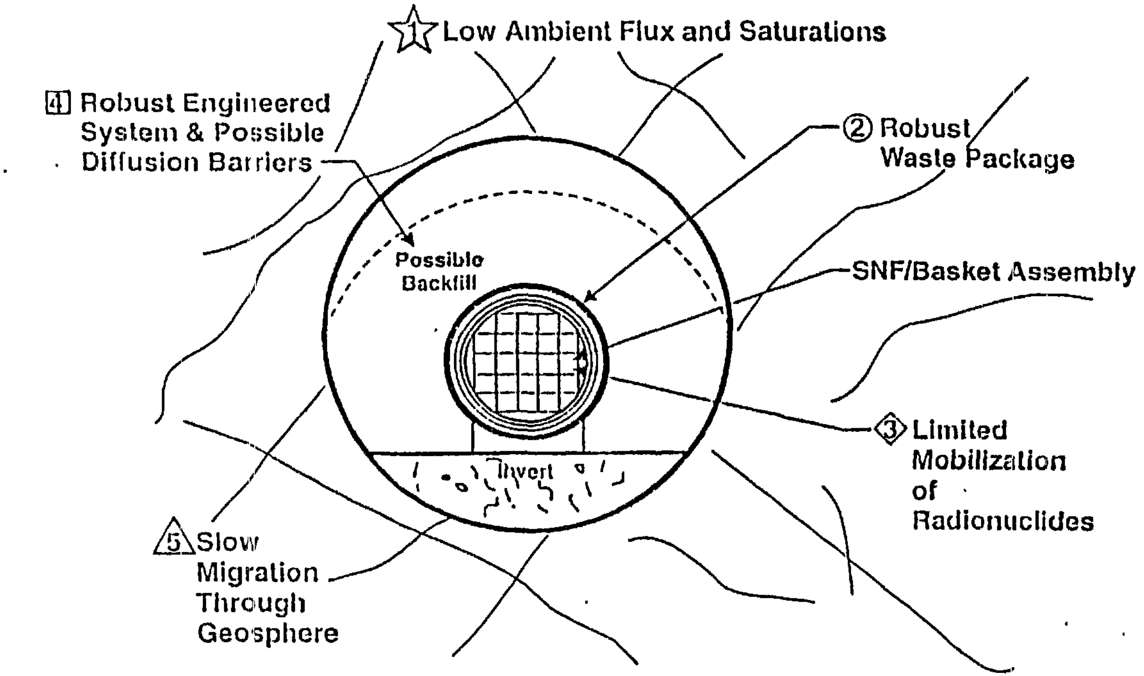


Figure 2.1. Drift-scale conceptualization of repository and multi-purpose canister (after Bhattacharayya, 1995).

The June, 1995 Study Plan for the characterization of the thermally perturbed zone provides a definition of "dry" conditions to be: no water arriving at the package for 95% of the waste packages, and less than 5L per package per year for the other 5%, during the first 300 y of repository operation. For the period between 300 and 1,000 y, the required percentages reduce to 90% and 10% for the two conditions, respectively. These definitions were not raised during the interactive PRT sessions, and discussions there implied even stricter limits might be required for water contact on containers. It is apparent that any attempt to counter thermohydrologic uncertainties through more robust or more flexible waste-package design would be accompanied by large increases in cost over the currently-favoured design.

Performance-assessment issues can be classified as preclosure or postclosure. Pre-closure performance assessment is concerned primarily with worker safety and is outside the PRT mandate. Postclosure performance assessment is driven by regulatory compliance criteria, which currently include standards associated with pre-emplacement groundwater travel time, inventory release rates, and cumulative releases to the accessible environment. The first of these has no thermohydrologic component, and the last could well be replaced by a risk-based dose standard at some time in the future, if the recommendations of the NRC (1995) are accepted. In any case, improved thermohydrologic conceptualizations and calculations are needed to feed into the simplified analyses used in the Total System Performance Analyses (TSPA). The most recent of these (TSPA-95) is the first to address thermohydrologic issues in any detail, but many simplifying assumptions are invoked, not the least of which is that all canisters are assumed to remain intact during the entire thermohydrologic pulse, so that release rates are controlled by ambient hydrologic conditions.

2.2.1 Program Approach

Over the past several years, a new approach to project development has been evolving at Yucca Mountain. This so-called "Program Approach" involves a step-wise approach to the determination of site suitability and to the licensing process. The main impact of this approach is a well-defined critical path to licensing the repository with the following milestones:

• Technical Site Suitability	1998
• License Application to Construct a Repository	2001
• Construction Authorization	2004
• License Application Update to Receive and Process Waste	2008
• License to Operate a Repository	2010

This schedule or newer variants reflect the reality that the YMSCP is proceeding under significant budget constraints with a strong need to demonstrate early progress toward licensing of the site The decision on technical site suitability is currently scheduled for 1998, with a license application for construction authorization in 2001. Even if these dates were to slip, the PRT was informed by Dr. Stephen Brocoum, YMSCP Assistant Manager for Suitability and Licensing, that an "investment decision" is required in the near future. A positive investment decision or site-suitability finding presumably requires compliance with siting guidelines and the existence of a credible design suited to the site conditions. Under the new "Program Approach", it is necessary to achieve a "broad understanding of nearfield thermal-hydrologic-mechanical-chemical (THMC) processes such that defensible calculations of postclosure performance can be made". A successful license application will require an "understanding of coupled processes" and "substantially complete containment".

The Program Approach has developed with the understanding that elements of the Site Characterization Plan (SCP) will not have been completed at the time that the license application goes forward. It is acknowledged that one cost of meeting the milestones in the Program Approach is greater expected uncertainty about aspects of the site and its performance when the initial license application is made. Although testing described in the SCP may not have been completed, opportunities remain to complete additional testing after the initial license application.

2.2.2 Thermal Loading Strategy

Thermal loading strategies are constrained by a set of design criteria. It is desired that, within 50 years after emplacement, temperatures not exceed: (1) 350°C at the centre of the waste package; (2) 200°C at the emplacement-drift walls; (3) 50°C in the access drifts; (4) 115°C in the rocks of the Calico Hills Formation and in the Topapah Spring Tuff (TSw3); and (5) the rise in temperature at the ground surface above the repository should not exceed 2°C. The decision variables that control the thermal loading include the spacing between emplacement drifts, the waste-package spacing within each drift, and the ageing of the fuel before emplacement. In order to meet contractual obligations with the utilities, a thermal load of at least 60 MTU/acre is required, and a value in the range 80-100 MTU/acre is preferred. These latter loadings would allow the expected waste volumes to be encapsulated in the primary emplacement block of Area 1 (see Figure 2.2) of the Yucca Mountain site. Lower loadings would require expansion to the lower emplacement block of Area 1 and/or the inclusion of additional Areas 2-6 with the concomitant large increase in required site-characterization funding.

In discussing thermal loading strategy, the PRT must address two different positions. One that holds that thermohydrologic issues can be made moot by adopting a low loading strategy and another, that high thermal loading provides an important opportunity for significantly improving the performance of the repository. To make this review manageable, the PRT will not discuss the various alternatives in between. Buscheck and Nitao (1995b) call these two philosophies the "minimally heated" repository and the "constructively heated" repository. (The latter has also been called "the extended dry repository").

The minimally heated repository depends upon low areal mass loadings to minimize the thermal perturbation to the system and to avoid the apparent process complexity caused by higher thermal loads. There is no attempt to derive performance benefits from heating. Instead, the system performance would come from the engineered barrier system and the geosphere. Minimal heating implies average temperatures in the repository horizon below boiling. Computations by Buscheck and Nitao (1995b) suggest that maintaining such temperatures would require waste loadings smaller than about 35 MTU/acre While there is no problem in achieving these loadings, an obvious concern is that its implementation would be difficult and expensive at Yucca Mountain. Bhattacharyya (1995) showed that loading at 24 MTU/acre would require four additional areas for the installation of emplacement drifts beyond the upper and lower blocks that constitute the primary area (Area 1 in Figure 2.2).

A strategy for constructively heating the repository can be implemented under a range of loading conditions (Buscheck and Nitao, 1995b). The "extended dry repository" envisions areal mass loadings in excess of 60 MTU/acre. Heat created by these high loadings drives liquid water, ultimately creating an extended superheated dryout zone around the repository. In this concept, average repository temperatures above boiling are calculated to last more than several thousand years. This approach potentially benefits performance by: (1) promoting less corrosive conditions at the waste packages through a reduction in relative humidity; (2) reducing the possibility that fast fracture flow could interact with containers; and (3) causing the repository to remain as a hydraulic sink for some period of time after boiling has ended and rewetting of the dryout zone occurs (Buscheck and Nitao, 1992). Water mobililized from the dryout zone condenses above and below the repository leading to increased moisture contents. Critical issues raised by this conceptual model are discussed in Chapter 3.

From the above, it is clear that important decisions with respect to repository design, waste-package design, repository performance, and site suitability rest on improved understanding and prediction of thermohydrologic processes under repository heat loading at Yucca Mountain. The following sections provide background information on the important aspects of the processes likely to be encountered during the YMP.

2.3 Yucca Mountain Site

A review of the pertinent geologic and hydrologic characteristics of the repository setting is presented to set the stage for our analysis.

2.3.1 Geology

Yucca Mountain is a fault- bounded volcanic plateau located in the arid, south-central part of the Great Basin (Figure 2.3). Within the 600 m thick unsaturated zone that will be affected by heat from a potential repository, the volcanic rocks are dominated by Miocene ash-flow and bedded tuffs that dip 5° to 30° to the east (Figure 2.4) (Montazer and Wilson, 1984). These tuffs vary considerably in welding,

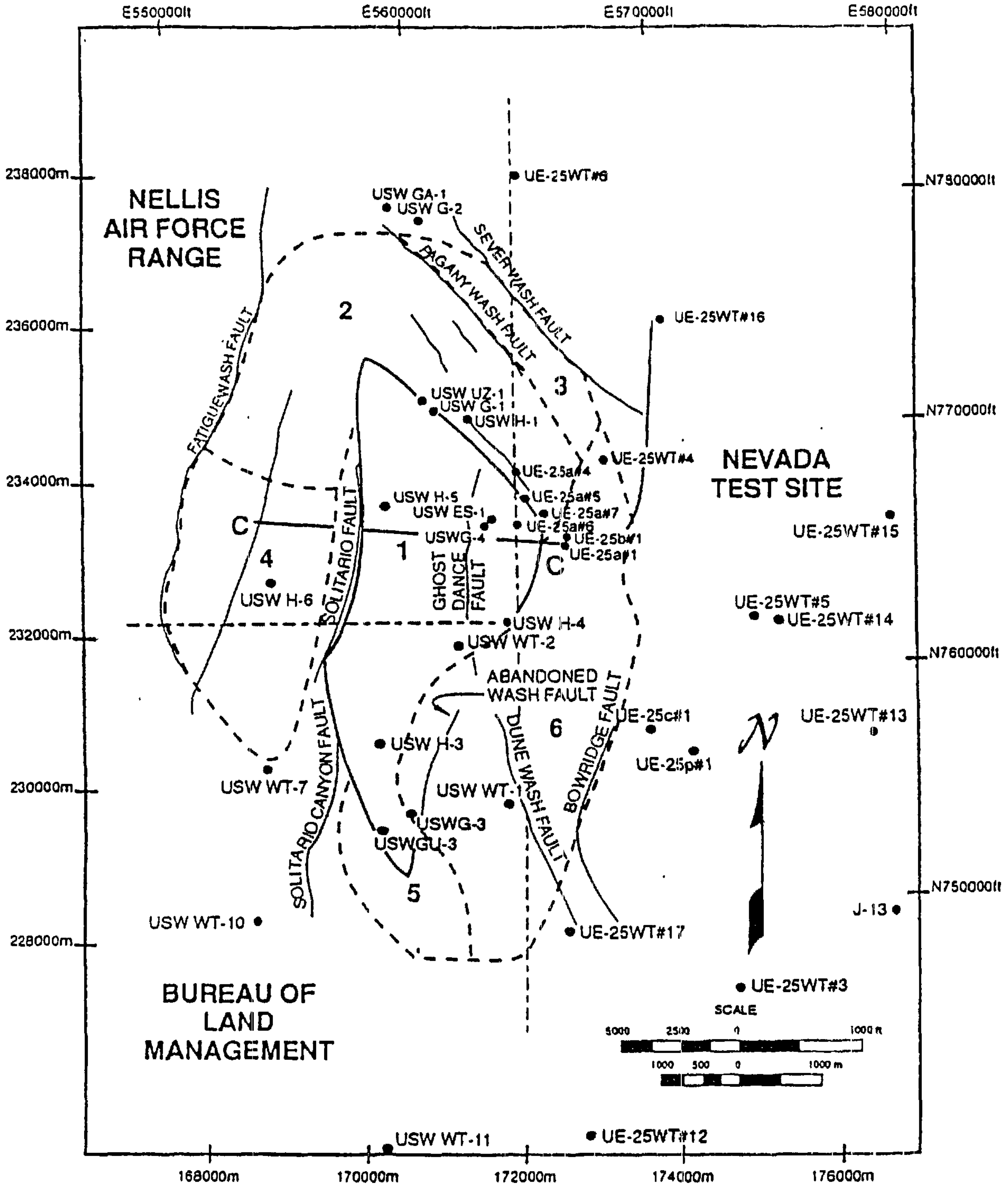


Figure 2.2. Potentially usable repository areas identified in SCP. Dots show locations of drillholes (after Bhattacharyya, 1995).

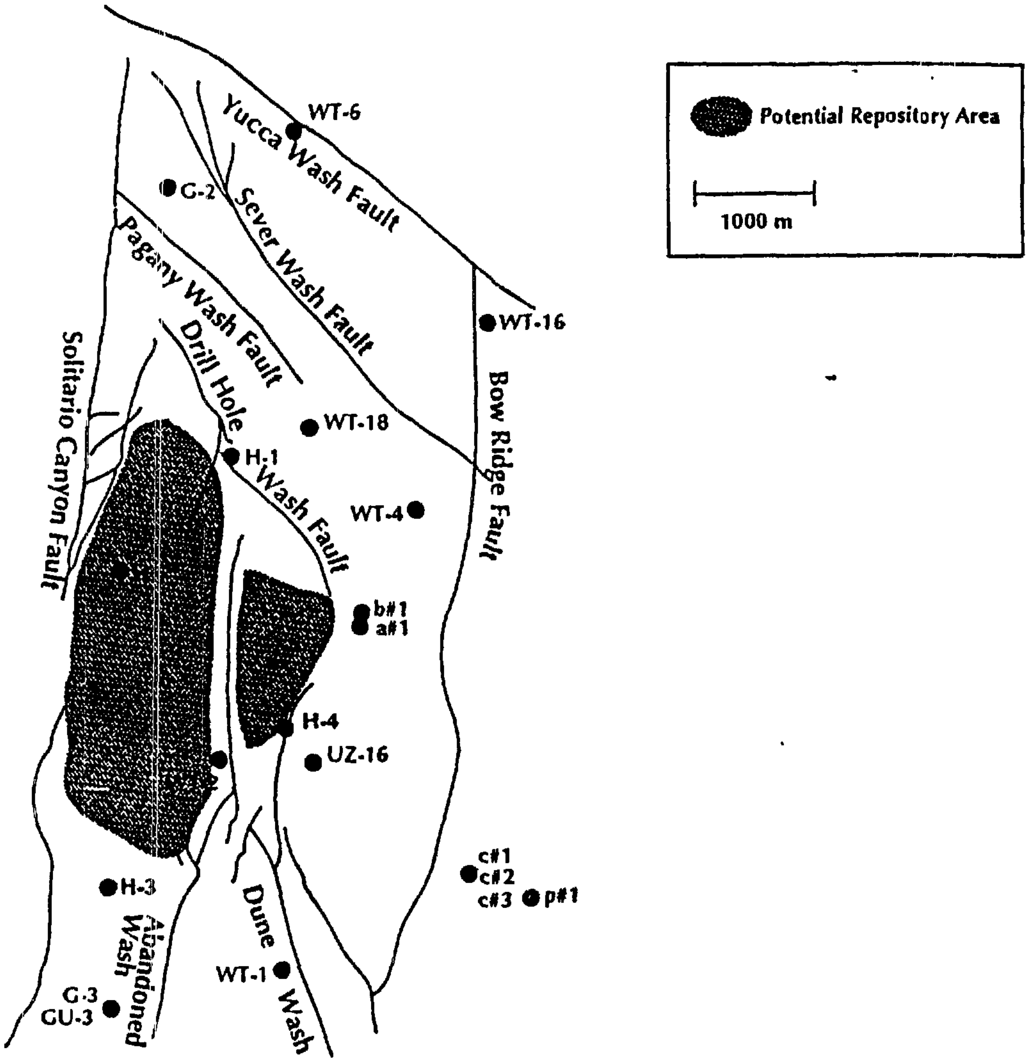


Figure 2.3. Schematic of Yucca Mountain showing location of potential high-level nuclear waste repository. Dots show locations of drillholes (from White Paper, DOE 1995a).

porosity, permeability, degree of saturation, fracturing, and alteration. As a result some of the volcanic units have the potential to focus fluid movement while others may retard it.

The various volcanic rocks within the unsaturated zone of the repository block at Yucca Mountain have been assigned to three formations. From youngest to oldest these include the Paintbrush Group, the Calico Hills Formation, and the Crater Flat Group (Scott and Bonk, 1984). The planned repository will be located in the densely welded Topopah Spring Tuff of the Paintbrush Group approximately 325 m below the surface and 225 m above the water table (Peters and Klavetter, 1988).

These tuffs are overlain by up to 30 m of Quaternary and Tertiary alluvium and colluvium (QAL), although these surficial deposits may be locally absent on ridge tops and side slopes. Beneath the tuffs, the basement consists of Paleozoic carbonate rocks that have been intersected at depths as shallow as 1200 m beneath the surface.

The rocks and overlying unconsolidated sediments within the unsaturated zone have been further divided into six hydrogeologic units, with the tuffs being distinguished largely on the basis of the degree of welding they exhibit (Montazer and Wilson, 1984) since this feature exerts primary control on the fluid flow within them Consequently the hydrogeologic units do not correspond exactly to the stratigraphic

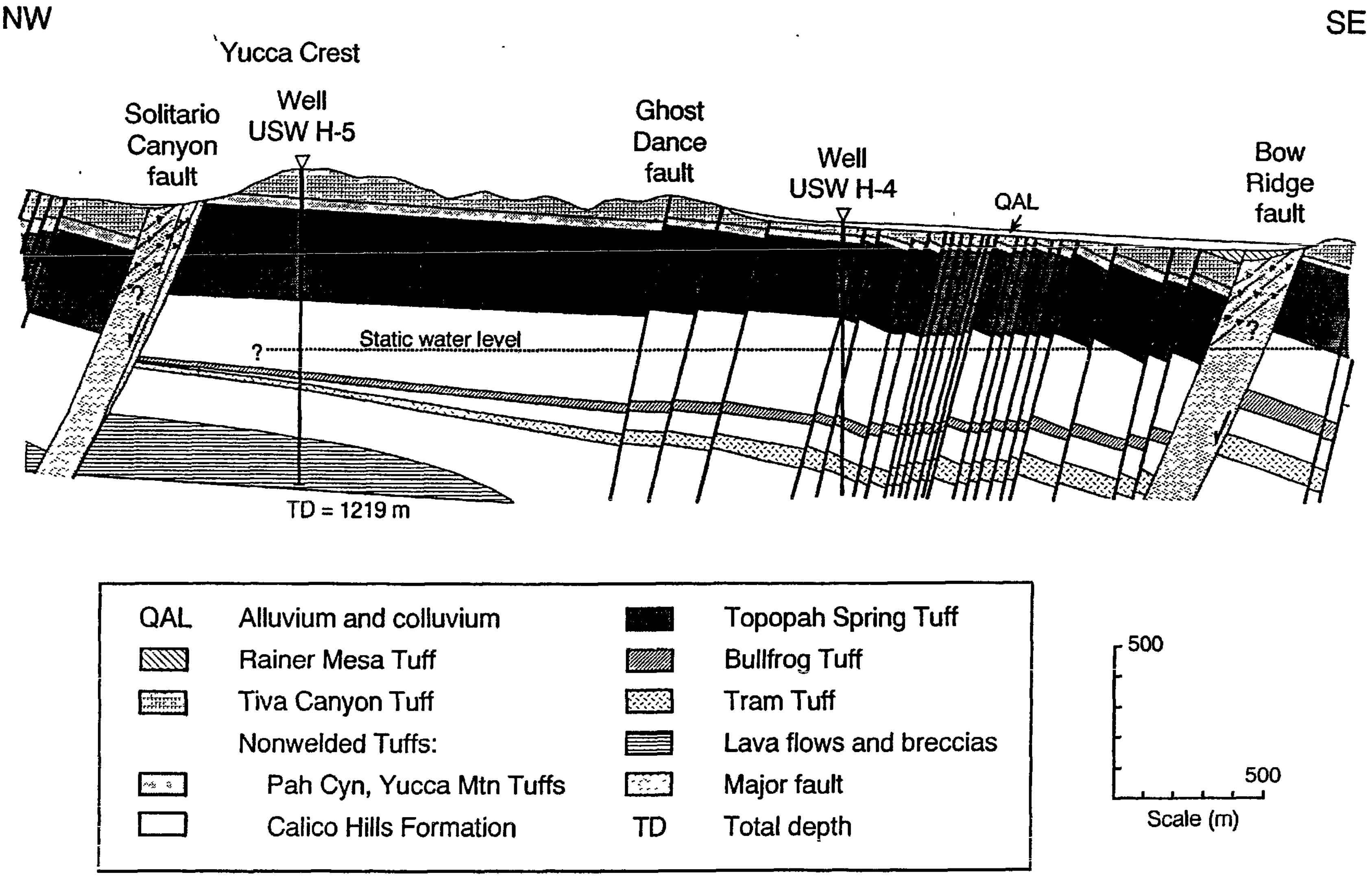


Figure 2.4. NW-SE vertical section through the site-scale model area (from White Paper, DOE, 1995a).

divisions. The geologic characteristics of the hydrologic units and their thicknesses are summarized in Table 2.2.

The uppermost hydrologic unit consists of the surficial sedimentary deposits designated as QAL. As discussed below, these deposits may play an important role in the storage and infiltration of moisture within the repository block (Flint and Flint, 1994).

The underlying Tiva Canyon (TCw) and the Topopah Spring (TSw) welded hydrogeologic units include generally similar moderately to densely welded ash-flow tuffs. With the exception of a basal vitrophyre in the Topopah Spring welded unit, the ash-flow tuffs are devitrified, fractured, and contain gas cavities (lithophysea) up to several cm in diameter. The matrix porosities (0.08 to 0.12, Flint et al., 1994a,b) and matrix permeablilites (2 to 4 x 10^{-18} m^2; Montazer and Wilson, 1984) of both the Tiva Canyon and Topopah Spring welded units are low and very similar. In contrast, fracture densities are

Table 2.2. Description of hydrogeologic units (from DOE, 1988).

Rock-Stratigraphic Unit		Hydrogeologic Unit[a]	Approximate Range of Thickness (m)	Lithology[b]
	Alluvium	QAL	0-30	Irregularly distributed surficial deposits of alluvium and colluvium
Paintbrush Group	Tiva Canyon Tuff	TCw	0-150	Moderately to densely welded, devitrified ash-flow tuff
	Yucca Mountain Tuff	PTn	20-100	Partially welded to nonwelded, vitric and occasionally divitrified tuffs
	Pah Canyon Tuff			
	Topopah Spring Tuff	TSw	290-360	Moderately to densely welded, devitrified ash-flow tuffs that are locally lithophysae-rich in the upper part, includes basal vitrophyre
	Calico Hills Formation	CHn CHnv CHnz	100-400	Nonwelded to partially welded ash-flow tuff Vitric Zeolitized
Crater Flat Group	Prow Pass Tuff			
	Bullfrog Tuff	CFu	0-200	Undifferentiated, welded and nonwelded, vitric, devitrified, and zeolitized ash-flow and air-fall tuffs

Sources: Montazer and Wilson (1984) except as noted.

[a] QAL = Quaternary alluvium and collumium; TCw = Tiva Canyon welded unit; PTn = Paintbrush nonwelded unit; TSw = Topopah Spring welded unit; CHn = Calico Hills nonwelded unit; CHnv = Calico Hills nonwelded vitric unit; CHnz = Calico Hills nonwelded zeolitzed unit; CFu = Crater Flat undifferentiated unit.

[b] Lithology summarized from Ortiz et al. (1985)

relatively high, ranging from 8 to $40/m^3$ (Scott et al.,1983). Saturations within the Topopah Spring Tuff are expected to be close to 65% (Montazer and Wilson, 1984).

The physical characteristics of these ash-flow tuffs are largely a result of welding and devitrification that occurred shortly after emplacement, and of the fracturing that followed. During devitrification and subsequent cooling, the originally glassy matrix of the densely welded Topopah Spring Tuff was converted to a granophyric mixture of alkali feldspar (65%), cristobalite (10%), quartz (25%), and clay (<1%) with low matrix porosities. Sparse, primary phenocrysts of sanidine, plagioclase, quartz, biotite, iron-titanium oxides, allanite, and zircon account for approximately 2% of the rock while lithic fragments comprise an additional 2 to 4% (Bish and Chipera, 1989). Common secondary minerals deposited on fracture surfaces include smectite, quartz, cristobalite, alkali feldspar, zeolites, and calcite (Carlos, 1985; 1989; Lin and Daily, 1989b; Carlos et al., 1991). These minerals were deposited at different times and under different conditions, but by and large, they represent only a small percentage of the total rock (up to 5%).

The densely welded ash-flow tuffs are separated by the intervening Paintbrush nonwelded unit (PTn) which includes poorly to partially welded ash-flow tuffs and bedded tuffs. The tuffs of this unit are generally vitric, porous, and only weakly fractured. Matrix porosities range from 0.08 to 0.41 (Flint et al., 1994), and matrix permeabilities are in the range of 10^{-13} to 6×10^{-15} m^2 (Montazer and Wilson, 1984; Flint and Flint, 1990). Fracture densities are low and average about $1/m^3$ (Montazer and Wilson, 1984). The higher porosities and the lack of fracturing in the Paintbrush nonwelded unit compared to the welded tuffs may buffer the movement of moisture and gas between the underlying repository in the TSw unit and the surface (DOE, 1995a).

The TSw unit is underlain by a second sequence of nonwelded to partially welded ash-flow tuffs and tuffaceous beds assigned to the Calico Hills nonwelded unit (CHn). This unit includes tuffs from the overlying Topopah Spring Tuff as well as rocks belonging to the underlying Crater Flat Tuff. Perched water has been found in the upper part of the Calico Hills nonwelded unit and at its contact with the TSw unit (DOE, 1995a).

The CHn unit is distinguished from the Paintbrush nonwelded hydrogeologic unit by the presence of both vitric (CHnv) and zeolitic (CHnz) tuffs, with the zeolitic tuffs predominating in the northern and northeastern part of the area where they are saturated (DOE, 1995a). In the southern part of the area, the rocks are unsaturated, and vitric tuffs overlie zeolitized rocks. The two facies have similar fracture densities ($2\text{-}3/m^3$; Scott et al., 1983) and porosities but substantially different matrix permeabilities. Porosities of the vitric rocks range from 0.08 to 0.48 compared to 0.15 to 0.35 for the zeolitically altered rocks while the matrix permeabilities range from 10^{-13} m^2 (vitric zone) to 10^{-16} m^2 (zeolitic zone) (Flint and Flint, 1990). Zeolitization is believed to have occurred when the water table was as much as 85 m above its present level (Scott et al., 1983). Thus, the upper extent of zeolite-bearing tuffs places a reasonable limit on the upward mobility of the water table under varying climatic conditions.

The Crater Flat undifferentiated hydrologic unit (CFu) is the lowest of the six unsaturated units. It is lithologically diverse, and includes variably welded, vitric, devitrified, and zeolitized tuffs deposited as ash-flows and air falls. The Bullfrog Tuff appears to be hydrologically similar to that of the TSw unit, with fracture densities ranging from 8 to $25/m^3$ and porosities of 0.23 (Scott et al., 1983; Montazer and Wilson, 1984).

The volcanic rocks have been disrupted by throughgoing faults that have the potential to act as "fast paths" in focussing fluid movement, or alternatively, to act as barriers. Several observations provide evidence for their importance in the unsaturated zone. These include: (1) pressure data indicating good connectivity between volcanic units (Bodvarsson, 1995); (2) the presence of young water within the deeper volcanic units (Fabryka-Martin et al., 1993); (3) mineral coatings deposited by downward infiltrating water (Whelan and Stuckless, 1992); and (4) observations from active hydrothermal systems elsewhere demonstrating that fluid movement in unsaturated regions is strongly influenced by faults.

Evidence of interconnected fracture networks, at least for the air phase, is provided by the observed propagation of pneumatic pulses through the upper stratigraphic units of the mountain. Indirect evidence of "fast-path" water flow is provided by isotopic data that demonstrates the presence of young water in fractures at depth (Yang, 1992; Fabryka-Martin et al., 1993). Furthermore, at locations between these young fracture waters, matrix waters do not contain tritium at concentrations indicative of similarly young water.

The majority of the mapped faults at Yucca Mountain are high angle, north- to northwest-trending normal structures with displacements of up to 100 m (Scott et al., 1983). Less commonly, the faults show evidence of strike slip movement with minor horizontal displacements. The most important structures include the west dipping Solitario Canyon and Bow Ridge faults which bound the west and east sides, respectively, of the proposed repository block, the Drill Hole Wash fault on the northeast side of the block, and the Ghost Dance fault, which separates the primary and secondary emplacement blocks of the proposed repository. Of these, only the Drill Hole Wash fault shows evidence of right lateral strike slip displacement; displacements on the other structures are dominantly dip slip.

Discontinuous fractures are also likely to play an important role in the storage and transport of moisture. Stuckless (1995) documented five sets of fractures with apertures ranging from 1 to 10 mm in the Tiva Canyon Tuff. Four of these sets were found to be high angle structures while the fifth set was subhorizontal. In general, however, the geometry and hydrologic characteristics of the faults and fractures are poorly known, and it can be assumed that the faults are substantially more complex than their current representation in numerical models. For example, Spengler et al. (1993) showed that the Ghost Dance fault is part of a larger disrupted zone, at least 213 m in width. Within this zone, they documented several subparallel faults and numerous fractures. The properties of the faults also vary in a vertical direction, as demonstrated by trenching along the Paintbrush fault at Busted Butte, where the fault displays a pronounced upward flaring and complexity (Stuckless, 1995). If there is a dominant direction for the fractures, more or less parallel with that of the faults, the overall rock mass will have a definite anisotropy.

2.3.2 Hydrology

Figure 2.5 shows the main elements of a conceptual model of the hydrology of the Yucca Mountain site in relation to a potential repository. Precipitation leads to infiltration into shallow units, and downward percolation through the unsaturated zone, the thickness of which varies between 500 and 750 m. Ultimately, water moving through the mountain joins a large-scale regional groundwater flow system. The following provides an overview of the main elements of the conceptual hydrologic model.

The present climate at Yucca Mountain varies as a function of elevation. At lower elevations, it is typical of southwestern deserts characterized by hot summers, mild winters, and limited precipitation (Wilson et al., 1994). The higher elevations are more characteristic of mid-latitude deserts, characterized by large temperature fluctuations and significant variability in precipitation on a year-to-year basis. This variability has important implications as far as deep percolation and recharge are concerned.

The mean annual precipitation is approximately 170 mm/yr, but exhibits considerable variation from year to year. Most of the precipitation falls during the cool season from October to April. Because of the elevation effects, however, the areal distribution of precipitation is quite variable, and typically, precipitation falling on the upper portion of the mountain is greater than at lower elevations.

The present-day climate at Yucca Mountain probably has existed for less than 10,000 years. The likely pluvial conditions at Yucca Mountain were characterized by average annual temperatures approximately 6° to 7° C cooler than present and winter rainfalls approximately 60% to 70% greater than present (Spaulding, 1985). By analogy with present-day conditions, this greater precipitation likely translated into significantly higher rates of infiltration and drainage.

Infiltration processes have been studied by the USGS (Flint et al., 1994a) by intensive monitoring of moisture in shallow units. The emerging picture is characterized by extreme variability in the spatial distribution of infiltration. A key feature in controlling infiltration is the thickness of alluvial cover. Relatively limited infiltration is associated with thick alluvial zones in the absence of runoff or ponding, where water moving into the ground will likely be evaporated shortly thereafter. Infiltration is much more significant in zones where alluvium is thin to absent. In these locations, water moves through the alluvium,

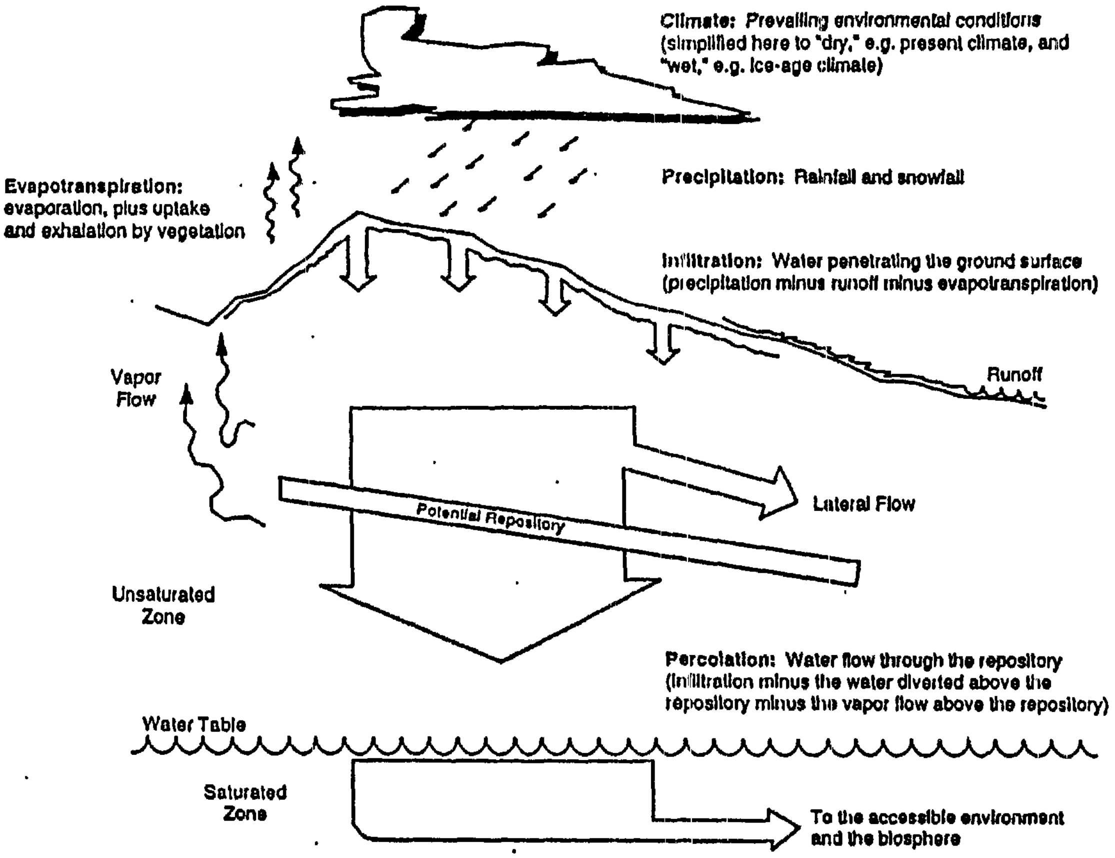


Figure 2.5. Conceptual model of the hydrologic system at Yucca Mountain including precipitation, infiltration and percolation (after Wilson et al., 1994).

enters the bedrock fracture system, and moves rapidly downward out of the evaporitic regime. Overall, infiltration is more effective on ridgetops and sideslopes as compared to alluvial terraces and channels.

Initially, percolation into the bedrock units occurs along fractures. Fracture flow is promoted in the near surface by relatively rapid infiltration rates, small matrix permeabilities and small moisture capacities (Montazer and Wilson, 1984). More recently, the possibility for fracture dominated flow has been explored by Nitao and Buscheck (1989) and Nitao (1991). The possibility of deep, relatively rapid, infiltration along so-called "fast paths" explains observations of rapid movement of water from the surface to the tunnels at Rainier Mesa (Russell et al., 1987), and the measured distribution of ^{36}Cl at Yucca Mountain (Liu et al., 1995).

An important feature of the unsaturated system is the significant heterogeneity in flow and transport processes related to the pattern of geologic layering, the variability in the extent of fracturing, and the presence of extensive primary and secondary faulting. An important consequence of the vertical variability in hydraulic properties is the significant local variation in the moisture content of some units. Figure 2.6 illustrates how capillary effects lead to relatively low water saturations in the PTn and CHnv. The capillary barrier that develops between TCw and PTn and the lateral dip of this interface may promote lateral flow in the TCw, as indicated by the conceptual model (Figure 2.5). Lateral flow is also likely to be promoted by the localized character of infiltration. The variability in geologic and hydrologic properties at YM has been the focus of several investigations (Montazer and Wilson, 1984: Wilder, 1993a,b).

Several investigators (e.g., Buscheck and Nitao, 1992; Finsterle et al., 1995) have history-matched their unsaturated flow models to the observed moisture content distributions. Under the assumption that capillary pressure equilibrium exists between fracture and matrix, these exercises typically yield very small percolation rates on the order of 0.1 mm/yr or smaller.

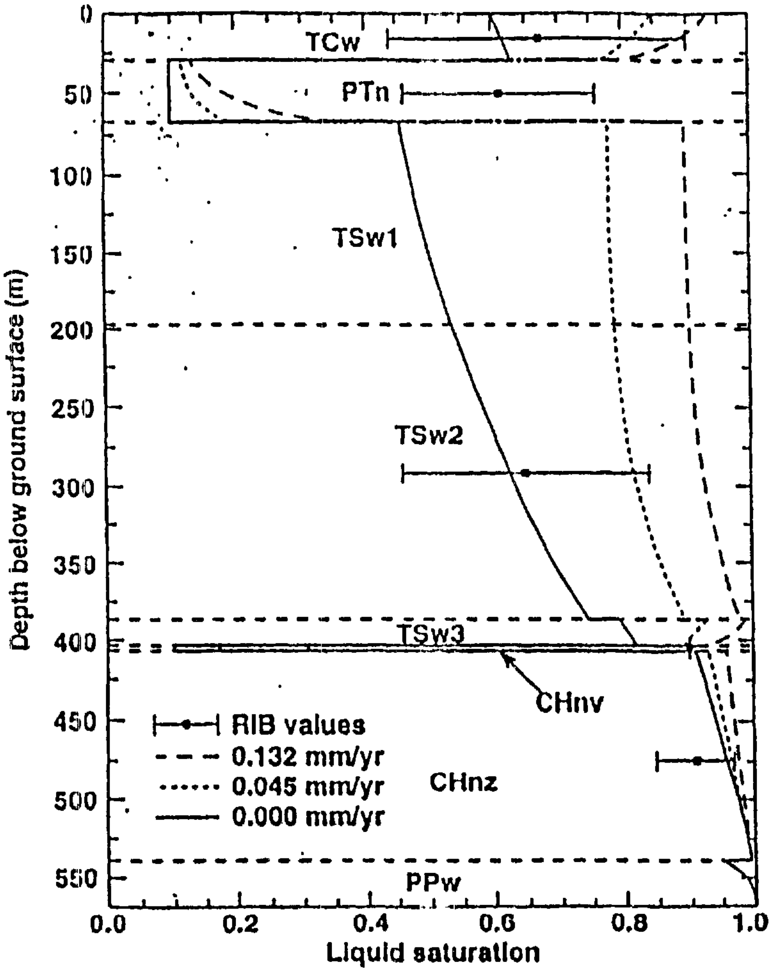


Figure 2.6. Comparison of calculated water saturations versus depth with measured saturations calculated from the RIB (after Buscheck and Nitao, 1992).

Zones of perched water are also related to the distribution of hydraulic properties. The USGS reports extensive zones of perched water along Drill Hole Wash, related to transition zones between relatively fractured and unfractured units. Typically, these zones occur near the bottom of the TSw unit, below the stratigraphic levels expected to be tested by the ESF. Perched zones occur in layered systems due to the difference in water entry pressures. At Yucca Mountain, they have been observed in wells UZ-1, UZ-7, UZ-9, and UZ-14, above zones with low fracture density, and above vitric/zeolithic boundaries. Hydrailic tests indicate that they are of limited size.

The existence of lateral flow at depth can be surmised on the basis of both direct and indirect evidence. The direct evidence early in the program was the migration of spiked drilling fluid from well UZ-1 to well G-1, which represents a distance of 1,000 ft. Indirect evidence is provided by the inversions with depth of ^{3}H and ^{36}Cl ages. For example, the ^{36}Cl ages in the Calico Hills formation are younger than the ^{36}Cl ages in the overlying TS, thus precluding direct downward migration. In any case, it seems reasonable to anticipate lateral flow of perched waters in their search for suitable entry pressures to allow downward gravity drainage.

The groundwater beneath Yucca Mountain is part of a larger regional flow system that encompasses a large area of southwestern Nevada and California, as far south as Death Valley. This system is recharged mainly in high elevation areas north of Yucca Mountain. In the vicinity of Yucca Mountain, groundwater flows to the southeast, as reflected by the map of the water table (Figure 2.7).

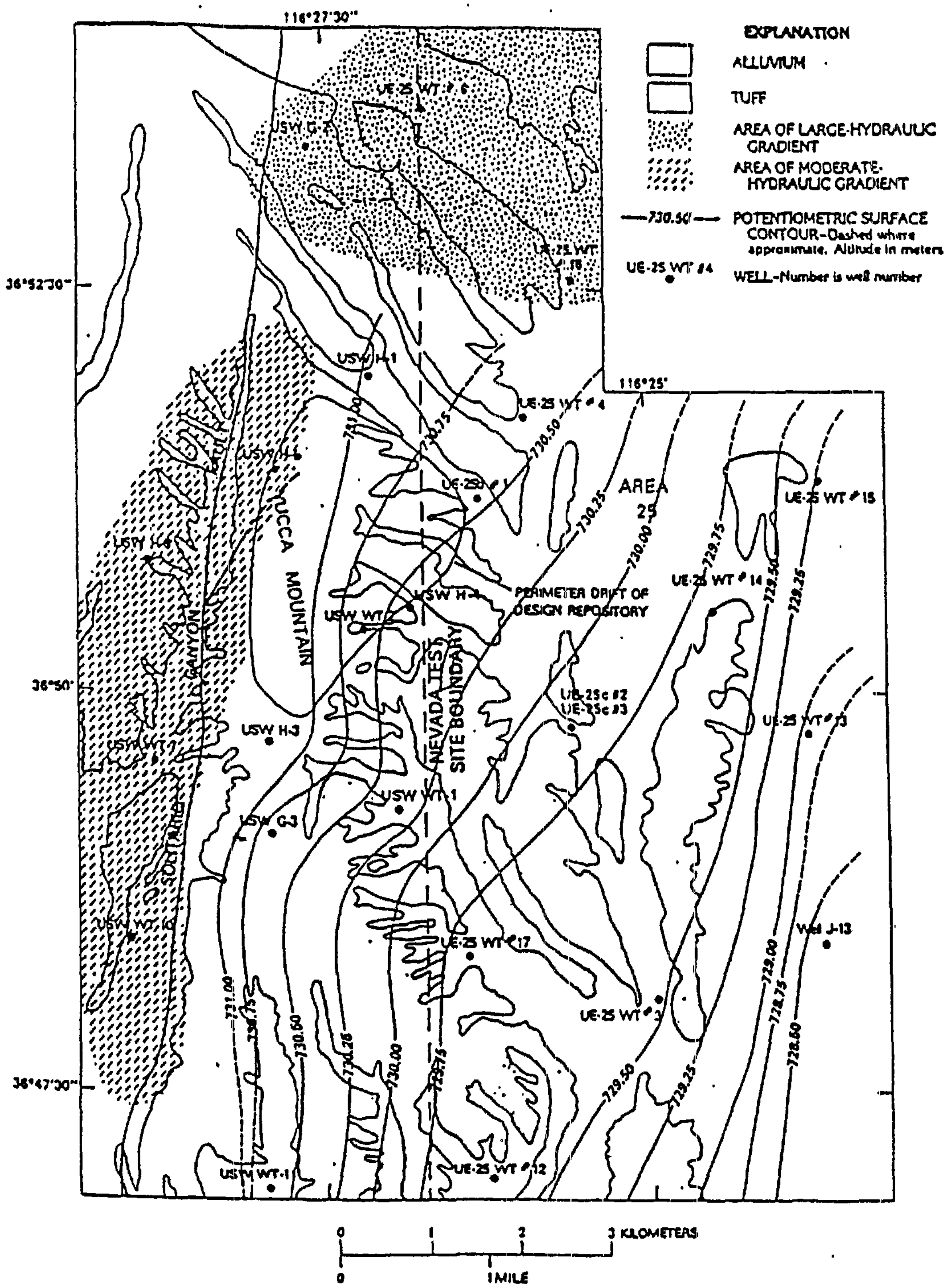


Figure 2.7. Map of the water-table configuration in the vicinity of Yucca Mountain (after Ervin et al., 1993).

Gradients on the water table are extremely variable. It is known that there are zones north and west of Yucca Mountain where the water-table elevations increase rapidly. These zones of high gradient contrast markedly with very low gradients beneath and southeast of the proposed repository. The origin of the high gradient remains unclear. A variety of models have been proposed to explain this feature including; simple changes in lithology and hydraulic conductivity, the presence of dikes or tight faults, the presence of a possible "drain" to the Carbonate Aquifer, or various conditions of perching (Luckey, 1994).

Pervasive fracturing of tuff units within the zone of saturation creates a modestly permeable hydraulic system. The system is extremely heterogeneous because extensive faulting on a regional basis disrupts the continuity of individual stratigraphic units. Average linear ground-water velocities are generally estimated in the in a range 2 to 20 m/yr (Barnard et al., 1992; Wilson at al., 1994).

2.4 Conceptual Models

Analyses of the TH processes and impacts are necessarily based on conceptual models and representations of the hydrothermal environment. Such a conceptualization is necessary, given the wide variability of properties and geologic characteristics over the site, and the spatial and temporal scales on which analysis is needed.

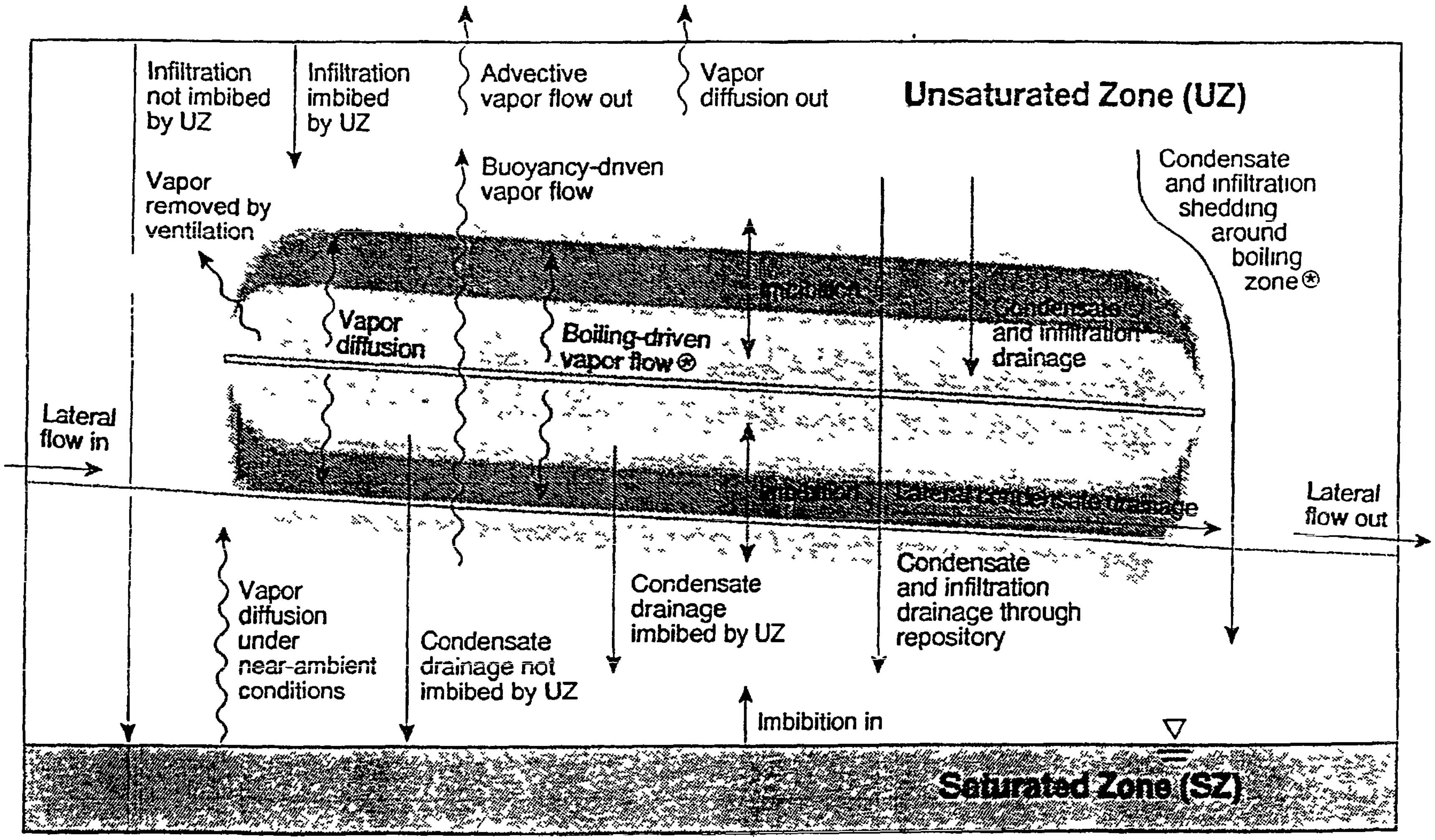
This section provides a brief overview of the conceptual models of the coupled processes that will occur in the thermally-perturbed environment.. All TH processes at the YMP will be driven by a time-varying heat source due to decay heat from the SNF and the areal mass loading, or areal power density, of the emplaced waste. Figure 2.8 shows a schematic diagram of the TH conditions affecting the moisture balance as a result of heating. The age of the SNF upon emplacement determines the specific power density, but the decay in power density is rather rapid. Figure 2.9 shows a plan view of potentially mined areas based on a total inventory of 63,000 MTU of spent nuclear fuel (SNF) at an aerial mass loading (AML) of 24 MTU/Ac

The various processes and impacts will be carried out within a "thermal framework" that has a rather rapid temperature rise as emplacement is completed and the period of monitored operation begins. This is followed by a long period in which TH processes in the near field environment and on the mountain scale are played out with a return to ambient thermal and hydrologic conditions at times on the order of 5,000 to 10,000 y. Figure 2.10 depicts this conceptualization with related comments on canister failure, average saturation, and climatic conditions.

The principal conceptual model of the TH coupling (supported by calculations and some measurements) involves an initial period in which heat is conducted into the rock on the repository scale (Figure 2.8). Temperatures in the vicinity of the repository rise above the boiling point (97° C) and vaporization of pore water may take place. This leads to a dried-out zone along fractures and in openings, and the transport of water vapor through fractures to cooler regions where condensation takes place. The condensate returns by either gravity or matrix capillarity to the area where it was originally heated. Thus, a reflux of water can be established both above and below the repository. However, there are alternative fates of the condensed water, including flow into the saturated zone below the repository, imbibition into the matrix, and transport along fast paths. There is also evidence that the the presence of the repository will result in a convective impact on the saturated zone (Buscheck and Nitao, 1993).

The severity of the TH impact on the hear-field environment can be estimated by the time variation of temperature at the repository center, where conditions are assumed to be most severe. The AML is the critical factor and Wilder (1993a) presents estimates of the centerline temperature history for AML's of 20 kW/Ac to 100 kW/Ac. Results that are most important for the TH problem are the times for temperature increases on the boiling point of 97° C, and the times necessary for the temperatures to return below the boiling point. Generally, boiling phenomena end at about 5,000 y, and temperatures at 10,000 y are significantly reduced below their peak values for all AML's considered. However, even at 10,000 y, the repository drifts will be warm and most likely very humid. Table 2.3 contains a summary of Wilder's results. Typical results for a two-dimensional areally averaged (i.e., "smeared") heat source presented by Wilder (1993a) indicate the sensitivity of drift wall temperatures with respect to the age of the SNF (Table 2.4).

As previously pointed out, processes at YMCSP fall into the category of "strongly coupled" processes with respect to repository impacts (Tsang, 1987). Related important couplings include thermal-hydrologic-chemical (THC) and thermal-mechanical (TM) processes. The TH processes appear to be the most important within the scientific-engineering-regulatory framework of licensing and operation (as well



⊛ Processes applicable to above-boiling conditions

Figure 2.8. Schematic diagram of thermohydrologic conditions affecting moisture balance as a consequence of heating. Shaded areas around repository mark the zone of dryout due to vapor diffusion or boiling-driven vapor flow (after Buscheck and Nitao, 1995b).

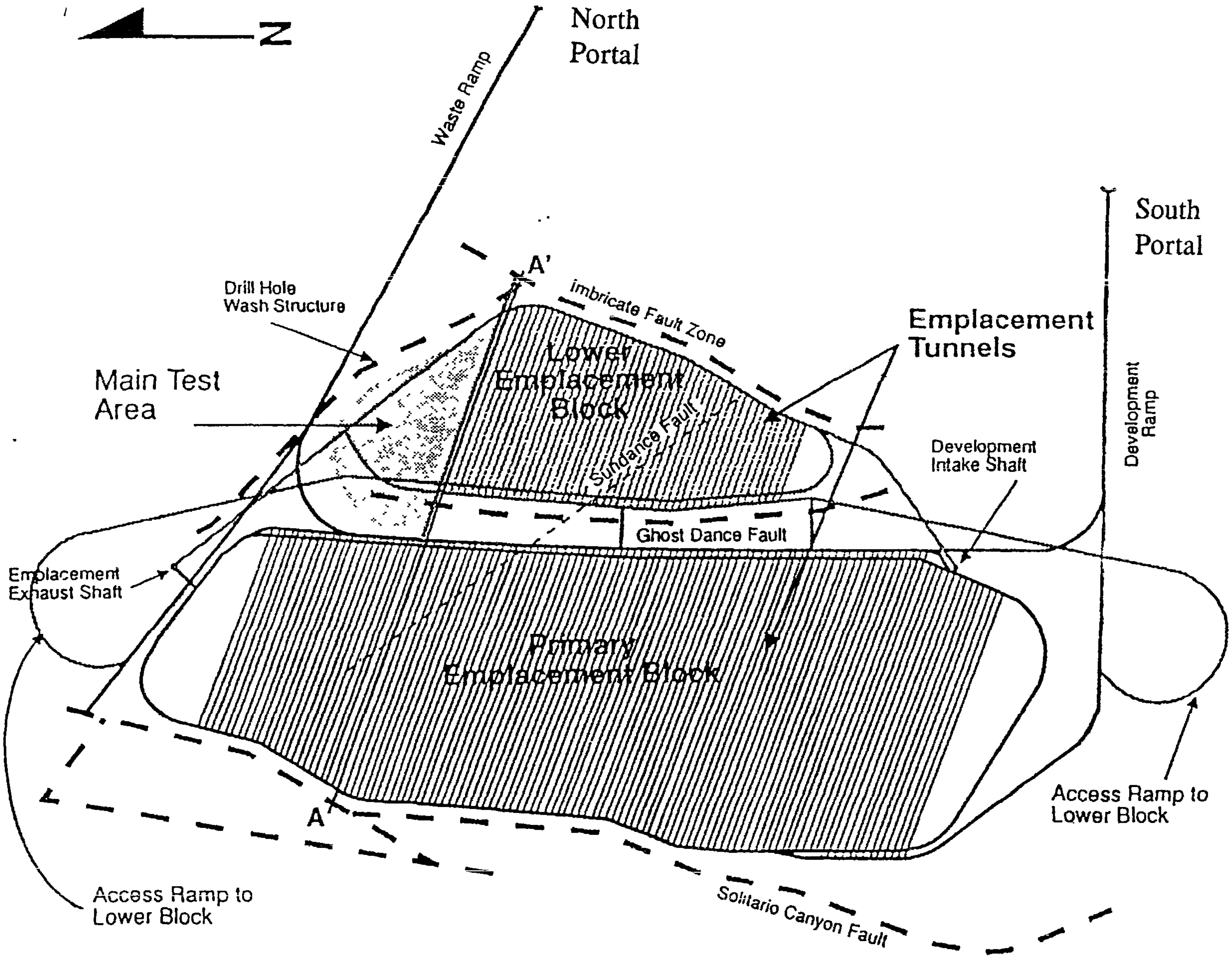


Figure 2.9. Plan view of potential repository based on an areal mass loading of 24 MTU/Acre and a total inventory of 70,000 MTU of SNF (after Bhattacharyya, 1955).

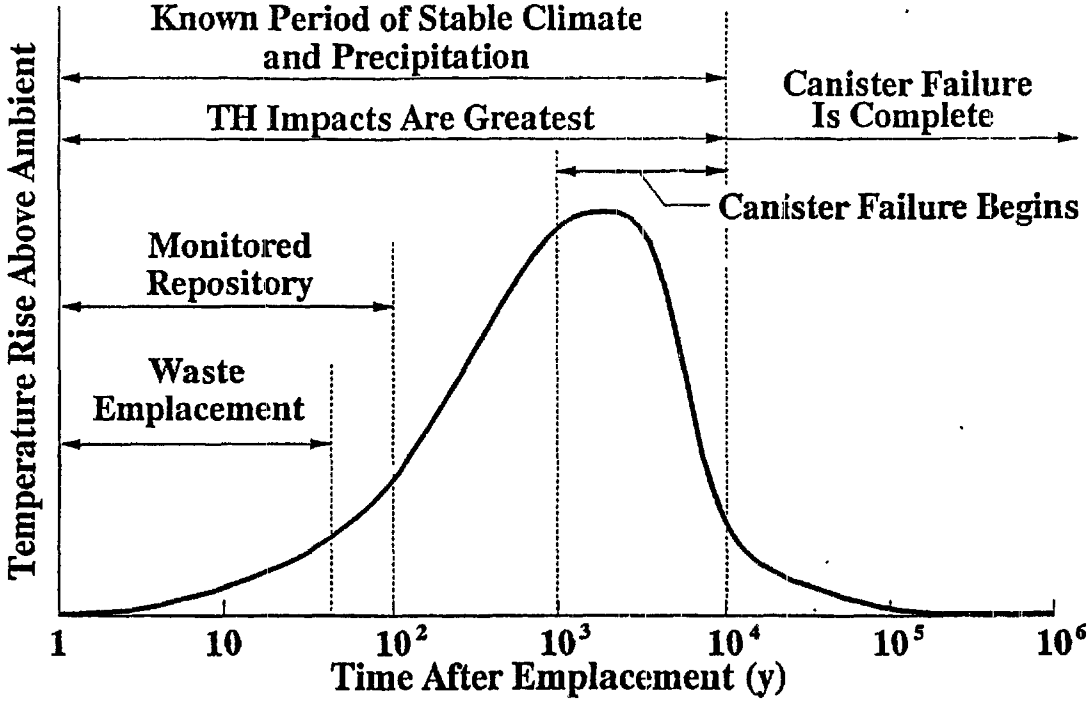


Figure 2.10. Conceptualization of thermal pulse in various time periods of repository operation. All significant TH impacts would occur within 5,000 y.

Table 2.3. Drift wall temperatures for various areal power densities (Wilder, 1993a).

Spent fuel age, y	Loading kW/Ac	Peak °C	Peak temp (°C) at time 100y	1000y	5000y
10	57	200	180	110	<100
30	20	60	60	57	38
	57	122	119	110	62
	80	153	147	134	76
60	57	147	132	138	82

Table 2.4. Repository centerline temperatues presented by Wilder (1993a). Values are taken from graphical results.

Loading kW/Ac	Peak °C	Time to Peak years	Return to 97°C years
20	60	500	-
36	85	500	-
80	145	750-1000	3000
100	175	750-1000	4500

as the charge to the PRT). Such processes involve all modes of heat and fluid transport in a heterogeneous and fractured porous medium. They are reviewed in some detail in subsequent sections.

The impact of the thermal load on the flow processes is intrinsically coupled to the hydrologic properties of the mountain and the infiltration rates. As shown in Figure 2.11, the hydrologic properties exhibit large variations both within and between geologic units. Such variations introduce a high level of uncertainty into the interpretation of modeling results and, to some extent, the design and evaluation of experimental efforts.

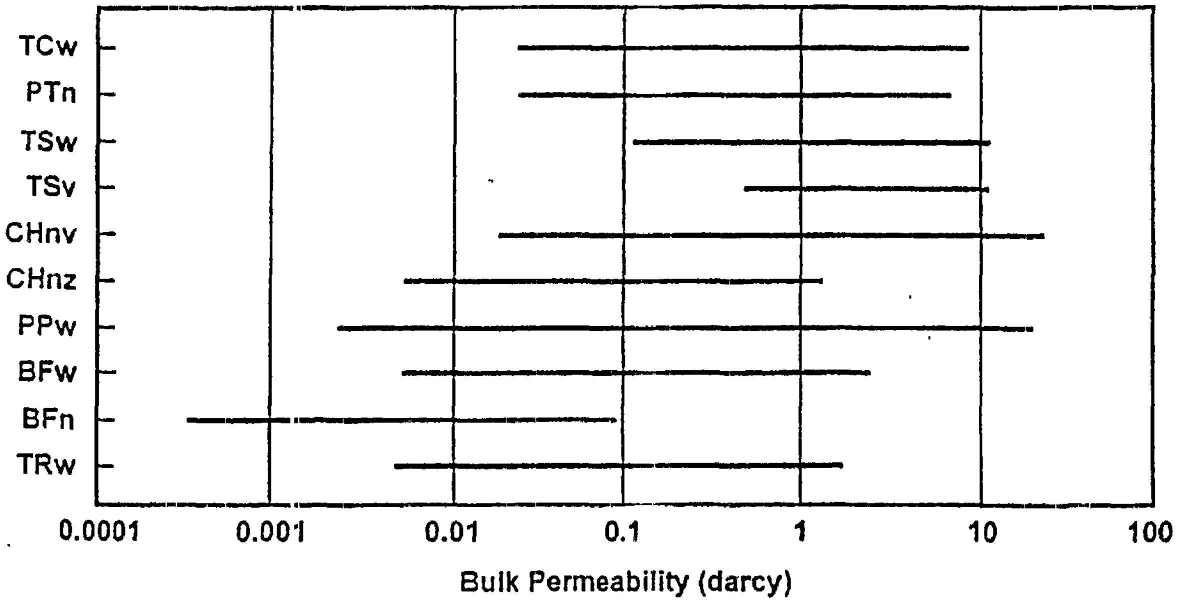


Figure 2.11. Ranges of bulk permeabilities for various geologic units at Yucca Mountain from air and water permeability testing (after Mishra, 1995).

Barr et al. (1995) have compiled a list of various possible scenaria, depending on the various hypotheses made. Determining the probability of the occurence of these various conceptualizations requires providing answers to questions such as: What is the nature of the liquid/vapor migration paths (more generally, of "heat pipes")? Will counter-current fluid flow develop primarily in the fast paths, and will this process be the same above the repository as it is below? What is the role of the imbibition of condensate into the matrix and its effect on counter-current flow in regions where fracture/matrix interactions occur? What role does gravity play in this process both above and below the repository? Is there danger that the repository may be breeched by any of these processes? If there is a dominant direction for the fractures, the overall rock mass will probably have a definite anisotropy, and what will the effect of anisotropy have on the various processes mentioned above? Are the recent estimates of Pruess and Tsang (1994) on the minimum infiltration rates for the breaching of the repository acceptable? What is the confidence on the estimates of future precipitation rates, given the recent findings of the USGS, which seem to indicate an infiltration substantially higher than originally determined? And can one use the ECM, in its present form, to correctly interpret these complicated phenomena?

Another question concerns the chemical reactions that will result from the rock-water interaction at elevated temperatures. Of particular importance are dissolution-precipitation processes in fractures and pores (Lin and Daily, 1989b). Related are also processes involving thermomechanical effects that occur as temperatures increase and the rock mass deforms. Because these chemical and mechanical interactions are coupled to the thermohydrologic behavior of the system, a critical question is the extent to which they may affect the overall fluid migration. For example, if their effect is to close fractures, will there be a significant reduction in permeability? Or, are thermochemical and thermomechanical reactions only second-order effects unlikely to have a significant impact on the overall process?

A great deal has been learned in the laboratory about these processes from extensive studies on rock cores and physical models. Much is still to be learned, however. These and other issues are critically discussed in this report.

2.5 Thermal, Hydrologic, Mechanical and Chemical Processes

To critically assess the adequacy and sufficiency of the present state of the art and the proposed program, the various THMC processes expected to impact significantly the performance of the YMSCP need to be reviewed. The following sections provide a summary review.

2.5.1 Fluid Flow Processes

The overall system performance will mainly be influenced by the following fluid flow processes: (1) flow in a dryout region and the adjacent heat pipe around the repository during the early part of the project (~1000 years); (2) flow of condensed fluids and/or of surface infiltration in the rock formation, particularly in fast paths; and (3) the re-wetting of the dry region when boiling ceases at the later stages of the project (>1000 years). The establishment of a dryout region and the delayed rewetting are the two key premises on which the concept of an "extended dry repository" is based (Buscheck and Nitao, 1992, see also below). All these involve the simultaneous flow and/or displacement of two immiscible phases (gas, or vapor, and liquid water). Understanding and prediction of such flows requires adequate knowledge of the flow characteristics of the formations comprising the site, namely the relative permeabilities and the saturation-capillary-pressure relationships. Of particular importance are flow and displacement across capillary barriers, in single natural fractures, in fracture networks, in the very tight porous matrix of the TSw, and in fault zones (Bodvarsson et al., 1994).

Flow properties depend on the particular displacement regime, namely whether it is counter-current flow (as in heat pipes) or displacement of a wetting phase (drainage) or of a non-wetting phase (imbibition) (for example, see Lenormand, 1990). The latter can be further distinguished as secondary or primary imbibition, depending on whether the medium is pre-wet or not. Surface infiltration is an example of secondary imbibition; rewetting of the dry region by condensed fluids is an example of primary imbibition. The recent experiments of water imbibition in TS tuffs by Lin et al. (1995) confirm the important role played by pre-wetting. Two-phase displacements in porous media or natural fractures, whether primary or secondary, that are solely controlled by capillarity (low capillary numbers, $Ca=u\mu/\gamma$, or gravity numbers, $B=g\Delta\rho k/\gamma$), are well understood. Less satisfactory is the knowledge of the mechanics of steam-water counter-current flows in porous media or fractures, of displacements in very tight porous media, and under conditions leading to gravity instabilities or channeling.

Significantly, the steam-water countercurrent flow (i.e., a heat pipe), and more generally, the boiling of liquid water in a single fracture or a fractured porous medium has not been well studied. At present, it is unclear whether the condensed water flows counter to steam in the fracture, in the network of fractures, or in the adjoining tight matrix. Identifying the flow mechanism is fundamental to the use of the relevant relative permeability formulation. Current simulators are based on a conventional description (Udell, 1985; Satik et al, 1991), using van Genuchten-type permeabilities (Buscheck and Nitao, 1992), thus neglecting important differences between steam-water counter-current flows and imbibition or drainage processes.

Two-phase flow and displacement in very tight porous media, such as TSw, are subject to the additional interaction between fluids and the rock minerals, surface adsorption, and the lowering of vapor pressure due to the high vapor-liquid interface curvature resulting from the small pore sizes. Typically, an equilibrium matric potential curve of water-gas (or vapor) is measured by applying Kelvin's equation, which has recently been extended to tight porous media by Nitao and Bear (1995). Then, parameters are extracted from the matric potential for subsequent use in a van Genuchten relative permeability model (Montazer and Wilson, 1984). The validity of this approach to the TSw matrix has not been demonstrated, however. This is particularly significant in view of the important role played by the capillary diffusivity, $D_c=-(k_m k_{rw}/\mu)(dP_c/dS)$, in estimating the re-wetting time.

Displacements in fractures, when capillary effects are not controlling, such as the gravity-driven infiltration of surface water or condensates, are subject to gravity fingering instabilities or to channeling, in the cases of random or spatially correlated apertures, respectively. Their relevance is measured by the gravity number, B, which for a relatively large fracture permeability k_{fr}, can be sufficiently high to give rise to gravity fingers. Experiments by a Sandia group (Nicholl et al., 1992; Nicholl and Glass, 1994; Tidwell and Davies, 1995) have clearly demonstrated this gravity instability in fractures. Under such conditions, displacements need to be simulated using a different formalism, perhaps similar to the effective viscous fingering models used in viscous instabilities in miscible displacements (e.g. Koval, 1963, Todd and Longstaff, 1975). Similar considerations may also apply to water-steam countercurrent flows (heat pipes) in such fractures.

Water propagation in the form of either fingers or channels is an example of a fast path (Tsang and Pruess, 1995). One possible definition requires an extended single fracture, or fault zone, where gravity controls the displacement over capillarity or viscous forces. An alternative definition of a fast path can be based on single-phase flow in media with wide distributions of (and perhaps spatially correlated) permeability (Chestnut, 1995). In such systems, most flow occurs over a single, connected path (Moreno and Tsang, 1994; Shah and Yortsos, 1995), which resembles the backbone of a percolation cluster. This effect is accentuated when, in addition, the system is spatially correlated. Wide distributions of (or spatially correlated) hydraulic conductivities are likely in the YM site.

2.5.2 Heat Transfer

Given the multitude of spatial and temporal scales that must be considered in the analysis of the YMSCP processes, many heat transfer mechanisms are expected to impact the performance of the repository. Excluding heat transfer in the drift and at the canister scale, which are outside the scope of the charge to the PRT, the following are the critical heat transfer processes.

Heat transfer in the matrix is expected to be dominated by heat conduction. In the near-field environment, this mode of heat transfer will be coupled with buoyant convection, in the dry-out region, and with two-phase convection in the heat pipe region. Heat conduction in the matrix is coupled to heat advection in the fractures, where fluid flow is expected to be focussed, at least under certain conditions. The development of heat pipes is likely owing to their substantial capacity to transfer heat compared to simple conduction (e.g. Udell; 1985, Stubos et al., 1993, also demonstrated in many geothermal systems). For the particular fractured rock mass, a good understanding of the heat pipe behavior is fundamental to the concept of an "extended dry repository", as discussed below. Buoyant gas-phase convection in the dryout region is also a possibility.

At the mountain scale, we expect, in addition, convective heat transfer in the saturated zone below the repository, and buoyant gas-phase convection in the unsaturated zone. The possible importance of the latter at higher values of effective permeability was emphasized in a recent study by Buscheck and Nitao (1995b), who differentiated between "throttled" and "unthrottled" boiling, depending on permeability. We point out, though, that the latter predictions are obtained from the ECM model and are subject to its constraints.

Characteristic time scales for diffusive transport ($t^* = L^2/D$, where D is the relevant diffusivity) point to heat conduction times for a distance of 1000 m on the order of 30,000 y for a typical thermal diffusivity value of 10^{-2} cm^2/s. This characteristic time is much greater than the expected decay time of the thermal pulse (Figure 2.10), and implies that the temperature response is likely to last much longer than the duration of the thermal pulse at the source. It must also be noted that the very low effective permeabilities of the site imply that heating on the mountain scale would need to be very strong to drive a purely convective system over the combined matrix-fracture system. However, convective heat transfer in the fractures is likely to be important, when matrix and fracture are at "non-equilibrium" conditions (see also below). Convective gas and vapor flows are also distinctly possible.

The interplay between all these heat transfer processes is significant and introduces considerable complexity into the development of predictive models and the interpretation of data from either field or laboratory tests.

2.5.3 Mass Transfer

With the exception of "enhanced vapor diffusion", the transport of chemical species in the YMSCP is due to advection and diffusion. Because of the importance of advection, relative to molecular diffusion or small-scale dispersion, the transport will be controlled by the flow of the particular fluid phases in the matrix, the fractures or the fracture network. Hence, resolving the various issues associated with the matrix-fracture interaction will also strongly affect the mass transfer rates. Enhanced vapor diffusion pertaining to the enhanced diffusive transport of water vapor through liquid films in an unsaturated air-water system, could be more significant under conditions of low-rate unsaturated flow.

Small-scale mass transfer is important to the various geochemical reactions involved (Glassley, 1995) and the process of fracture healing (Lin and Dailey, 1989b), although its incorporation in models is, at present, only qualitative. The only quantitative study of chemical transport reported (Robinson, 1995) has addressed large-scale issues using the ECM approach. Larger-scale mass transport is subject to the heterogeneity of the fracture network, hence to the possibilities of channeling and spreading (i.e.,macro-dispersion). Predicting the fate of chemicals at the larger scale is tied to the adequacy of the description of heterogeneity at these scales. We expect that passive tracer tests at the field scale would help uncover the connectivity of the fracture network and shed light on corresponding "fast paths". Such tests are proposed in Section 4.

2.5.4 Chemical Processes

As a result of the strong thermal disturbances that will occur in the vicinity of the repository in response to heating, the following main classes of chemical processes are likely to occur: (1) dissolution-precipitation involving an aqueous phase and the enclosing rock matrix; (2) solid-solid phase transformations; and (3) mineral precipitation from an aqueous phase in response to changing temperatures or vaporization. Minerals whose solubilities are strongly temperature-dependent, such as the silica polymorphs and the carbonates, will be most affected. Because many of these reactions involve a change in the volume of the solid phases and the release or uptake of water, they have the potential for altering the porosity, permeability and moisture budget of large volumes of rock. These changes will, in turn, affect the hydrologic and mechanical properties of the repository block.

Mineral deposition in fractures and matrix pores will become particularly important if thermal loadings are sufficiently high to cause boiling and the generation of heat pipes. The net effect of this process will be to plug fluid pathways, and divert or pond water. Lining of the fracture-matrix interface with deposited minerals will affect the matrix-fracture interaction during two-phase flow by restricting imbibition of liquid water into the matrix or, inversely, by restricting the availability of pore water. Water movement between the matrix and fractures may be further affected by changes in the vapor pressure of the pore waters as salinity increases during vaporization. Within the heat pipe, deposition of silica at the advancing boiling front may lead to the formation of an effective seal that can substantially affect the thermohydrologic behavior of the repository block.

The vitric tuffs are most susceptible to the formation of hydroxyl-bearing clays and zeolites through dehydration reactions because of the instability of glass at even low temperatures (Bish et al., 1995). However, the extent of the alteration reported is restricted to relatively narrow zones around the fractures. Similar secondary mineral assemblages can be expected to develop in the relatively porous, nonwelded and bedded vitric tuffs. In view of their potentially higher water contents, this alteration may extend over greater volumes of rock. In contrast, the densely welded TSw and TCw in the near-field environment may be largely immune to the formation of new secondary minerals because these rocks are already devitrified.

However, the TS may be altered by other chemical transformations, that result in a net change in volume. Most important is the transformation of alpha to beta cristobalite, which involves a net volume reduction of 12% (Bish et al., 1995). This transformation will occur within the core of the repository, if temperatures exceed about 220° C. Within the near field environment, the most significant alteration will probably involve silica dissolution and precipitation (Lin and Daily, 1989b; Robinson, 1995).

Although the kinetics of some of these reactions are known, many questions remain open (Glassley, 1995). Included among them are the effects of flow rate, mass transfer and pH on the reaction rates, the difference between dissolution and precipitation rates, the possible influence of microbial effects, and the relation between porosity, volume change, and permeability. Significantly, the effect of the confining stress on the reaction rates (pressure solution) and the resulting permeability change is not known. Current models have utilized an ad-hoc porosity/permeability relationship (Robinson, 1995). Likewise, the extent of the hydrothermal alteration of a fracture-matrix system that will occur within the heat pipes is unknown. In this process, dissolution and precipitation in the fractures are complicated by the presence of a low-salinity water originating as condensate, while the behavior of the pore fluids is influenced by mineral deposition in the pore throats. Reaction processes in small volume pores, such as found in the matrix of the TS, are not well understood.

Finally, we note that there is ample evidence from active geothermal systems that water-rock interactions will occur in the near field environment at Yucca Mountain, and that they will affect the hydrologic and mechanical properties of the rock at some scale. However, the overall importance of these reactions in modifying the large-scale behavior of the repository block is unknown at present and remains to be demonstrated. In general, we expect the effects of thermochemical couplings to depend on a number of factors which include the rock flow properties, water and steam flow rates in the heat pipe (hence, the thermal load), water composition, and reaction kinetics. In later sections, we describe the necessary experimental and theoretical studies needed to address these issues.

2.5.5 Mechanical Processes

When the temperature of a fractured rock mass increases significantly, the rock mass will undergo thermally induced displacements and changes in stress that, in addition to the material properties, will depend on: (1) the frequency and orientation of the fractures that are present, and (2) the aperture distribution. As the temperature first changes, both the displacements and stresses rise very rapidly over a relatively short period of time. Thereafter, the rate of increase becomes more gradual, so that over longer periods of time, nearly asymptotic values are approached.

For given material properties of the rock (linear coefficient of thermal expansion, Poisson's ratio, and Young's modulus), the theory of linear thermoelasticity can be used to compute the displacements and stresses for the rock matrix, in response to the thermal load. However, the presence of the fractures introduces a complication because they represent a discontinuity in the material properties. Depending on the geometry of the fracture network, the overall rock deformation will take place in the normal and/or shear modes. As a result, apertures will generally tend to close as the matrix expands, and the net displacements for the rock mass will be less than what is predicted for an unfractured rock. The corresponding implications on fluid permeability and flow paths are important.

Another mechanical effect in response to the temperature increase is thermal degradation due to microcracking. Such cracking is a function of the confining stress and can occur during the opening of an extensile crack being subjected to changes in compressive stress (Blair, 1994). According to Blair (1995a), water can enhance the propensity for cracking at the tip of an existing crack, and rock failure can occur when the temperature exceeds 100° C. Points of contact at the asperities on rough fracture surfaces can also develop stress concentrations as the fracture deforms and produce microcracking.

Understanding the importance of TM coupling necessitates a better understanding of these issues. In particular, such information would be vital to repository design, especially the question of adequate support for the underground openings. This design must take into consideration the rock-mass characteristics, the pre-existing in-situ state of stress, and the geometry of the mined excavations. From the standpoint of the thermohydrologic issues, this information is also needed in determining whether the permeability of the rock mass may be adversely affected by the changes in apertures of the fractures.

2.6 Summary

The potential horizon for a repository at Yucca Mountain (YM) is in the Topopah Spring Formation which is a heavily fractured tuff in the vadose zone some 325 m below the surface and about 250 m above the water table. A decision on technical site suitability is currently scheduled for 1998, with a license application for construction authorization in 2001. Under the new "Program Approach", it is necessary to achieve a "broad understanding of nearfield thermal-hydrologic-mechanical-chemical (THMC) processes such that defensible calculations of postclosure performance can be made." A successful license application will require an "understanding of coupled processes" and "substantially complete containment".

Thermal loading strategies are constrained by a set of design criteria as to maximum temperatures at key points, but in order to meet contractual obligations with the utilities, a thermal load of at least 60 MTU/acre is required, which could be accomodated within the primary emplacement block of Area 1. Lower loadings would require expansion into a larger percentage of the total available area with a significant increase in costs.

The geology and hydrology of the YM site have been studied extensively, and the cumulative picture is continually being expanded as excavations in the ESF go forward. Yucca Mountain is a fault bounded volanic plateau located in the arid, south-central part of the Great Basin. The Topopah Spring Tuff is enclosed in a series of ash-flow tuffs whose characteristics are largely a result of welding and devitrification that occurred shortly after emplacement. The volcanic rocks have been disrupted by throughgoing faults that have the potential to act as paths of high permeability. The majority of the mapped faults are high angle, north- to northwest-trending normal structures, and there is extensive associated fracturing. Faults and connected fracture networks can provide "fast paths" of focussed fluid flow through the mechanisms of fingering and channelization. Communication in the vadose zone, presumably through fast paths, is indicated by several factors, such as the pneumatic pressure communication between the volcanic units, and the presence of young water at depth. Since the matrix permeability in the TS is of the order of 10^{-18} m^2, it is apparent that the fast paths are significantly more permeable to be able to provide the observed communication.

The hydrologic system at Yucca Mountain depends on precipitation, infiltration and percolation. Mean annual precipitation at present is 170 mm/yr, but the amount of infiltration is an important issue that has not been resolved. Model results have given values as low as 0.1 mm/yr; however, significantly higher values from field measurements have recently been reported. A major feature of the unsaturated system is the significant heterogeneity in flow and transport processes. An important consequence is the significant local variation in the moisture content of the geologic units. The average water saturation in the TS is 65%, whereas layers immediately above and below have much lower saturations. The matrix porosity of the TS is 0.08 to 0.12.

As the repository is subjected to a thermal load, all TH processes will be driven by a time-varying heat source due to decay heat from the SNF and the areal mass loading of the emplaced waste The various processes and impacts will be carried out within a "thermal framework" that has a rather rapid temperature rise at first, followed by a long period in which TH processes in the near field environment and on the mountain scale are played out.

The principal conceptual model of the TH coupling involves an initial period in which heat is conducted into the rock on the repository scale. Temperatures in the vicinity of the repository rise above the boiling point (97° C) and vaporization of pore water takes place. This leads to a dried-out zone along fractures and in openings and the transport of water vapor through fractures to cooler regions where condensation takes place.

The overall system performance will mainly be influenced by the following fluid flow processes: (1) flow in a dryout region and the adjacent heat pipe around the repository during the early part of the project (~1000 years); (2) flow of condensed fluids and/or of surface infiltration in the rock formation, particularly in fast paths; and (3) the re-wetting of the dry region when boiling ceases at the later stages of the project (>1000 years). The establishment of a dryout region and delayed rewetting are the two key premises on which the concept of an "extended dry repository" is based. All these processes involve the simultaneous flow and/or displacement of two immiscible phases (gas, or vapor, and liquid water). Understanding and prediction of such flows requires adequate knowledge of the flow characteristics of formations comprising the site, namely the relative permeabilities and the saturation-capillary pressure relationships.

Heat transfer in the matrix is expected to be dominated by heat conduction. In the near field environment, this mode of heat transfer will be coupled with buoyant convection in the dry-out region, and with two-phase convection in the heat pipe region. The likely development of heat pipes is significant to heat transfer, due to their substantial capacity to transfer heat compared to simple conduction. At the mountain scale, we expect, in addition, convective heat transfer in the saturated zone below the repository, and buoyant gas-phase convection in the unsaturated zone.

As a result of the strong thermal disturbances that will occur in the repository in response to heating, the following main classes of chemical processes are likely to occur: (1) dissolution-precipitation involving an aqueous phase and the enclosing rock matrix; (2) solid-solid phase transformations; and (3) mineral precipitation from an aqueous phase in response to changing temperatures or vaporization. Minerals whose solubilities are strongly temperature-dependent, such as the silica polymorphs and the carbonates, will be most affected. Because many of these reactions involve a change in the volume of the solid phases and the release or uptake of water, they have the potential for altering the porosity, permeability and moisture budget of large volumes of rock.

When the temperature of a fractured rock mass increases significantly, the rock mass will undergo thermally induced displacements and changes in stress that, in addition to the material properties, will depend on: (1) the frequency and orientation of the fractures that are present, and (2) the aperture distribution. Depending on the geometry of the fracture network, the overall rock deformation will take place in the normal and/or shear modes. As a result, apertures will generally tend to close as the matrix expands, and the net displacements for the rock mass will be less than what is predicted for a homogeneous rock. The corresponding implications on fluid permeability and flow paths are important.

These chemical and mechanical effects create the difficult problem of trying to predict the overall behavior of a rock mass that is being subjected to changes in temperature. Laboratory measurements can provide reliable values for the material properties of fractured rock samples subject to chemical and/or mechanical processes; and presumably, field data on the chemical environment, state of stress and the fracture geometry are, or will be, available. However, without data on the actual *in situ* behavior of the Topopah Spring Tuff as it is exposed to a changing thermal field, it will not be possible to develop a reliable procedure for predicting the magnitude, nor the degree of coupling, of the thermochemical and thermomechanical effects of this extensively fractured rock.

The impact of the thermal load on the TH processes is intrinsically coupled to a significant number of factors. Determining the probability of occurence of the various conceptualizations that can be raised requires providing answers to questions such as: What is the nature of the liquid/vapor migration paths? Will counter-current fluid flow develop primarily in the fast paths, and will this process be the same above the repository as it is below? What is the role of the imbibition of condensate into the matrix and its effect on counter-current flow in regions where fracture/matrix interactions occur? What role does gravity play in this process both above and below the repository? If there is a dominant direction for the fractures, the overall rock mass probably will have a definite anisotropy, and what will the effect of anisotropy have on the various processes mentioned above? Is there danger that the repository may be breeched by any of these processes? Are the recent estimates on the minimum infiltration rates for the breaching of the repository defensible? What is the confidence on the estimates of future precipitation rates, given the recent findings of the USGS, which seem to indicate an infiltration substantially higher than originally determined? And can one use the ECM, in its present form, to correctly interpret these complicated phenomena?

3. CRITICAL ISSUES

In order to determine the adequacy and sufficiency of the existing and proposed thermal testing program, the PRT first identified certain critical issues, the resolution of which it considers necessary. They are presented in this section, in the following classification: (1) Technical issues, which deal with site characterization, physical processes, their modeling, and parameter estimation; (2) Thermal loading strategy, with emphasis on the concept of the "extended dry repository"; (3) Validation and calibration of the models developed; and (4) Reduction of uncertainty.

3.1 Technical Issues

The thermohydrologic performance of the repository is expected to be dominated by certain key boundary conditions, parameters and processes. The successful prediction of their effect requires a reliable mathematical model. The following subsections identify critical issues related to these. They include: Infiltration, the Impact of Heterogeneities, the Fracture-Matrix Interaction, Thermochemical and Thermomechanical Effects on Fracture Permeability, and Process Scale-up.

3.1.1 Infiltration

The rate of natural infiltration from precipitation at the ground surface constitutes the upper hydrologic boundary condition. Infiltration flux provides a source of water to the condensation zone expected to form above the repository horizon, and this additional flux must be considered in the prediction of the extent and duration of the thermohydrologic impact. It is conceivable that if infiltration rates are sufficiently high, they could overwhelm the dryout region.

Infiltration rates are likely to show great variability, both spatially and temporally. As discussed in Section 2.3.2, spatial variability is due to: (1) differences in topography over the site; (2) differences in climatic input over the site; and (3) differences in surface geology and soil cover over the site. Temporal variability is due to: (1) differences in storm-to-storm rainfall intensity; (2) seasonal climatic differences; and (3) longer-term climatic cycles.

Early efforts to determine a numerical value for infiltration attempted only to provide an estimate of the average annual value in mm/year. The estimate was based on one-dimensional model calibration to measured saturation profiles in boreholes, using the equilibrium assumption inherent in the ECM representation for fracture/matrix interaction. An average value of 0.1 mm/year was obtained and has been widely used ever since in model calculations. This value represents a very small percentage of the average annual precipitation of 170 mm/year, and it is very favourable to the "extended-dry-repository" concept.

To provide more defensible infiltration estimates, the YMSCP has recently established a network of 84 neutron-probe boreholes to shallow depths over the mountain. Infiltration is calculated on the basis of field-measured water contents and lab-measured rock and soil properties. Initial interpretations of this data (Flint and Flint, 1994) produced estimates as low as 0.02 mm/year for areas where the TCw outcrops (66% of the area) and as high as 13.4 mm/year for areas where the PTn outcrops (11.5% of the area). Rates were highest in the north, lower to the south. The overall average was 1.4 mm/year.

During the course of the peer-review deliberations, the PRT learned that a more recent interpretation of the data, as yet preliminary and unpublished, indicates much higher infiltration values. The latest analysis produces maps that show great variability areally and temporally, but indicate values as high as 32 mm/year, and an average annual value in excess of 20 mm/year. There appears to be a feeling within the infiltration study team and within the YMSCP at large that these values are too high; further assessment of the data is ongoing.

A variety of issues lead to uncertainties in the neutron-probe measurements and their interpretation. The measurement issues include:

(1). Factory-provided neutron-probe calibration curves (relating counts-per-minute to moisture content), have apparently been used to date by the study team. In applications elsewhere, it is often found that separate calibrations are required for each soil type. and/or each individual borehole.

(2). The neutron probe measurements are made in holes much larger than the diameter of the measurement tool, and there is an annular air gap between the borehole casing and the formation at many of the holes. The influence of these conditions requires careful consideration.

The interpretation issues include:

(1). Infiltration is a non-linear function of precipitation. There may be a threshold value of precipitation below which infiltration is essentially zero. Wet years therefore bias the average annual estimates upwards. The infiltration program involves field measurements over a 10-year period, but not all of the neutron holes have existed for the full period. Three of the past five years have been very wet, and 24 of the 84 holes were only monitored during this period. Information provided to the PRT suggests that corrections for this bias have not yet been carried out.

(2). Each measurement location could be viewed as a microenvironment deserving of individual analysis. Consideration of the data at this level of detail has apparently not yet been carried out.

(3).The infiltration flux calculations are made for a depth 6 feet below the alluvial/bedrock contact. At some sites, it is possible that evapotranspiration could extend beyond this depth.

(4). It is recognized in the project that the PTn may smear the fluxes, reducing very large local values, and leading to more uniform recharge rates below the PTn. On the other hand, the isotopic evidence reviewed in Section 2 indicates the likelihood of rapid infiltration to significant depth via fast flow paths. It must be recognized, however, that isotopic data, while indicating short travel times for some flow paths has little to say about overall infiltration flux rates.

The PRT is very concerned about the large range of reported estimates of average annual infiltration (from 0.1 mm/year to greater than 20 mm/year). The hydrologic system is very sensitive to the infiltration rate. For example, for a rate of 0.1 mm/year, fast paths are unlikely to be critical because groundwater travel times to the water table are in excess of 300,000 years. On the other hand, for a rate of 10 mm/year, fast paths are likely to be critical because travel times could be orders of magnitude smaller. From a thermohydrologic perspective, if one accepts the arguments of Pruess and Tsang (1994), an infiltration rate greater than 4 mm/year could overwhelm the thermohydrologic pulse.

The PRT concurs with the conclusion that infiltration rates are likely to show great variability over space and time. Even if the latest infiltration calculation proves to be an overestimate, it will be difficult to deny the possibility that infiltration rates could attain values up to 10 mm/year, at some points in space and time. If fact, one of the arguments put forward in support of the higher recent estimates is that it reflects an episodic climatic cycle of higher precipitation associated with the El Niño event of 1992-93. The same period featured anomalously higher winter-season precipitation.

These seasonal and longer-term anomalies will undoubtedly continue to occur over the postclosure period, and they may lead to transient fluctuations in the extent of the boiling zones and heat pipes associated with the thermohydrologic pulse. It is the conclusion of the PRT that it will be difficult to proceed to the necessary decisions with respect to repository design, waste-package design, and site suitability without a significant reduction in uncertainty as to the likely spatial and temporal patterns of infiltration, and its average annual value.

3.1.2 Impact of Heterogeneities

As described in Section 2, the tuffs of Yucca Mountain exhibit heterogeneity in their lithology, stratigraphy, structure, and in their thermohydrologic properties, at several scales, from canister-scale (~1 m), through drift (5-10 m) and near-field (50-500 m) scales to a regional scale (1-5 km). At the larger scales, heterogeneity reflects the horizontal layering of welded and non-welded units, variable patterns of alteration (such as the zeolitization of non-welded tuffs), and large-scale discontinuities, such as faults and major shear zones. At the smaller scales, it reflects detailed layering within volcano-stratigraphic units, lateral changes in lithology and degree of welding, variable local-scale alteration, and local-scale discontinuities in the form of individual fractures and lithophysal development.

Faults and fractures are of particular interest. Faults are large through going features, exhibiting shear zones up to 100 m or more in width near the surface, narrowing in a "horsetail" fashion with depth. It is likely that such fault zones can be treated as porous media in hydrologic modelling. They are likely to feature a high saturated hydraulic-conductivity and a step-function relationship in their unsaturated characteristic curves. They also are likely to be vertical conduits, but may form barriers to lateral flow in non-welded units, where shearing and the formation of fault gouge, rather than more brittle deformation, can occur. Large uncertainties still exist as to their role in the regional hydrogeologic regime, but it is anticipated that some of these uncertainties will be reduced by proposed fault-zone studies in the ESF.

Individual fractures are thought to be connected, although they are likely to be very heterogeneous in their aperture, roughness, coatings, and hydrologic characteristics. Furthermore, the predominant dip of fracture planes suggests a strong degree of anisotropy, which must be taken into consideration in the modeling of the various THMC processes. This local heterogeneity will lead to fingering and channeling on fracture planes similar to the experiments of Nicholl et al. (1992) and Nicholl and Glass (1994). These authors found that episodic infiltrating water tended to preferentially follow the paths of earlier fingers and channels. Such persistent channels through the interconnected fracture systems in the welded units may constitute one class of fast paths.

Geological heterogeneity has a substantial impact on both the ambient hydrologic system and on the thermohydrologic system that will exist during repository operation. The impact on the ambient system includes: (1) very irregular infiltration fluxes; (2) a complex saturation field; (3) the existence of saturated perched zones within the vadose zone; (4) the possible occurrence of lateral flow; (5) the presence of fast paths, and (6) the creation of a preferred flow direction due to fracture anisotropy.

In spite of significant advances in several of these areas, tremendous uncertainty remains as to how the heterogeneous features of YM influence flow. The issue of temporal and spatial heterogeneity in infiltration fluxes has already been taken up in Section 3.1.1 as one of the key controls on moisture flow and transport. The next issue, as to how the spatial variability in saturation as a function of the major stratigraphic units has developed, is reasonably well defined As depicted in Figure 2.6, capillary effects have led to relatively low moisture saturations in PTn and CHn. Model studies have suggested that the overall variation in moisture content represents gravity-capillary equilibrium, developed under essentially zero recharge (Wilder, 1993c). However, this interpretation is at odds with measurements of recharge fluxes, and suggests that there remains a knowledge gap with respect to the nature of fracture-matrix interactions. Again, this manifestation of the heterogeneous nature of the medium is sufficiently important to be discussed at length in a subsequent section.

Heterogeneity in hydraulic conductivity and recharge appears to be responsible for the development of perched zones within the unsaturated zone. While several of these perched zones have been discovered, it is not exactly clear why they have formed. The most important problem related to perched water concerns the question of how these zones might develop in the future as a consequence of changing climate or moisture redistribution during repository heating. Clearly, one important influence of heterogeneity may be to produce additional zones of saturation in as yet undetermined locations.

Another manifestation of heterogeneities in hydraulic conductivity is the possibility for lateral flow in some units. As was described in Section 2.3.2, the capillary barrier that develops at the PTn could promote lateral flow above the repository (see Figure 2.5). If this lateral diversion along the so-called "tin roof" of the repository does in fact occur, a mechanism exists for significant infiltration to bypass the repository. Model studies indicate that lateral diversion is most effective under conditions of ideal layering. However, broad variability in hydraulic conductivity or the presence of fracture zones within the PTn could reduce the tendency for lateral diversion. Thus, understanding how flow occurs above the repository will require detailed information on the heterogeneous nature of geologic units.

Lateral diversion, like spatially heterogeneous recharge, has the ability to focus flows of water along particular zones. These zones could be fractures or continuous zones of saturation adjacent to fractures. Until recently, these zones of focussed flow have not received attention. Pruess and Tsang (1994), however, make the point that formational heterogeneities make strong spatial focussing of flow "not only possible but likely". They go on to infer that these focussed flows have the potential to create areas locally within a hot repository where flows are sufficient to overwhelm vaporization. These ideas have been extended beyond recharge to zones of condensate that could form above a repository. However, there is modeling evidence to suggest that much of the condensate that could form above a repository will occur in the matrix and be incapable of rapid return as cooling takes place (Buscheck and Nitao, 1995b).

The presence of fractures in otherwise low permeability materials has the potential to create complex patterns of fracture-matrix interactions. There is compelling evidence from studies at Rainier Mesa and isotopic measurements at YM to suggest the possibility for fast fracture flow.

There are a variety of ways in which heterogeneity can influence the thermohydrologic response at YM. Under ambient conditions, heterogeneity appears to play an important role in determining the quantity, timing, and distribution of flows. Similarly, the features of repository heating will also be sensitive to heterogeneities. The PRT believes that dryout will be sensitive to fracture properties (as suggested by Eaton, 1994), and that because of the heterogeneity of these properties, there is considerable uncertainty in the predictions of the size and duration of the dryout zone. Conduction may serve to homogenize dryout somewhat, but heterogeneities in the fracture system and in the infiltration flux are likely to create a complex saturation field in the dry-out region and in the condensation region, rather than the smooth fields indicated by idealized models (Figure 2.8).

The PRT concludes that predictions of thermohydrologic conditions during repository heating will have to be based on an analysis that includes consideration of irregular infiltration fluxes, development of time-dependent zones of saturation, the possibility of lateral flow in specific lithologic units, and the presence of channelized fast paths in discrete, possibly anisotropic, fracture systems. Of these, it is the first and the last issues that are most problematical. The "fast-path" issue bears directly on the equivalent-continuum concept, which is treated as a separate critical issue below.

3.1.3 Fracture-Matrix Interactions

A key feature of the near field environment is the extensive natural fracturing of the tuff (spacing of 0.3 m/fracture). The ability to successfully model and assess the thermohydrologic conditions depends to a large degree on the understanding of the flow and displacement in this complex fracture-matrix system. Although fracture characterization is not complete, certain features have been identified: (1) nearly straight fracture traces, but with a small tortuosity; (2) some variations in dip, but a large fraction of fractures with nearly vertical dip; (3) widely variable apertures; and (4) some degree of interconnection of fractures leading to a fracture network. The analogy of the fracture network to that of the well-studied Stripa site has been frequently cited (Pruess et al., 1995).

Flow and transport in fractures have been well-studied. Single-phase flow permeability has been studied in terms of the fracture mean aperture, its statistics, and its spatial correlation. Capillary-controlled displacement, such as drainage, in a rough fracture has been modeled in analogy to porous media. Because of the quasi 2D aspect of fractures, however, saturations of trapped phases can be considerably higher than in porous media. As previously pointed out, Sandia researchers have studied gravity-driven displacements in rough fractures. Preliminary work on boiling in a fracture has also been reported (Tsang and Pruess, 1995). Single-phase flow in networks of fractures is also reasonably well understood for a variety of networks (including self-similar fractal networks, Acuna and Yortsos, 1995). Less advanced, however, is the understanding of two-phase flow in a fracture network and, more generally, in a matrix-fracture system.

Flow processes that would predominate during the life of the YMSCP include: countercurrent steam-water flow in the heat pipes following the onset of boiling, flow of surface infiltration and/or condensate water, and the re-wetting of the dry region, following the boiling period. Both of the latter are imbibition processes. These processes critically affect the extent of the heat pipe, hence the volume of the dryout region, the assessment of scenaria of focussed liquid water flow (including water condensate) and the advance of the re-wetting front.

To our knowledge, the countercurrent flow of steam and water in a fracture-matrix system has not been studied. Assuming coexistence of two phases in the fracture, the liquid in the tight matrix must be superheated, due to the substantial vapor pressure lowering and the capillary pressure barrier for steam penetration of the matrix. It can reasonably be concluded that in such heat pipes, steam will flow only in the fractures. What is not known, and needs to be determined, is the return flow pathway of the water condensate. Condensate can drain as a liquid film on the interface, possibly in the form of gravity fingers, or it may slowly return by imbibition through the matrix. The particular mechanism, hence the flow conductivity, would depend on factors such as the surface roughness of the matrix-fracture interface, the fracture and matrix permeabilities, and more generally, the nature of the connected fracture network. The mechanisms will also be dependent on the steam flow rates, which in turn depend on the applied thermal load.

Heat pipes inside the matrix are possible, although the small matrix permeability could substantially limit their extent (Satik et al., 1991). However, for a matrix embedded in a network of fractures, the return of the condensate through the network of fractures is a more likely possibility. This feature has important bearing on the possibility of "focused" flow (Pruess and Tsang, 1994). Little is known at present about any of these effects. Equally unknown is the effect of focused liquid flow resulting from anomalously high episodic infiltration on existing heat pipes and the dryout regime. This knowledge gap is of obvious significance to the validity of the "extended dry repository" concept. Current models treat the steam-water countercurrent flow as a conventional displacement (imbibition) in the ECM framework (discussed in Section 5.1.2). However, an analysis of the results from the G-tunnel tests suggests that the return condensate flow is through a large fracture (Zimmerman et al., 1986). Nitao and Buscheck (1995) confirmed the effect of a discrete single fracture, using a conventional ECM-based flow description. Assuming a worst-case scenario of focused flow only, Pruess and Tsang (1994) estimated minimum infiltration rates for the breeching of the dryout region. The implications of their findings call for a better understanding of steam-water flow in fractured rock.

The other aspect of two-phase flow in a fracture-matrix system relates to imbibition of water under unsaturated flow conditions. The basic issue relates to the condition under which water will flow through the fracture, and more generally through the fracture network, only, or through the matrix. Clearly, this condition is fundamental to the question of focussed flow discussed earlier. Nitao (1991) considered the problem of primary imbibition of water in the simplified geometry of a 2D matrix, single-fracture system. Based on certain simplifications and the use of a continuous approach, he showed the existence of the following critical value,

$$q^{*} = \phi \, (S_f - S_i) \, D_m \tag{3.1}$$

below which the imbibition front in the matrix advances much faster than in the fracture (also termed condition of "equilibrium" between fracture and matrix), and above which the reverse occurs (condition of "non-equilibrium" flow). This condition essentially expresses a balance between viscous forces in the fracture and capillary suction forces of the matrix. For homogeneous systems, the capillary diffusivity, D_m, is proportional to the matrix hydraulic conductivity, as discussed previously. However, D_m will also be affected by the transport and capillary characteristics of pore-lining minerals at the fracture-matrix interface, in the case of THC effects. A similar criterion, but based on a pore-network approach, was also derived by Haghighi (1994).

Under ponding conditions, equation (3.1) can be equivalently translated into a condition on the fracture permeability (hence the aperture, b). Therefore, preferential flow in the fracture will be favored at conditions of higher aperture and lower matrix permeability (but also of a reduced permeability due to deposited minerals at the fracture-matrix interface, although this was not quantified by Nitao, 1991). Partial experimental support of the above can be found in Mattax and Kyte (1962), and in unpublished work by Nitao (1995). Although the existing evidence appears to support the validity of Equation (3.1), stringent laboratory investigations must be conducted, in view of the important implications for the modeling of flow in naturally fractured systems.

3.1.4 Thermochemical Effect on Fracture Permeability

Self-sealing of fractures by mineral deposition or by dissolution and reprecipitation sequences is an on-going process in hydrothermal systems with direct consequences on the system permeability and the flow of fluids. The possibility exists that it would also develop during the life of the YMSCP. The process affects both the saturated and unsaturated zones. In active hydrothermal systems, self-sealing is most strongly developed when temperatures are sufficiently high to form heat pipes. Under these conditions, mineral precipitation and hydrothermal alteration occurs primarily in regions where boiling or condensation occur. Water-rock interactions may be enhanced by the presence of H_2S or CO_2 because of their strong effect on fluid pH. During boiling, the loss of CO_2 will increase the fluid pH leading to the deposition of carbonates. Silca minerals (e.g., quartz) may also precipitate in response to increasing concentrations and solubilities that are strongly temperature dependant.

By contrast, the dissolution of these gases in the condensate lowers the fluid pH, resulting in the formation of mineral assemblages dominated by clays. However, the seals that form in reponse to these interactions may be only transient features that are subject to recracking. It is also possible that the resulting "throttled boiling" would lead to renewed cracking. The possibility that dissolution and precipitation processes will effectively seal fractures (or otherwise reduce their permeability) in the near field environment of the repository is currently an open question. The experiments of Lin and Daily (1989a,b) and Lin et al. (1995) indicated substantial and relatively fast permeability reductions of single fractures resulting from silica remobilization at temperatures and pressures that may develop within the respository environment. Both these effects can critically affect the TH response. The precise mechanism responsible for this effect is still under study, however.

The issues that need to be better understood include: the dependence on applied pressure and flow rate; the relevant time scales; the development of a predictive model; the permeability reduction in the fracture-matrix system under heat pipe conditions; and the change in the water-matrix imbibition rates resulting from the mineral precipitation.

3.1.5 Thermomechanical Effect on Permeability

As discussed in Section 2, changes in the aperture of a fracture, induced by changes in temperature, can produce a very significant change in the permeability of the fracture. For a fracture with planar surfaces that are roughly parallel and separated by a mean aperture b, the single-phase flow rate per unit width, q, is:

$$q/\Delta h = (W_{fr}/L_{fr})\,(\rho g/\mu)\,(b^3/12) \qquad (3.2)$$

This equation ("cubic law") has been derived for an "open" fracture, namely under the condition that the planar surfaces remain parallel and not in contact at any point. Romm (1966) has shown that it holds for fractures made of optically smooth glass with apertures as small as 0.2 μm.

In the case of a rough fracture, deformed under the effects of normal stress, the cubic law still holds if allowances for the roughness are taken into consideration in determining the mean aperture (Witherspoon et al., 1980). In laboratory investigations, the normal stress - flowrate curves are characterized by large decreases in permeability with increase in normal stress in the low stress region (<3 to 5 MPa), although the decrease is much smaller as the normal stress is increased to higher levels (Gale et al.,1993). These can have important effects in the hydraulic conductivity of the fracture network as it is subject to the thermal load.

In the case of a rough fracture deformed in a shear mode, the size of the asperities and the magnitude of the effective normal stress are other important factors to be taken into consideration. The effects on flow can be rather complicated. In laboratory studies on rough fractures with small-scale to large-scale asperity ratios that varied from 1 to 20, Gale (1995) observed that the permeability decreased logarithmically with the increase in normal stress, and decreased further as the sample was sheared. Fluid flow parallel to the direction of shear was reduced to nearly zero, while flow parallel to the large scale roughness was significantly increased. If the normal stress is sufficiently low, shear may simply cause the rough surfaces to ride up the sides of the asperities, but if the normal stress is high enough to prevent such movement, then asperities will be ground off.

The effect of an increase in temperature will tend to increase the effective stresses on the fractured rock mass, hence the permeability of the fractures will decrease as a result of the deformations that take place in both normal and shear modes. However, if the changes in temperature also cause microcracking, an opposite effect may take place. Certain aspects of this problem can be investigated in the laboratory, but it is not clear what the thermomechanical effect of a change in temperature will have on the permeability of the TSw under field conditions, where temperatures may reach 200° C. Nor has any work been done to determine the extent to which there will be a coupling of the thermomechanical and thermochemical effects. This is an important issue that needs investigation, possibly in a large scale, long duration test.

Both of the above are prototypical examples of the complex THMC coupling. They demonstrate that the net effect of chemical and mechanical interactions involving rock surfaces cannot be predicted by isolated studies of their interactions alone in the absence of flow and confinement. Their overall effect on the performance of the YMSCP, however, is unclear and needs to be evaluated.

3.1.6 Scale-Up

The geometric length scales characterizing the YMSCP are: (1) a heterogeneity scale of the matrix, L_m (order of cm); (2) the characteristic fracture spacing, L_{fr} (order of m), which also measures the typical matrix block size; (3) a heterogeneity scale of the fracture network, L_{fn} (unknown); (4) the grid block scale of numerical simulations, L_n (order of 100 m); (5) the drift scale, L_d (order of 1000 m); (6) the scale of fault spacing or other large-scale features, L_{fa} (order of km); and (7) the mountain scale, L_M (order of tens of km). In the above, we excluded phenomena at the pore-scale.

Relevant time scales for the TH process (see Figure 2.10) are the following: (1) 0-100 y, during which there is a high level of thermal activity and large TH impacts in the NFE; (2) 100-1000 y, during which there is a decline of thermal power pulse at the repository horizon, with continued TH activity, and mountain-scale TH impacts; (3) 1,000-10,000 y, during which mountain-scale TH impacts are significant, as the thermal pulse reaches its maximum spatial extent; and (4) 10,000-1,000,000 y, during which the thermal pulse has ended and ambient hydrology controls release and transport of radionuclides.

Phenomena at different scales affect the physical processes in different ways. Implicit in process modeling at the various scales is an averaging process, the validity of which depends on the various assumptions made. A critical evaluation of these procedures is important, particularly in regard to the development of numerical models.

The impact of heterogeneity in properties is the product $v\lambda$, where v is the variance of the distribution of the property, and λ is the spatial correlation length. For example, depending on the nature of the process and the degree and correlation length of heterogeneity, two-phase flow may be dominated by fingering, dispersive flow or channeling phenomena (Gelhar and Axness, 1983; Waggoner et al., 1991). At present, little is known about the heterogeneity of the matrix or the fracture network in the units of the YMSCP. However, measurements have shown a great degree of variability (large v) in the matrix and fracture permeabilities (see Figure 2.11). Therefore, we should expect a significant effect from this heterogeneity, particularly at the scales L_{fr} and L_{fn}. Studies in this direction have yet to be performed.

The characteristic scales L_n, L_d, L_{fa} and L_m are deterministic and fixed. In published studies, the fracture spacing is assumed deterministic and constant (of the order of 0.3m). There is no explicit account of the heterogeneity at the other two scales L_M and L_{fn}. Most numerical studies proceed with the assumption of constant matrix and fracture properties (Buscheck and Nitao, 1993, Bodvarsson et al., 1994). The implication of this assumption is that it tends to underestimate the degree of dispersion and/or channeling of the various processes modeled, particularly infiltration, heat pipes, and thermal and chemical transport.

Model representations, such as ECM, deal with scaling-up to the scale L_{fr}, to incorporate the matrix-fracture interaction. A discussion of the ECM is presented in Section 5. Here, we briefly point out that it relies on two key premises, a simplified geometric representation of the fracture system and the assumed equilibrium between the matrix and the adjacent fractures. A more appropriate model at this scale should be based on a dual-porosity/dual-permeability description that allows for transient, as opposed to instantaneous, coupling between matrix and fractures, at least as far as capillary and mass transport is concerned. An even greater challenge is to scale-up the process at the numerical grid scale adequately. Mountain-scale simulations have a grid block linear length, L_n, of the order of tens to hundreds of meters (Pruess et al., 1995). At this scale, each grid block is likely to contain a multitude of matrix blocks and their adjacent fractures.

Currently, there is a general consensus among investigators on the existence of large-scale "fast paths", namely of flow pathways correlated over distances of scales L_{fn} and larger, as evidenced from pneumatic pumping and movement of radionuclides (Bodvarsson, 1995). These paths have been identified as faults, by some authors (Bodvarsson et al., 1994), and as planar fractures of a large vertical extent, by others (Tsang and Pruess, 1995). Chesnut (1995) proposed a simplified transport model based on vertical layered flowpaths with a wide permeability distribution that implicitly accounts for large-scale heterogeneity. A similar concept is to be implemented by Nitao to model condensate flow at the repository scale. In this context, it must be mentioned that the existence of fast paths does not necessarily require large-scale (large λ) correlated structures (such as faults). Even in single-phase flow in an uncorrelated medium, but with a wide distribution of permeabilities (large v), most of the flow occurs over a connected subset of large permeabilities, which effectively plays the role of a fast path, as discussed in Section 2. A similar result could apply to a fracture network with a wide size distribution.

The PRT concludes that the development of appropriate scale-up models of the various processes in the highly heterogeneous and anisotropic rock system at YM is largely unexplored.

3.2 Extended Dry Repository

The efficacy of the extended dryout approach has remained controversial since it was first proposed in the late 1980's. The daunting complexity of dealing with the thermohydrologic processes that is forced by the high thermal loading and an overall lack of related engineering experience has prompted some to conclude that avoiding the thermal issue altogether with the minimal heating alternative provides the most logical design alternative. The PRT has briefly examined the issue of what thermal effects might be evident under minimal waste loading. Bounding calculations by Halsey (1994) showed that creating thermal fluxes comparable to ambient or natural conditions would require 500 square miles over which to emplace the waste. Thus, any practical loading scheme at the repository will create significant thermal perturbations. Another feature of the minimal heating approach is that heating is minimal on *average* over the repository. With the use of MPC containers, however, heating would be highly heterogeneous *across* the repository. Zones of local boiling in the rock might persist for hundreds of years (Halsey, 1994). Conductive heat flow calculations by Benton (1995) showed boiling up to five meters away from the emplacement drifts. Thus, boiling-related processes and inherent complexities will be manifest at a local scale even under minimal heating conditions.

In looking at this evidence, the PRT concludes that no simple argument can be made for accepting the minimally heated repository over the extended dry approach as the "simpler" approach. At any practical waste loading, the thermal perturbation will give rise to complex thermal effects at both the repository and local scale. The selection of the MPC container requires that thermohydrologic processes be investigated both theoretically and experimentally.

The repository design will be judged according to how well it performs in relation to regulatory standards. Initially, the concept of an extended dry repository was developed in the context of regulations that limited releases from the repository and to the accessible environment after 10,000 years. Given the relatively long duration of boiling and rewetting times, a strong case could be made that this approach would improve overall performance. The main improvement in performance would come from providing more reliable containment at the repository for thousands or tens of thousands of years. During the period of boiling, the possibility of low relative humidities could substantially reduce the rate of container corrosion. In addition, for a long time, there could be an absence of mobile water. Moreover, it is argued that heating could mitigate the uncertainty and lack of predictability associated with fast fracture flow.

This extended dry repository concept is based on two key premises: that a robust, extended dryout region would prevail for a long time around the repository, and that following the cessation of boiling, at the latter stages of the life of the repository, the re-wetting of the dry region would lag significantly behind the thermal front, and occur mostly in the matrix. Both these premises, however, need to be critically evaluated.

A main cause of concern is the large volume of condensate likely to occur above the repository. For several years, it was believed that this repository-scale redistribution of water was a direct result of boiling. New calculations, however, indicate that even for a minimally heated repository (AML of 27.1/acre and on average below boiling), moisture could be redistributed due to large-scale, buoyant gas convection (Buscheck and Nitao, 1994; Buscheck and Nitao, 1995b). If the bulk permeability of the fracture network is relatively high (e.g., k ~ 40 darcy), buoyant vapor convection is found to create regions of dryout below the repository and a zone of condensate buildup above the repository.

It is also possible that fracture heterogeneity can lead to episodic selective fast-path reflux of channelized saturated flow. Such a scenario is supported by conditions observed in the G-tunnel heater tests (Zimmerman et al.,1986, see also Ho and Eaton, 1995), wherein fractures served as the predominant flow paths for both gases and liquids. It is conceivable that if infiltration rates are sufficiently high, they could overwhelm the dryout region, in contradistinction to an earlier claim by Buscheck and Nitao (1992) that the spatial extent and duration of boiling is insensitive to recharge flux. Under these conditions, the possibility raised by Pruess and Tsang (1994), that some of the canisters may get wet some of the time, during the period of thermohydrologic impact, cannot be dismissed.

The other assumption of the lag of the re-wetting front, which is crucial in the latter stages, is based on the hypothesis of matrix imbibition, which involves small capillary diffusivities. Questions can be raised on the role of the fractures in this process, however, which may be the dominant path for flow. More importantly, at this point this premise is only a theoretical prediction from the ECM approach, and has not been tested experimentally at any scale (laboratory or field).

The PRT identifies the concepts associated with the extended dry repository as main issues of concern. Reliable predictability requires one to develop knowledge about the processes, the controlling parameters, and the complex interactions involved that is sufficient and verifiable for the purposes of engineering design. Some PIs argue that larger dryout zones would accompany significant heating and would yield the greatest benefits in performance (Ramspott, 1991; Wilder, 1993b). However, others claim that there may be deleterious consequences that will result in diminished repository performance over more moderate heating strategies

Some of the deleterious consequences that have been suggested include; the possibility of focused flow, discussed above, as well as far-field changes in the thermomechanical and thermochemical properties of the rocks. If confirmed, these effects could lead to unacceptable increases in ground-surface temperatures, and enhanced migration of radionuclides to the accesible environment. As indicated in Section 3.1.1, there is also the completely independent problem concerning the large range of reported estimates for the average annual infiltration. All these issues will impact the necessary decisions with respect to repository design, waste-package design, and site suitability.

3.3 Model Validation and Calibration

There are two main issues to be considered with respect to validation and calibration. First, are the general questions as to what is the present state of validation of thermal, hydrologic, chemical, and mechanical models, and whether experiments are in place to accomplish validation. Second, is the issue of whether calibration of large-scale field tests necessarily demonstrates the predictive capability of models at an even larger scale.

Testing the validity of a model is ideally accomplished by using the model to simulate behavior measured in well-characterized field or laboratory experiments. Rigor in the testing is achieved through an independent measurement or estimate of every parameter in the model in advance of the modeling exercise. Validation implies testing in advance of any practical application of the model. Some workers use the term validation to describe one final test with a calibrated model against an independent set of field data.

Realistically, a true model validation is seldom if ever achieved, as it is almost impossible in field experiments to measure or estimate parameter values without uncertainty (NRC, 1990). This leads to non-uniqueness in interpretation, wherein parameter uncertainty and process uncertainty cannot really be distinguished from one another. With complex process models, validation proceeds in a much less satisfying manner through a history of "successful" applications of the model. In theory, if a model is not valid, this eventually should be discovered. Unfortunately, models often have so many adjustable parameters that model applications are almost always deemed to be successful.

Calibration is the process of selecting model parameters that provide an acceptable match between observed (i.e., historical or known) behavior and simulated system responses. Successful calibration of a model is taken as one demonstration of its predictive capability. In effect, if a model can reproduce the known or historical response of a system, it should be capable of making predictions in the future. Common practice is to set calibration targets in advance of the actual modeling to assure that appropriate calibration is achieved. Many calibrations involving distributed parameters, however, are nonunique.

It is commonly acknowledged in the hydrologic sciences in general, that efforts in developing theory and models have outpaced the collection of data that might serve to constrain parameter estimates or to validate models. The state of affairs at Yucca Mountain is similar with theoretical and modeling efforts far ahead of confirmatory field testing. The field testing has been delayed by the need to develop an appropriate and defensible set of methodologies, and by difficulties in accessing the site for testing.

As indicated earlier in this report, thermal effects will dominate the performance of the repository at any practical waste loading. This statement implies that fluid flow and mass transport processes will also be strongly influenced by thermal effects. While there has been considerable scientific progress in the theoretical formulation and mathematical modeling of coupled phenomena (particularly involving heat), there has been a dearth of field-oriented experimentation. What progress is evident is mainly related to large-scale geothermal systems, and the subsurface storage of hot water. Similarly, there has been relatively little work related to systems as unique as Yucca Mountain, featuring unsaturated and fractured porous media.

The relatively limited experience of the scientific community in complex coupled problems, and the unique conditions at Yucca Mountain impose a significant burden of proof to assure proper validation of the models. In the opinion of the PRT, this burden has yet to be met because appropriate field and laboratory experiments are not sufficiently far advanced.

The validation of mountain-scale thermohydrologic modeling should be of great concern to the Yucca Mountain Project because of the direct link to design decisions. The presently limited number of available thermal experiments means that the thermohydrologic models are largely unvalidated for Yucca Mountain conditions. This problem, in and of itself, is not critical to the scoping and process oriented calculations that are being undertaken by the modeling group at LLNL. However, consumers of the modeling studies must be aware that as validation data become available, there remains a strong possibility for surprises in the understanding of how processes are conceptualized. The "aura of correctness" (Bredehoeft and Konikow, 1993) that is attached to simulation models of all kinds requires extreme caution in the interpretation of simulation results.

The heater experiment carried out in the G-Tunnel complex of the Nevada Test site (i.e., Prototype Engineered Barrier System Field Test; PESFT) has played a significant role in validating the current thermohydrologic modeling. As Buscheck et al. (1993a) indicate, the detailed quantitative examination of the PESFT test results provided surprises that led to modifications in the conceptual understanding of thermal processes. Recent reinterpretations of the experimental data (Nitao and Buscheck, 1995) illustrate yet again the complexity of the thermohydrologic processes, and the important role that large-scale experiments will play in validating theoretical models. These observations provide significant justification for the need for expedited thermal testing underground at Yucca Mountain.

The Yucca Mountain project has sponsored a variety of laboratory-scale experiments, some of which logically might have been used to validate conceptual models of the thermohydrologic system. With the exception of some of the work at Sandia National Laboratory related to the question of fast-fracture pathways, there is relatively limited laboratory data available for model validation. The previous laboratory work was focussed on more fundamental questions related to the examination of thermochemical, and thermomechanical processes. The PRT was presented with plans for thermal experiments (Tsang and Pruess, 1995) that could provide important laboratory information to assist with model calibration. Clearly, appropriately designed laboratory experiments take on more importance for model validation given the budget constraints that may limit field testing.

3.4 Reduction of Uncertainty

There is considerable uncertainty associated with thermohydrologic processes and parameters at Yucca Mountain. It is the reduction of these uncertainties that is the primary goal of the laboratory and field testing programs, and the modeling program, that are being reviewed in this report.

Uncertainty is a critical issue for several reasons. First is the fact that thermal processes are sensitive to small changes in parameters. Secondly, performance may be strongly influenced by a few key parameters. Lastly, there are large irreducible uncertainties because of the fractured-rock environment. There is a potential for significant surprises due to the large uncertainties on this project.

The types of uncertainty faced in the project can be classified into five groups: (1) Process Uncertainty; (2) Geologic Uncertainty; (3) Parameter Uncertainty; (4) Uncertainties in Model Idealization; and (5) Uncertainty in the Performance of Engineered Components.

Under the first category of Process Uncertainty, we include the current uncertainties associated with predictions of the duration and extent of the thermohydrologic response to heat emplacement. This includes the processes of boiling, dryout, condensation, reflux, and the formation of heat pipes. The physics of these processes are reasonably well understood in porous media, although some additional work is needed (see Sections 4 and 5). The underlying process uncertainties here relate to two-phase fluid-flow in fractured media, in particular to the fracture/matrix interactions outlined in Section 3.1.3, and the potential for channelized "fast paths". This process uncertainty is exacerbated by the large uncertainties associated with current estimates of the spatial and temporal distribution of infiltration, as discussed above.

The uncertainties associated with the second and third groups listed above are often combined, but we choose to differentiate between geological uncertainty and parameter uncertainty. Geological Uncertainty refers to the uncertainties associated with the locations, extent, and three-dimensional distribution of horizontal geological units and vertical structural features. These include faults and "fast-path" fracture interconnections in the vertical sense, and horizontal capillary conduits and barriers caused by differences between welded and non-welded units, and vitric and zeolitized altered rocks.

Parameter Uncertainty refers to the uncertainty associated with the representative values of hydrologic and thermal properties assigned to each of the identified geologic features and units. These include saturated hydraulic conductivity and porosity, thermal conductivity and capacity, and all other flow requires specification of the two characteristic curves relating capillary fluid pressure, water saturation, and relative permeability (or hydraulic conductivity) for both the matrix and the fractures. The parameter uncertainty of greatest sensitivity may well be that associated with the parameters of the double-hump unsaturated characteristic curves used in the ECM representation.

Model Idealization Uncertainty relates to such issues as the use of the ECM representation, discussed in Section 5, and the use of 2D representations of the 3D system, also discussed in Section 5. The first of these is closely related to the primary process uncertainty identified above.

Uncertainty in the Performance of Engineered Components such as waste-package canisters will not be discussed further here.

Of the first three types of uncertainty, it is the opinion of the PRT that reduction of process uncertainties should take the highest priority, with geological uncertainty second, and parameter uncertainty third. Reductions in process uncertainty will be achieved largely through laboratory and field experimentation, and associated model validation and calibration. It is unlikely that it will be possible to develop a quantitative measure of the degree of uncertainty reduction achieved for process uncertainties. The acceptable level of uncertainty reduction will tend to be a subjective judgement that will require peer review and acceptance.

Parameter uncertainty is the type of uncertainty that is most amenable to traditional geostatistical analysis. The degree of uncertainty reduction achieved by parameter measurements taken in the site characterization program can be estimated on the basis of conditional geostatistical analysis using either a classical or Bayesian statistical framework (Freeze et al., 1992). However, this step requires the definition of probability density functions and autocorrelation functions for the various parameters, and this task will be hindered by the sparseness of the available data base.

There is growing recognition among hydrgeologists that geological uncertainties have greater impact than parameter uncertainties on overall hydrologic (and presumably thermohydrologic) response. Geological uncertainty, because it relates to the location of geological features, is more involved with the uncertainty in positioning and continuity of planar features and boundaries. Uncertainty analysis of geologic uncertainties thus requires the application of non-traditional indicator statistics that are still emerging from the current research efforts in the geostatistical community. The YMSCP should continue to investigate the potential usefulness of these geostatistical techniques in the study of thermohydrologic uncertainties.

Traditional geostatistical analysis usually involves Monte Carlo simulation, which requires many model runs. It is unlikely that this will be a feasible approach for the complex 2D and 3D thermohydrologic models being applied in the YMSCP. It is possible, hoever, that some simpler type of stochastic modeling, perhaps based on first-order approximations, could be developed. Such approaches deserve consideration. This question is further addressed very briefly in Section 5.2.6.

3.5 Summary

The PRT has identified a set of critical issues that must be resolved by the testing and modeling program of the YMSCP. These have been classified as: (1) technical issues; (2) issues associated with the extended-dry-repository concept; (3) model calibration and validation issues; and (4) issues associated with uncertainty reduction. The technical issues include: (a) infiltration; (b) heterogeneities; (c) fracture-matrix interactions; (d) thermochemical effects; (e) thermomechanical effects; and (f) scale-up issues.

Infiltration rates are likely to have considerable impact on the extent and timing of the thermohydrologic response of the mountain to repository heating. It is conceivable that if infiltration rates are sufficiently high, they could overwhelm the dryout region. Measured infiltration rates show great variability, both spatially and temporally, and there is currently much uncertainly as to the average annual value and the breadth of the spatial and temporal ranges. It will be difficult for the YMSCP to proceed to the necessary repository-design decisions without a significant reduction in uncertainty with respect to infiltration rates.

The tuffs of Yucca Mountain exhibit heterogeneity in their lithology, stratigraphy, structure, and thermohydrologic properties at a variety of scales. This heterogeneity has substantial impact on both the ambient hydrologic system and on the thermohydrologic system that will exist during repository heating. In particular, the dryout, condensation, and possible reflux of moisture during the period of thermal load is likely to be very sensitive to the heterogeneity of the fracture networks in the rocks. Predictions of TH conditions during repository heating will have to include consideration of irregular infiltration fluxes, irregular time-dependent zones of saturation, possible lateral flow in specific lithologic units, and the presence of channelized fast paths in discrete interconnected fracture systems.

Fracture-matrix interactions are still poorly understood, even for single-phase fluid flow, and especially for two-phase flow of steam and water. The nature of these interactions will control, to a large degree, the nature of the heat pipes that may develop, and the potential for reflux of water that condenses above the repository. Understanding the controls on imbibition from the fractures into the matrix, and on the potential for channelized flow in the fractures, needs to be improved.

The possibility that mineral dissolution and precipitation may effectively seal fractures or otherwise reduce their permeability in the nearfield environment of the repository is still an open, but important, question. Similarly, reductions in permeability due to mechanical changes in fracture apertures under a thermal load have been predicted but not confirmed. Some have suggested that such effects will be secondary, but as yet their overall importance in the proposed repository is uncertain.

Phenomena at different scales affect the physical processes in different ways. Implicit in the passage from one scale to another is an averaging process, the validity of which depends on the assumptions made. The development of numerical models, in particular, requires critical consideration of upscaling procedures. The numerical studies of the YMSCP have proceeded on the assumption of constant matrix and fracture properties over considerable distances. Such studies tend to underestimate the degree of channeling that may occur during infiltration or within heat pipes, and with respect to thermal and chemical transport. The ECM approach also relies on scale-up assumptions regarding the geometric representation of the fracture system and the assumed equilibrium between matrix and fractures. These assumptions require investigation.

The concepts associated with the extended-dry-repository continue to be issues of concern in the project. The extended-dry-repository concept is based on two key premises: (1) that a robust extended dryout region will prevail for a long time around the repository under high thermal loadings; and (2) that the rewetting of the dry region will lag significantly behind the thermal front. Theoretical calculations that lead to these premises require experimental support. There are contrary scoping calculations, that cannot be easily dismissed, suggesting that fracture flows are not properly considered in the theoretical calculations, and that deleterious consequences could arise from high thermal loadings.

The relatively limited experience of the scientific community in modeling complex thermohydrologic problems and the unique conditions at Yucca Mountain, impose a significant burden of proof to assure proper validation of the process models used in the project. This burden has yet to be met because appropriate field and laboratory experiments are not yet sufficiently far advanced. Consumers of the modeling studies in the repository-design and performance-assessment teams must be aware that until more-defensible validation data becomes available, there remains a strong possibility for surprises at the process understanding level.

There is considerable uncertainty associated with thermohydrologic processes at Yucca Mountain. The three main types of uncertainty can be classified as process uncertainty, geologic uncertainty, and parameter uncertainty. Of these, it is the opinion of the PRT that reduction of process uncertainties should take the highest priority. This can be achieved by laboratory and field experimentation, and associated model validation and calibration. The of use of geostatistical analyses to describe reductions in geological uncertainty and parameter uncertainty will be hindered by the sparseness of the available data base.

4. LABORATORY AND FIELD TESTING

In this section, we review past and planned activities in the laboratory and field testing program contained in the White Paper (DOE, 1995a) and comment on their adequacy to build confidence in the understanding and prediction of TH processes. We address sequentially, activities related to site characterization, laboratory experiments and field tests, as they address boundary conditions, small scale processes and larger scale processes, respectively. Site characterization activities are not included, *per se*, in the charge of the PRT. In fact, a program on site characterization was not included in the White Paper (DOE, 1995a). However, in view of its expected crucial effect on the TH processes, the PRT considered it necessary to proceed with an assessment of their status. This section is organized as follows: (1) activities in the various categories are, first, reviewed, and then; (2) the adequacy of the overall program is discussed.

4.1 Site Characterization

Yucca Mountain is a large, geologically and hydrologically, complex system, of which the main properties at the various scales are only now starting to be understood. Evaluating the large-scale properties has proven to be a difficult task. Continuing efforts are necessary as they bear directly on our ability to model and predict the various TH processes.

4.1.1 Past and Present Activities

The geology of the site, including the distribution of rock types and the surface and subsurface traces of the faults, has been mapped in considerable detail, where accessible. The key results have already been summarized in Sections 2 and 3. Investigations on estimates of the infiltration rate and the principal hydrologic features of the mountain have been conducted and are currently active. The relevant information was summarized in Sections 2 and 3, where some of the difficulties associated with reliable measurements were pointed out.

Of significant interest are large-scale hydrologic properties, which are associated with faults and the fracture network As previously mentioned, under some conditions, these features may provide preferential flow paths. Past activities in this area included indirect estimates using geochemical tracing and pneumatic testing of boreholes. The latter is a more recent activity. Because of their relevance, the two activities are discussed more extensively in the following sections.

Measurements of the ^{36}Cl, ^{14}C, and ^{3}H levels in water samples collected from different geologic units have provided direct evidence of young waters, and, by extension, of fast paths, within the unsaturated zone (Fabryka-Martin et al., 1993, Yang, 1994). Bomb-pulse levels of ^{36}Cl were found in two drill holes (UZ-14, near the surface, and UZ-16, at depths exceeding 375 m in the CH formation). Samples from the TS in the ESF have also been collected, but they are currently under study.

Elevated levels of ^{14}C were found in several wells in the TC and in drillhole UZ-1 in the TS. The deepest bomb-pulse signal was found from samples collected at a depth of 125 m. The conjecture that these elevated ^{14}C levels are indicative of fast paths is based on the fact that concentrations of these radionuclides exceeded natural levels during the 1950s and early 1960s as a result of nuclear weapon testing in the near vicinity. Hence, the presence of waters with bomb-pulse levels of radionuclides must be due to fast fracture flow, with effective flow velocities exceeding estimates based on the average infiltration rates (Section 2). However, these data cannot yet be used to distinguish between lateral movement along capillary barriers and vertical infiltration along faults. Nor are they able to identify the nature of these paths, namely whether they pertain to faults, single fractures, fracture networks or other connected pathways.

It should be pointed out that although the overall conclusions based on ^{36}Cl and ^{14}C are similar age determinations for water based on ^{14}C measurements (modern to 10,000 y) are one to two orders of magnitude lower than those based on ^{36}Cl (which are modern to 700,000 y). Liu et al (1995) offered several possible reasons for this discrepancy, with perhaps the most likely being the mixing of waters of different ages. Despite these uncertainties, such studies clearly hold the potential for unraveling issues concerned with unsaturated flow in the vadose zone.

A more direct determination of large-scale hydraulic properties was recently provided using air injection tests in the three wells UZ-16, NRG-6 and NRG-7, and the subsequent analysis of the resulting pressure response. This technique has provided values for the effective, large-scale air permeabilities in the regions probed, which range between 1×10^{-15} m^2 in the non- to partially-welded Calico Hills Formation to about 5×10^{-11} m^2 in the densely welded Tiva Canyon Tuff (Hoxie, 1995). Permeability values for the Topopah Spring Tuff varied between these two limits, with most in the range 1×10^{-13} to 2×10^{-11} m^2.

Permeabilities were also estimated from measurements in wells NRG-6 and NRG-7a (Bodvarsson, 1995, Hoxie, 1995) in the absence of air injection, using pneumatic testing. This novel technique is based on a model analysis of large frequency pressure variations, which reflect fluctuations in atmospheric pressure. From the analysis of the lag and attenuation observed, large-scale permeability estimates can then be made. Moreover, the observed significant attenuation of pressure changes in the TS, compared to TC, has reinforced the belief that the intervening tuffs (PTn) act as a "tin roof". The implications of this behavior in the TC are important regarding water infiltration. Pneumatic testing is an attractive and relatively simple characterization test and has rapidly emerged as a potentially useful tool.

4.1.2 Planned Activities

A specific program of site characterization activities was not explicitly formulated in the White Paper. However, the PRT singled out efforts to: (1) update site-specific data, including the delineation of hydrostratigraphic units and faults; (2) determine saturation profiles in boreholes and identify the locations of perched water; and (3) characterize water movement through radioisotope investigations. Furthermore, the PRT was informed that activities will continue in the areas of pneumatic testing, which appears to be a high priority item, and on the further estimation of infiltration rates. In addition, mapping of the fracture network in the access tunnel of the ESF will continue.

4.2 Laboratory Investigations

Knowledge of the thermal, hydrologic, chemical, and mechanical properties of the host rock at YM and of the various THMC processes at a small scale is essential for the development of predictive models for flow and transport, as well as the interpretation of the results of various *in situ* tests. This section summarizes activities in the areas of properties and processes at the laboratory scale.

4.2.1 Past and Present Activities

Rock properties are generally determined from measurements obtained either in controlled laboratory experiments or from *in situ* tests. Several reports and papers made available to the the PRT illustrate the types of data for characterizing the site under ambient hydrologic conditions. These include the reports of Montazer and Wilson (1984), Wilder (1993a,b), Flint et al. (1994b), White Paper (DOE, 1995a), and Zimmerman et al. (1986, 1987). Properties can be categorized as hydraulic, thermal, chemical and mechanical. With the exception of hydraulic properties, and to some extent chemical properties (Bish et al., 1989, 1995; and Glassley, 1995), the characterization has been extensive and largely sufficient for the needs of the YMSCP. In terms of hydraulic properties, matric potentials at various locations have been determined. However, relative permeabilities of the various rock types have not been measured, and they are currently estimated by applying the van Genuchten model (see Section 3).

In contrast to the large number of measurements made on the thermal, chemical, and mechanical properties of rocks, relatively few laboratory studies have been conducted on the various THMC processes that will occur in the repository block. Those that have been carried out focussed on flow processes and, to some extent, on geochemical processes. Few laboratory investigations of the full TH processes expected in the fractured TSw have been conducted.

Nicholl et al. (1992) investigated gravity-driven fingering due to wetting-front instabilities in unsaturated, rough-walled fractures. Once a finger structure develops in an initially dry fracture, the structure was found to persist in subsequent infiltration events. Additional work by a Sandia group (Tidwell and Davies, 1995) investigated further aspects of flows in isolated fractures, accompanied by matrix imbibition. In other investigations of two-phase flow, Persoff and Pruess (1995) developed a laboratory flow apparatus that was used to visualize and measure relative permeability data in natural rough-walled fractures. Visual observation of changes in the occupancy of the various pores by different fluids, showed that instabilities develop from an interplay between capillary effects and pressure drop due to viscous flow. A strong phase interference reduces the relative permeabilities to very small values at intermediate saturations for both wetting and nonwetting phases. Fracture-matrix interaction has not been systematically investigated (although a preliminary unpublished experimental study was reported by Nitao, 1995). Significantly, no studies of water-steam flows have been conducted, in either homogeneous or in fractured systems, with the exception of recent work by Lin et al. (1995) to be discussed below.

More emphasis has been placed on chemical effects, particularly as they relate to the possibility of fracture healing and the importance of mineralogical changes. Lin and Daily (1989b) and Lin et al. (1995) examined the effects of mineral precipitation and dissolution on fracture permeabilities in the densely welded TSw. In these experiments, natural fractures were saturated under various temperatures and confining pressures that ranged up to 150°C and 5 MPa, respectively. The tests involved both natural fractures that were reopened, and tensile and saw cut fractures in samples that were originally unbroken. It was found that permeabilities decreased by several orders of magnitude, when water (or steam) flowed through the fracture, at temperatures exceeding 90°C and pressures above 0.5 MPa, but that no change occurred in the permeability of an unfractured sample or in a fracture containing stagnant water under similar conditions. Lin and Daily (1989b) concluded that the permeability changes occurred because silica dissolution and precipitation was able to reduce asperities along the fracture walls, allowing the fracture apertures to be reduced at the confining pressures to which they were being subjected.

In a second set of experiments, Lin et al. (1995) initiated investigations to evaluate the interrelationships between fracture aperture, initial water saturation, and water imbibition in the surrounding matrix. In these experiments, water is allowed to flow down a vertically oriented fracture of fixed aperture. Movement of the water can be determined by X-ray scanning or electrical resistivity methods. These techniques allow visualization of the water movement through the rock throughout the experiment. They found that dissolution and deposition of minerals on the fracture surfaces by hot water/steam led to fracture plugging. In addition, the experiments revealed substantial differences in the rate of imbibition, depending on whether imbibition occured in a pre-wet sample or not.

Glassley (1995) investigated water-rock interactions and mineralogical changes as a function of temperature. The rate at which steady states were approached was found to depend on the kinetics of mineral dissolution and precipitation and the small-scale mass transfer. The primary impact of secondary mineral development is on porosity-permeability and is related to changes in pore structure, pore volume, fracture roughness and connectivity, etc. However, the state-of-the-art currently does not allow for a conclusive statement to be made on how chemical changes impact a permeability-porosity relationship.

In view of the ion-exchange capacity of zeolites and their common occurrence in the altered rocks at Yucca Mountain, a series of experimental studies have also been conducted to determine the thermodynamic properties of ion-exchange. Murphy and Pabalan (1994) obtained data on cation exchange equilibria at 25°C between clinoptilolite, the most abundant zeolite at Yucca Mountain, and binary solutions of various concentrations. The results were used to develop a model to predict ion exchange equilibria between aqueous solutions and clinoptilolite over a range of fluid and zeolite compositions. This model may prove useful in assessing the composition of groundwater in equilibrium with this zeolite.

Studies at Yucca Mountain show that with increasing depth, clinoptilolite is replaced by analcite. The formation of analcite may become important when temperatures are perturbed within the repository block. The breakdown of clinoptilolite results in the release of silica and water, and a large decrease in volume (Bish et al., 1995). Murphy and Pabalan (1994) measured the solubilities of these zeolites at 25^{o} C, and determined equilibrium constants and free energies of formation for the appropriate dissolution reactions. These thermodynamic properties will be used in fluid-mineral equilibrium calculations.

4.2.2 Planned Activities

The White Paper (DOE, 1995a) describes the following laboratory tests to be undertaken:

(1). Thermally-driven fracture flow test (Fig. 4.1a). This test will use a small-scale, transparent replica of a rough fracture to investigate patterns and rates of water flow along the fracture. The heterogeneity of the fracture will be preserved in order to probe effects of surface roughness, distribution of asperities and aperture heterogeneity. The test will be performed under non-isothermal conditions, including the possibility of water injection in a superheated system. Provision will be made to orient samples at various inclinations to explore effects of gravity and convection patterns. Information from this test will address preferential flow paths within a single fracture under non-isothermal conditions, and imbibition under conditions of non-isothermal flow and gravity orientation. Some information on chemical changes and possibly on heat pipe development would also be collected.

(2). Laboratory evaluation of heat pipes in fractured rock. This test will use fractured rock samples and an imposed heat flux (Fig. 4.1b), as well as individual fractures in the presence of a heater (Fig. 4.1c), to study the development and patterns of heat pipes in the respective geometries. Additional information to be collected will include the change of salinity content near heaters.

(3). Measurement of gas-phase buoyant flow in a temperature gradient. The test focuses on the possibility that gas-phase natural convection may be sufficiently strong to establish a fast path of gas-phase radionuclides that may potentially be released. Here, the proposal is to use gas tracers in real or replica fractures, at various inclinations, to study vapor flow in the presence of a temperature gradient.

(4). Enhanced vapor diffusion. The test will be conducted in partially liquid-saturated fractures at the boiling point and with various temperature gradients (Fig. 4d). An effective vapor diffusivity will be inferred for potential use in simulation.

In addition, the PRT has learned of planned experiments by the USGS for the measurement of relative permeabilities of various rock matrix samples using a newly acquired centrifuge apparatus.

4.3 Field Tests

4.3.1 Past and Present Activities

To date, no *in situ* thermohydrologic tests have been carried out at Yucca Mountain because access to the underground location of the potential repository in the Topopah Spring Tuff has only recently become possible with the excavation of the ESF. However, useful information has been obtained from thermomechanical and thermohydrologic testing at other sites.

Experimental field testing of thermomechanical processes has been carried out in granitic rocks at several different locations (DOE, 1995b). Although these thermal tests were carried out under saturated conditions in igneous rocks, with few similarities to tuff, the results from two different locations wereessentially the same and illustrate important aspects of rock behavior. One thermal test was performed in the Stripa underground facility in Sweden where three electric heater experiments were carried out from 1977 to 1980 at a depth of 340 m in drifts excavated in a saturated and fractured granite (Jeffry et al.,

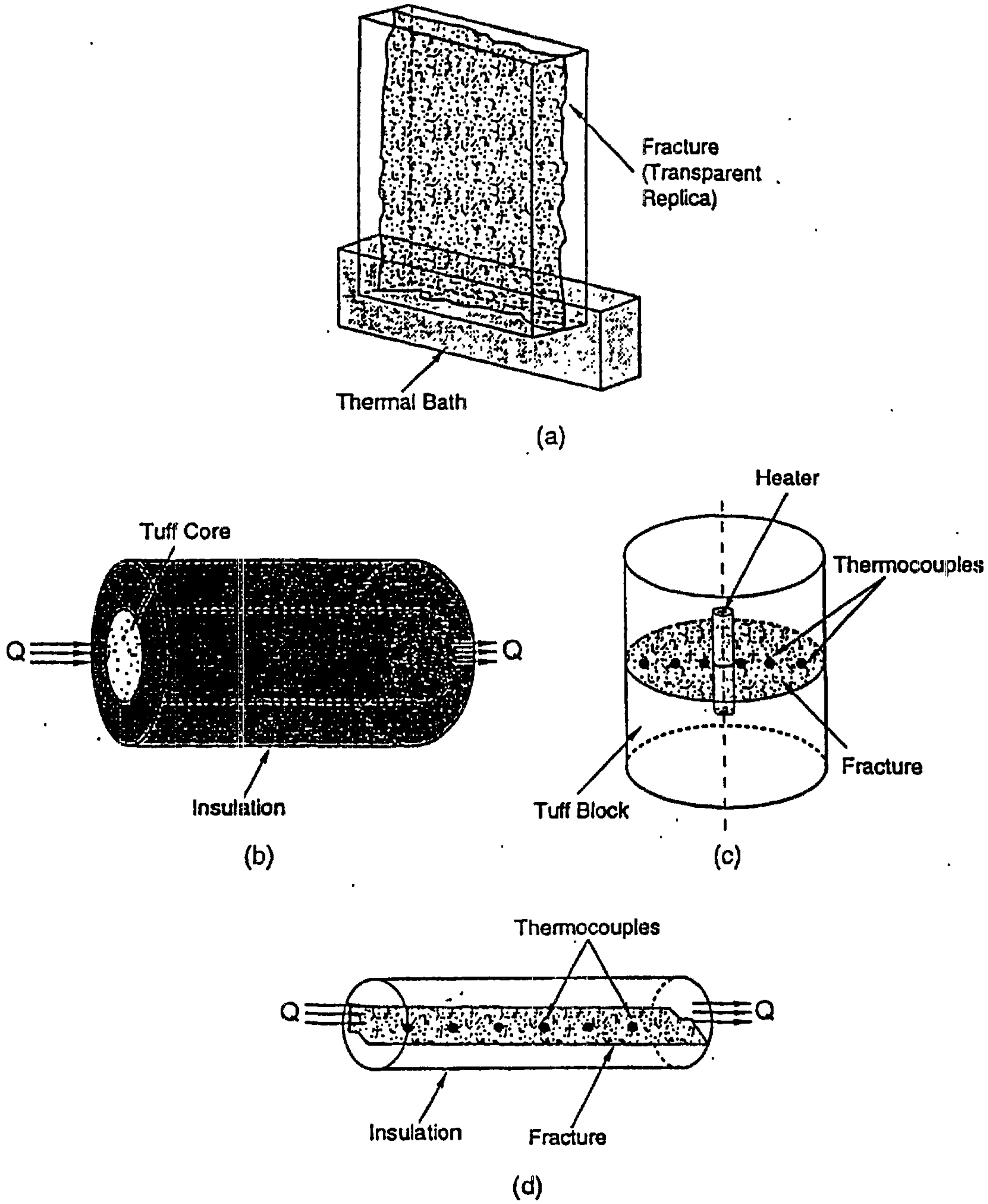


Figure 4.1. Proposed laboratory thermal process tests: (a) Laboratory thermally driven fracture flow test, (b) and (c) Laboratory evaluation of heat pipe test, (d) Laboratory vapor diffusion test (from DOE, 1995a).

1979; Hood et al., 1979). The other thermal investigation was performed in the spent fuel test (SFT) that was carried out in the early 1980's in a saturated and fractured granite in the Climax Mine in Nevada (Wilder, 1995). The lessons learned from these two tests were:

(1). Flow of heat in the rock mass is predominantly by conduction and theoretical calculations using laboratory values of thermal parameters can be used to predict rock temperatures reasonably well despite the presence of fractures,

(2). Thermally induced displacements, calculated using linear thermoelasticity theory were found to be significantly larger than actually measured, probably because rock expansions were being taken up by fracture closure, and

(3). The majority of the changes in stress and displacement occured in a relatively short period of time contemporaneously with changes in temperature.

In situ experimental field testing of TH processes have been carried out in the G-Tunnel underground facility at Rainier Mesa on the Nevada Test Site between 1980 and 1990. The G-Tunnel experiments have considerable relevance to the Yucca Mountain site. They are in similar rock types, at a location quite near to the Yucca Mountain site, and they include experiments that were specifically instrumented to investigate TH processes at relevant temperatures. In fact, many of the TH concepts and theories that have recently been developed in the project emerged in response to the observations of boiling, vaporization, condensation and reflux observed in the G-Tunnel experiments.

The G-Tunnel underground facility has hosted a large number of single heater tests and heated-block experiments. In a block heater test that took place as early as 1980, water was observed to flow out of an inclined heater hole. Recently, Ho and Eaton (1995) carried out an after-the-fact thermohydrologic modeling of this test that clarified the roles of outward gas-phase advection and diffusion of water vapor, condensation in the outer cooler regions, and drainage of the condensed water into the heater hole.

In the period 1983-1985, several small-diameter heater experiments and heated-block experiments were carried out in G-Tunnel (Zimmerman et al., 1986. 1987). These were primarily thermal and thermomechanical in nature, but they did include the first vestiges of hydrologic instrumentation in the form of neutron probe measurements of moisture content and measurements of water accumulations in emplacement holes. Testing was limited to the very near field over relatively short testing periods. Results indicated that water migration could affect temperatures over localized regions of the rock. Moisture contents around the neutron probe holes rose during the early stages of heating and then fell at a later time under the dewatering effects of vaporization. Thermohydrologic processes were identified, including water vapor migration away from the boiling region, and later liquid migration from condensing regions into the surrounding rock. Qualitative comparisons of the observed phenomena and numerical modeling results indicated relatively good agreement between the experimental trends and the modelling concepts.

A fully instrumented TH heater experiment was carried out in the G-Tunnel in 1988-1989 (Ramirez et al., 1991). A 1.1 kW/m heat loading was used for 130 days, followed by a 65-day linear rampdown. Measurements included temperature and moisture content in the rock, and pressure, humidity and temperature in the gas phase. The sensor distribution was designed to allow consideration of radial profiles out from the heater in all three dimensions. Observations confirmed the occurence of boiling, vaporization and condensation. The measurement of a constant-temperature plateau in the vicinity of 100° C in some thermocouples indicated the existence of a heat pipe. However, condensation was not symetric above and below the heater, as expected on the basis of ECM modeling of the fractured rock. Rather, it occurred preferentially above and to the sides of the heater, raising the possibility of condensate shedding around the boiling zone. This finding, together with other conceptual discrepancies between predicted and observed moisture conditions along the radial profiles point to the importance of discrete fractures in the migration and reflux of water during drying and re-wetting. Qualitative observations during the test suggested that flow in the fractures was channelized.

Recently, an after-the-fact remodeling of the 1988-1989 G-Tunnel heater experiment has been carried out (Nitao and Buscheck, 1995). This remodelling used the NUFT code to model the effect of discrete fractures on the thermohydrologic behavior observed in the test. With this formulation, nonequilibrium fracture-dominated flow resulted in rapid condensate drainage around the boiling zone in a manner similar to that observed in the test. The discrepancies between observed and predicted radial moisture profiles were also removed. These results further confirm the importance of fracture flow in near field thermohydrologic processes. Large scale tests of longer duration, as outlined in subsequent sections of this report, are needed to diagnose whether these fracture-dominated processes are important at the drift and repository scale.

4.3.2 Planned Activities

The planned *in situ* thermal experiments presented to the PRT during the review (Datta, 1995) included the following:

(1). **Large Block Test (LBT).** Considerable effort was expended in 1994 to isolate a block of TS about 3 x 3 x 4.5 m in size at Fran Ridge on YM (Lin et al., 1994). Because the block was exposed at the surface, it was planned to enclose it in a load-retaining frame that would have maintained a constant stress of about 4 MPa both vertically and horizontally during the test. The frame was designed but never constructed. When the PRT visited the test site (9/25/95), the isolated block was only partially instrumented. The test was scheduled to start 2/96 and run for one year to provide a means of investigating the coupled THMC processes that will take place in the TS under the influence of a thermal load. Were it to be carried out, the test would accomplish three objectives: (a) gather data on THMC processes for model development; (b) gather preliminary data to be used in predicting quality and quantity of water in the near-field environment of the repository; and (c) develop and evaluate the various measurement systems and techniques to be used in large scale in situ tests.

(2). **Single-Heater Test.** This is a simple, small-scale field test that is primarily focussed on TM coupled effects (DOE, 1995b) and is intended to set the stage for design and implementation of larger scale THMC testing. The test consists of emplacing a long heater rod in a horizontal (or slightly updip) hole so that a significant volume of rock can be heated to approximately 200° C. Appropriate instrumentation will be provided to measure temperature, stress, displacement, fluid saturations, changes in permeability, and water chemistry. It is scheduled to start 6/96 with a 12-month heating period followed by a 12-month cooling period.

(3). **Spatially-Distributed Single-Heater Tests.** These are two tests, similar to the Single Heater Test described above; each test will have a 12-month heating period followed by a 12-month cooling period. These experiments will provide a means of carrying out a short-term heater test in locations with significantly different rock conditions. They are scheduled to be started 6/97 and 6/98.

(4). **Drift Scale Test with Flatjacks (DSTFJ).** This test uses a single drift with the desired thermal field created by emplacing heaters in the drift, plus auxiliary "wing" heaters on both sides along the length of the drift. The design of this test will focus on determining the distribution of temperature, moisture, stress and displacement in the near-field environment and the associated rock-water interactions. The DSTFJ appears to be an outgrowth of an earlier design for a large-scale test that was described in the Study Plan for Engineered Barrier System Field Tests (DOE, 1995c) released April 27, 1995. In the EBSFT, an arrangement of three parallel drifts was to be equipped for an 18-month heating period and a 6-month controlled cool-down period. The work of Buscheck et al. (1993b) is cited in the EBSFT to explain the need for three parallel heater drifts. During the PRT review, Buscheck explained that by using only one drift with wing heaters in the DSTFJ, the test conditions and results envisioned in the short-term test described in the EBSFT could be duplicated. The test is scheduled to start 12/96 with an 18-month heating period followed by a cooling period extending to 2001.

(5). **Large-Scale Long-Duration (LSLD) Test.** According to the EBSFT, the test design is to include five parallel drifts, and the test duration may be changed based on the actual response of the rock mass. The design of this test will focus on determining the distribution of temperature, moisture, stress and displacement, the effects on permeability, and the associated rock-water interactions. The longer time period will provide a thermal perturbation over a much larger rock volume than any other in situ test as well as the development of a significant dry-out region to allow investigation of the re-wetting process. The test is scheduled to be started in 6/98 with a 4-year heating period and a controlled 12-month cooldown period followed by a natural cooldown period.

(6). **Use of Natural Analogues.** Glassley (1995) describes the use of natural analogue systems to: (a) identify and reconcile disparities between laboratory and field studies; and (b) refine conceptual models of processes. The effects of thermal, hydrologic, mechanical and chemical processes can be observed in active geothermal systems that have operated in time frames of tens to hundreds of thousands of years. Bruton et al. (1994) concluded that geothermal systems in New Zealand are particularly appropriate for testing geochemical codes because these systems are hosted in volcanic rocks similar to those found at Yucca Mountain. A significant amount of geologic and geochemical data including mineral and temperature distributions, and fluid and rock chemistry is readily available and can be utilized in these studies.

4.4 Adequacy of Laboratory and Field Testing

In this section we discuss the adequacy of the proposed program. It should be pointed out that during its deliberations and the previous two meetings with the PI's, it has become evident to the PRT that the particular program proposed is not actually fixed, but rather it is in a state of flux, as a result of new budgetary realities, etc. The important issues raised by such programmatic constraints are postponed to Section 6. Here, the PRT will proceed with the assumption that its charge is to address only the program described in the White Paper (DOE, 1995a). In commenting on the adequacy of the program, we will also compare the relevance of the activities proposed to the critical issues of Section 3.

4.4.1 Site Characterization

The PRT believes that a program in site characterization is absolutely necessary in helping to reduce uncertainties; this was identified as a critical issue in Section 3. We believe that the following investigations should be pursued:

(1). Continue and refine measurements and estimates of infiltration rates through a reliable analysis of the saturation profiles. Additional efforts should be placed on bounding the infiltration rate, in view of its potential significance on the viability of the "extended dry repository" concept (see Section 3). It would be highly desirable to extend infiltration flux calculations to depths deeper than 2m below the alluvial bedrock contact. Efforts in this direction will help address Critical Issues 3.1.1 and 3.2.

(2). The measurement of the radionuclide levels (^{36}Cl and ^{14}C) in pore and perched waters should be continued. At present, only a small percentage of samples collected from boreholes and the ESF drift have been analyzed, and it is unclear what is the future of this program. The PRT believes that this effort should be continued, by further enlarging the data set. Efforts should also be made to resolve the discrepancies reported in the radionuclide ages based on such data (see Section 4.1.1).

(3). Air injection and pneumatic testing have proven to be effective for evaluating large-scale air permeabilities. The effort should continue and be expanded, so that a broader coverage of lithologic units and fault zones in the mountain can be obtained.

(4). Continued emphasis should be placed on identifying the heterogeneity of the large-scale features. Detailed geologic mapping has provided the basic framework for the numerical models developed and needs to continue. The drilling of additional boreholes within the ESF is of paramount importance, as they will provide valuable data on the expected heterogeneity under NFE conditions. In particular, the fracture mapping effort in the ESF drift should continue. Efforts should be also directed to understand whether or not faults act as capillary barriers, and to quantify lateral flow along discontinuities.

(5). In addition, the PRT believes that useful hydrologic information that would confirm the existence and possibly help define the location of fast paths, is possible through tracer tests. Vapor-phase tracers, such as SF_6, may be suitable for these experiments. One envisions injecting tracers into boreholes drilled in the ESF and monitoring their movement by sampling at different locations. Information to be obtained from such tests would be of high value in identifying fast paths, which is a recuring issue in this project. We note that such a testing program is currently not in place.

(6). The characterization of fractures (distribution, permeability, and connectivity) remains largely unresolved. Fracture characterization has a large uncertainty, and is an area where much remains to be done. Conceptual models of TH processes that are presently in use rely on crucial approximations of the fracture permeability and distribution. These models assume isotropic conditions, and if the fractures have a dominant orientation, the rock system could be highly anisotropic (see Section 5.1.2). Given the important role fractures play in TH processes and predictive models, efforts in this direction must continue.

Investigations in (2) through (5) above will address in some detail Critical Issues 3.1.2, 3.1.6, and 3.2 of Section 3.

4.4.2 Laboratory Investigations

The PRT believes that the laboratory and field activities proposed should be viewed as components of an integrated experimental testing program, where processes must be investigated at three different scales: (1) the laboratory scale; (2) an intermediate scale involving pilot tests; and (3) a large scale involving *in situ* tests. The program recommended below is guided by this general philosophy. In this section, we comment on the adequacy of the laboratory program by distinguishing activities in property measurements and in process understanding.

A program in property measurement was not included in the White Paper (DOE, 1995a). The PRT concurs that the characterization of thermal (such as conductivities, heat capacities, etc.), mechanical, and thermodynamic properties of the host rock has reached a sufficiently high level, such that additional advantages to be gained from extensive additional programs of property measurements will be small. We note, however, that the available information on adsorption and fluid-solid interaction in the tight TS matrix, as well as information on chemical rate properties is not extensive. Therefore, further advances in these areas would provide useful information that would benefit the modeling of the TH behavior in the matrix and the THC behavior in the fractured rock.

To reduce uncertainty in the modeling of the two-phase flow properties in the matrix, we suggest that the following investigation be undertaken:

(1). Measurement of the water relative permeability (and capillary pressures) in the tight TSw matrix under various infiltration conditions (primary, secondary, and under heat-pipe conditions). Uncovering the dependence of these properties on temperature will be desirable. More generally, a further investigation of adsorption and Kelvin effects in the very tight matrix pores would be useful. These studies would not only test the empirical van Genuchten formalism currently used, but would also shed light on unsaturated flow and displacements in very tight porous media, and provide confidence on the capillary diffusivity in the matrix, D_m, which depends on both relative permeability and capillary pressure (Section 2). As discussed in Section 3.1, D_m determines both the critical rate, q^*, which sets the condition for matrix infiltration, as well as the re-wetting time. Both concepts are fundamental to the concept of an "extended dry repository", identified as Critical Issue 3.2.

The need for additional laboratory investigations on chemical processes is discussed below in conjuction with the fracture healing problem. In the area of processes, the White Paper (DOE, 1995a) contains several proposed activities. Section 3 of this report suggested key areas, where our current understanding of TH, THC and THMC processes, limits our ability to correctly predict the mountain response to the thermal load to be applied. Despite the limitation of scale, a laboratory program is fundamental to build confidence and improve significantly our understanding and the ability to predict. To advance the state of the art and to reduce uncertainty in the representation of the physical processes, we propose that the following laboratory studies be undertaken or continued:

(2). Steam-water countercurrent flow (heat pipes) in single fractures and in fractured rock. A clear understanding of these process, as outlined in Critical Issue 3.1.3. is crucial to the accurate prediction of heat transfer in the NFE and the return condensate rates. Experiments (1) and (2), described in Section 4.2.2 and contained in the White Paper (DOE, 1995), address these issues specifically and are, therefore, deemed quite appopriate. However, we propose that these tests be further expanded to attempt to evaluate, even at the small laboratory scale, the two key premises of the concept of "extended dry repository", identified as Critical Issue 3.2. A similar experimental set-up could be used to test at the laboratory scale the scenario of Pruess and Tsang (1994). Experiments could be designed to test the concept of a lag between thermal and rewetting fronts. Further continuation of the type of experiments of Lin et al (1995) on the different infiltration behavior, depending on the history of the process, must also be considered. However, efforts should be taken to test such processes in geometries as realistic as possible, including a representative fracture-porous medium network.

(3). Experimental verification of the concept of critical rate, q^*, during infiltration of a matrix-fracture system, under various conditions (infiltration in a dry or pre-wet matrix, and under heat-pipe conditions), in conjuction with the proposed experiments (1) and (2) above. This study would confirm the importance of the critical rate of (3.1) and build confidence in the simplified computer models used or to be developed. Experiment should also be conducted to evaluate the effect on the validity of (3.1) of pore-lining minerals deposited at the matrix-fracture interface as a result of precipitation, perhaps in conjuction with experiment (4) below.

(4). Continuation of the fracture healing experiments of Lin and Daily (1989b) to test their relevance under conditions to be encountered during the YMSCP and to build confidence in the corresponding chemical models (Robinson, 1995). These studies should aim at defining more precisely the general permeability-porosity relationship expected to govern the evolution of hydrologic properties during mineralogical changes. In particular, fracture healing under conditions of steam-water counterflow should be tested, in view of the proposed scenaria of precipitation at the boiling front and dissolution at the condensation front (Glassley, 1995). The deposition of precipitated minerals at the matrix-fracture interface could affect the critical rate, q^*, as emphasized above. It is conceivable, then, that in this context a parallel series of experiments in chemical kinetic rates may become necessary

The PRT had long discussions on the necessity of TM experiments. The absence of compelling scoping experiments of the type reported by Lin and Daily (1989b) led the PRT to the conclusion that, at this stage, TM experiments should be of a lower priority However, it was stressed that in carrying out the experiments described above, particularly experiments (2) through (4) where fractures are involved, attention be placed on the mechanical stress conditions applied. The PRT also noted that useful TM information would be obtained from the LBT test to be described in a later section.

Finally, the PRT finds that given the current state-of-the-art, experiments (3) and (4) of Section 4.2.2 on buoyant transport and enhanced vapor diffusion, although interesting, would be of a lower priority. In particular, experiment (3) addresses radionuclide transport in the vapor phase, which is outside the scope of this review.

4.4.3 Field Tests

In commenting on the adequacy of the field-test program it is important to differentiate between the LBT, which is actually a pilot test in an environment that is as well chacterized as possible, and the other *in situ* tests.

4.4.3.1 Large Block Test

The LBT is the only field test that was nearing completion of the construction phase when the PRT began its peer review. The LBT has subsequently been removed from consideration for funding in the FY96 budget of theYMSCP This test was designed to provide a means to investigate TH and related processes that will take place in a large block of Topopah Spring Tuff as the temperature attains a maximum of 135°C.

After a lengthy debate on the scientific and engineering merits of this test, five of the six members of the PRT have concluded that this test will be useful in addressing TH issues on length and time scales that lie in between the laboratory and *in situ* field tests. As such, the LBT should not be compared, or ranked, with other field activities. Specifically, the system is well suited to investigate the following important hypotheses:

(1). The two premises of the "extended dry repository", namely the development of a robust dryout region around the heaters to be emplaced, and the lag of the re-wetting front, after cessation of boiling.

(2). The scenario of Pruess and Tsang (1994) on the possibility of quenching the dryout region at selective points, due to fast paths.

(3). The development of heat pipes and the role of fractures in the reflux of the condensed water. One should note that fracture mapping over all five exposed sides of the block is finished, which will allow a much more discriminating evaluation of fracture effects than in any *in situ*, "blind" test.

(4). The effects of changes in chemistry and mineralogy, and concommitant effects in hydrology.

(5). Last, but not least, the LBT will allow a rigorous testing of field equipment, and of the various computer models in existence. Testing the ECM in a predictive mode would be an important exercise to establish confidence in a code that is being used to make important design decisions.

The PRT does, however, appreciate and understand the technical and scientific implications of the possible shortcomings of the experimental design: (1) the low state of stress in the rock will make it difficult to obtain TM effects that can be translated to the stress conditions at the repository level; and (2) the existence of some three dozen boreholes in the block that will support the extensive set of probes and instruments that are needed may affect the mechanical and hydraulic integrity of the block and may also perturb the thermal and moisture fields.

However, from an overall standpoint, the LBT is deemed a very useful device and should be exploited as much as possible. Inasmuch as the installation of the LBT is well advanced, it is the opinion of the PRT that this test should be supported and continued to completion.

One member of the PRT believes that the LBT will present difficulties in the interpretation of results on the thermal and hydrologic responses of the rock primarily due to length scales and the inherent variability of the thermal boundary conditions in the microclimate at the location of the experiment. Additionally, he believes that the dynamics of the dryout and re-wetting will not adequately be represented over the length scale of the block and in the presence of the fracture network of limited extent and that experimental uncertainty will provide no inherent advantage over the results that could be obtained with a controlled drift-scale program.

4.4.3.2 Intermediate Scale Underground Testing

In the opinion of the PRT, the different Single Heater Tests and the Drift Scale Test with Flat Jacks (DSTFJ) can be considered intermediate scale underground tests, because of the similarities in objectives and overall testing plans. They are therefore reviewed together in this section.

The Single Heater Tests were designed to run for a 12-month heating period which we do not think will provide an adequate test. As will be discussed below in connection with the LSLD test, there are a number of critical problems facing the YMSCP that need to be addressed by thermally perturbing an appropriate volume of rock under conditions approximating that of the near field environment. This will not be possible using single heater tests. Furthermore, these tests are somewhat similar to the heater experiments already carried out in G-Tunnel and other locations, and the PRT is concerned that there may not be that much new experience to be gained. In the opinion of the PRT, these heater tests are not needed.

The DSTFJ was designed to run for an 18-month heating period, and again, the PRT does not think this will provide an adequate test. As indicated above, this test was designed to use a single drift with an arrangement of auxiliary wing heaters to develop a thermal field that would be similar to that generated by three parallel drifts with the same areal loading. Although the rock volume being perturbed is substantially more than in the case of the single heater tests, the length of the heater period is such that we do not believe the DSTFJ will provide a means of addressing the critical problems that are discussed below and that must be solved before DOE will be able to settle the question of site suitability.

The PRT recognizes that a potential use of intermediate scale underground tests would be to calibrate instrumentation of various kinds, but this is also an important objective of the LBT program. We believe such investigations are much more likely to be successful in the LBT because the degree of geologic characterization and the control of the experiment in the block will be difficult, if not impossible, to obtain in underground tests.

If the LSLD test can go forward as recommended below, the PRT believes the results would provide a much more comprehensive investigation of repository behavior. These results would easily encompass those of the DSTFJ, which means that a possible duplication of effort could be avoided. Five of the six members of the PRT recommend dropping the DSTFJ. The same dissenting member of the PRT has indicated that, in view of the limitations of the LBT mentioned in the section above, an accelerated schedule of intermediate-scale underground testing using the DSTFJ would better serve the objectives of the YMSCP.

4.4.3.3 Large-Scale Long-DurationTest

The PRT strongly supports the need for a large-scale, long-duration (LSLD) test. The concept for such a test was apparently first developed in the Study Plan for Engineered Barrier System Field Tests (DOE, 1995c). The EBSFT includes a long-term test that was set up to have a 48-month full-power

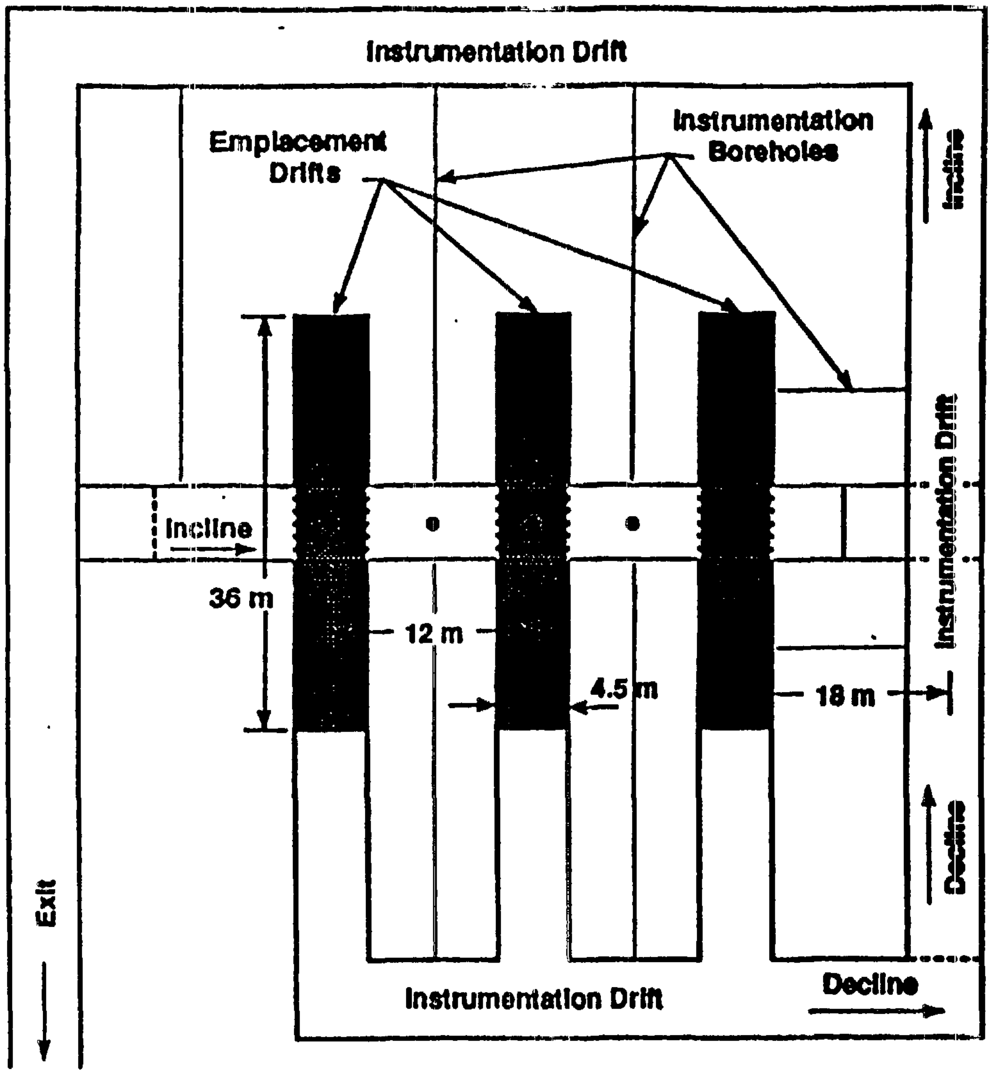


Figure 4.2. Plan view of general layout of emplacement drifts, instrument drifts, and instrumentation boreholes for LSLD test (from DOE, 1995c).

heating period and a 12-month controlled cool-down period, followed by a natural cool-down period. The EBSFT also includes a short-term test with a layout of three parallel drifts as shown in Figure 4.2; the layout for the long-term test is to expand this design to five drifts, presumably with the same dimensions and spacing.

As has been discussed in Section 3, the process of increasing the temperature of a very large volume of the Topopah Spring Tuff, possibly up to maximum levels of about 200° C, raises some issues about rock system behavior, for which there is little or no field experience to serve as a guide to the expected response of the system. A number of complicated phenomena will occur, some interactively, as this highly fractured rock mass is thermally perturbed. It is the opinion of the PRT that these phenomena are unlikely to be sufficiently clarified by shorter, smaller tests, and that an LSLD test must be given the highest priority in the YM thermohydrologic testing program.

The planning of an LSLD investigation must endeavor to understand the nature of these phenomena to the extent possible, but planners must also be aware of the implications where our knowledge of the behavioral characteristics of this welded tuff is incomplete. One of these phenomena involves the complicated process of the manner in which moisture migrates through the rock mass. Boiling at one location near the heat source with condensation in adjacent cooler regions will involve the simultaneous flow and/or displacement of two immiscible phases in a fractured rock under conditions that are not well

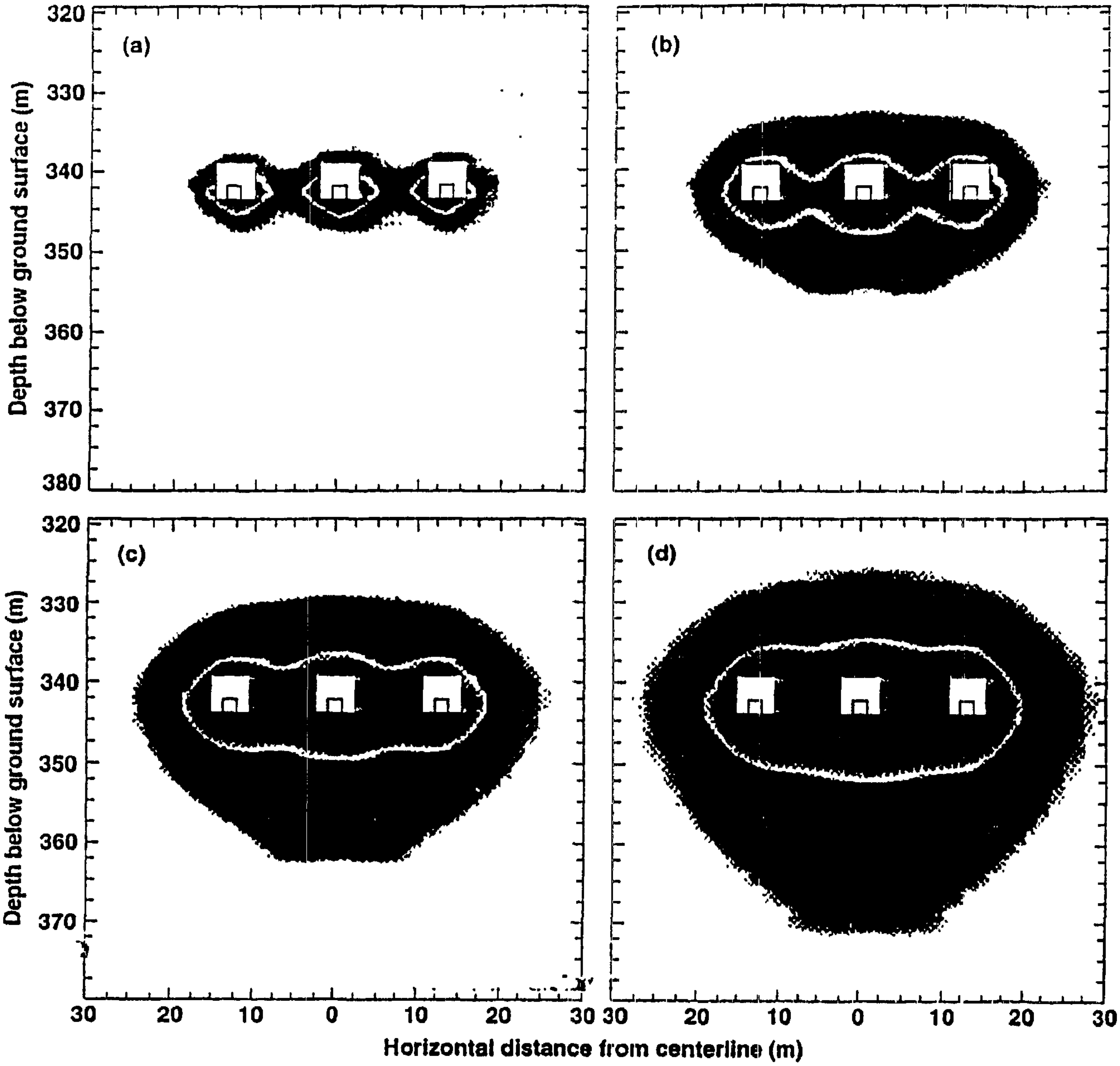


Figure 4.3. Dimensionless liquid saturation distribution orthogonal to an array of three infinitely long, parallel heater drifts, each generating 1.0 kW/m of drift. Time = (a) 1, (b) 2, (c) 3, and (d) 4 years. Shaded areas inside white line are dry-out zones and outside, are.condensation zones (after Buscheck, et al., 1993b).

understood (see Section 2 and Critical Issue 3.1). Because this two-phase process of fluid migration will occur in all directions away from the repository, it is also not clear that the same fluid flow mechanisms that prevail above the repository will control migration beneath it. These issues must be investigated in an LSLD test.

Another issue involves the development of a dryout zone that will grow in size as the available water boils away and the two-phase region propagates away from the heat source under the influence of higher temperatures. The development of a dryout zone over a four-year period for a three-drift system is illustrated in Figure 4.3. It can be seen how the areas inside the white rings, which encloses the dry out zones, grow and merge with time. Supposedly, all of the matrix water boils away within the dryout zone, but this is another issue that needs to be investigated because a complete dryout of the matrix may not actually take place. Furthermore, rewetting of the dry mineral surfaces of the fracture walls will be subject to a condition of primary imbibition as opposed to the secondary condition of imbibition that controls migration in the two-phase regions. This is another factor whose influence on fluid migration is not well understood and which needs investigation.

The presumed coalescence of the condensate and dryout zones, depicted in Figure 4.3, is based on the results of modeling exercises using ECM (Buscheck et al., 1993b), which has incorporated many simplifying assumptions, as discussed below in Section 5. The predictive integrity of the ECM representation has not yet been confirmed. For example, the ECM assumes isotropic conditions, but the underlying geometry of the model is strongly anisotropic. As mentioned in this review, the underlying geology of Yucca Mountain appears to be anisotropic, although the actual extent of anisotropy in the TS is not completely known. Thus, the actual times for the dry out and condensation zones to reach the stages of development shown on Figure 4.3 could be much different than predicted.

Another issue is the effect of infiltration on on the entire TH process. What is the present rate of infiltration, and will the effects noted above actually take place as depicted in Figure 4.3? Or, will there be an unexpected and substantially different result?

Of particular concern is the location of the test, which, in our opinion, should be conducted in a highly fractured area where the effects of moisture redistribution will be most pronounced Because it appears that the near vertical fractues may have a dominant orientation along one azimuth, placing the orientation of the long axes of the parallel drifts along the same azimuth would enable one to investigate the degree to which the various effects listed above are controlled by anisotropy in the fractured rock mass.

Another factor that may also have a bearing on the LSLD test is the changes in permeability that may result from the thermochemical and thermomechanical processes, as discussed in Section 2. As presently formulated, these processes are not included in the ECM, and from the discussions during meetings with the PIs, it was not clear that these effects on permeability are necessarily of second order and can therefore be ignored. It is the conclusion of the PRT that both processes will likely lead to changes in the permeability of the fractures, but it is not clear what the nature and magnitude of these changes will be. This is an another issue of some importance that requires investigation with an LSLD test.

All of these factors indicate that LSLD design needs to be re-evaluated, so that the planned geometry and test schedules reflect not just the most likely scenario, as indicated by deterministic ECM-based models, but also the potential range of uncertain responses. It is very important that this test fully reveal the nature of the controlling factors in thermohydrologic behavior.

The PRT believes that important results will be obtained from the LSLD, both from early and later results, and that subsequent analyses of the cumulative data will produce a picture that becomes increasingly more clear as those components of the controlling mechanisms are revealed. Therefore, the PRT favors a flexible schedule. It could be that, during the heating period, sufficient results will be obtained more quickly than expected and the planned length can be shortened. On the other hand, with a flexible schedule, the planned length might have to be extended to achieve the desired goals.

If our recommendations on underground testing are accepted, we suggest that the LSLD test be started as soon as possible.

4.5 Summary

The question of whether the laboratory and field testing programs are adequate to build confidence in the understanding and prediction of thermohydrologic processes at Yucca Mountain are examined in Section 4. We have reviewed sequentially, activities related to site characterization, laboratory investigations, and field tests as they address the problems of boundary conditions, small scale processess, and large scale processes, respectively. Site characterization activities were not included in the charge to the PRT, but in view of their expected effect on the TH processes, it was considered necessary to proceed with an assessment of their status.

Site Characterization. Site characterization at YMSCP has been on going for over ten years, and is not yet fully complete. The site is geologically complex and obtaining thermal, physical, hydrologic and geochemical properties of the host rock has proved to be a challenging task The characterization activities have reached the point where the physical geology of YM is sufficiently understood to support currently planned and future modeling and field test programs. However, the hydrogeology of the mountain, particularly in the Topopah Spring Tuff, where the potential site for a repository has been selected, is less well understood; and it is in this area where YMSCP needs to focus most of its future efforts.

One of the crucial items is the question concerning the existence of "fast paths". Measurements of the ^{36}Cl, ^{14}C, and ^{3}H levels in water samples collected from different geologic units have provided direct evidence of young waters, and, by extention, of fast paths within the unsaturated zone. In addition, elevated levels of ^{14}C were found in several wells in the Tiva Canyon Tuff at depths down to 125 m, and it is conjectured that these elevated ^{14}C levels are indicative of fast paths

Another crucial item is the measurement of large-scale hydraulic properties. Air injection tests haveprovided air permeabilities in the regions probed, which range between $1\text{x}10^{-15}$ m^2 to about $5\text{x}10^{-11}$ m^2. Permeability values for the Topopah Spring Tuff varied between these two limits, with most in the range of $1\text{x}10^{-13}$ to $2\text{x}10^{-11}$ m^2. A new and novel technique, pneumatic testing, has been developed that is based on a model analysis of large frequency pressure variations, which reflect fluctuations in atmospheric pressure. Large-scale permeability estimates can then be made. With this new technique, the observed significant attenuation of pressure changes in the Topopah Spring Tuff, compared to Tiva Canyon Tuff, has reinforced the belief that the intervening poorly welded tuffs act as a "tin roof". The implications of this behavior in the Tiva Canyon Tuff are important regarding water infiltration. The characterization of fracture flow paths and air permeabilities remains a critical, high priority need of the YMSCP, because an improved data base and process-related information play a key role in the model development and their validation.

The PRT recommends that future activities must focus on: (1) updating the characterization of hydrostratigraphic units and fault zones; (2) determining saturation profiles and identifying perched water zones; (3) characterizing water movement especially with respect to infiltration; (4) continuing the application of pneumatic testing; and (5) continuing the fracture mapping in the access tunnel of the ESF. Characterization studies related to possible fast paths for fluid flow should receive the highest priority

Laboratory Investigations. A program of laboratory experimentation and testing has been supported by the YMSCP to determine properties and process-related quantities that bear on modeling and repository design. Extensive data have been compiled on the thermophysical and mechanical properties of the TS host rock, but there are much less data available on several potentially important geochemical, multi-phase flow and mass transfer processes.

From the existing thermophysical property and hydrological data (i.e., bulk permeabilities), the picture that emerges at this point is that the natural variation in properties is extensive within the mountain. This introduces uncertainty into the results of predictive models which use volumetrically averaged properties. However, the PRT believes that no significant advantage to model development, model validation, and fundamental understanding of the relevant TH processes can be gained from additional laboratory programs of property measurement in these areas.

The YMSCP in the White Paper (DOE, 1995a) has indicated that the following laboratory investigations will be undertaken: (1) thermally-driven fracture flow; (2) evaluation of heat pipes effects in fractured rock; (3) measurement of gas-phase buoyant convection; and (4) measurement of enhanced vapor diffusion. While each of these studies is believed to address several key issues related to model development and validation, the PRT suggests that experiments (3) and (4) should be of lower priority. The PRT also suggests the addition of the following investigations to the laboratory program: (1) measurement of matrix water relative permeability at various infiltration rates; (2) studies of steam-water countercurrent flow in single fractures and in fracture networks; (3) experimental verification of the critical rate concept for infiltration of a matrix-fracture system, and (4) continuation of the fracture healing experiments of Lin and Daly (1989b) to test their relevance under repository conditions and build confidence in THC models.

Field Tests. Field experiments and tests to address YMSCP needs in characterization and modeling have provided property data and measures of TH impacts on the host rock. The most important experiments have been conducted in G Tunnel at Rainier Mesa in the late 1980s and involved small diameter heater experiments, a heated block test, and thermohydrologic field tests (i.e., single heater experiments). The G-Tunnel experiments have considerable relevance to the Yucca Mountain site. They are in similar rock types, at a location quite near to the Yucca Mountain site, and they include experiments that were specifically instrumented to investigate TH processes at relevant temperatures. In fact, many of the TH concepts and theories that have recently been developed in the project emerged in response to the observations of boiling, vaporization, condensation and reflux observed in the G-Tunnel experiments.

In an effort to expand the understanding of TH phenomena at YM, a series of five *in situ* thermal experiments has been planned that will start in 1996 and continue beyond 2006. They include: (1) a Large Block Test (LBT); (2) Single Heater Test; (3) Drift Scale Test with Flatjacks (DSTFJ); (4) Spatially Distributed Single Heater Tests; and (5) Large-Scale Long-Duration Test (LSLD).

After a lengthy debate on the scientific and engineering merits of the LBT, the PRT concluded that this test addresses TH issues on length and time scales that lie in between the laboratory and *in situ* field tests. As such, the LBT should not be compared, or ranked, with other field activities. The PRT is aware that this test has been removed from consideration for funding in the FY96 budget, and that the test has certain shortcomings that are concerned with the low state of stress on the block. However, five of the six members of the PRT believe the LBT is well suited to investigate a number of important hypotheses that are concerned with the TH behavior of the Topopah Spring Tuff. We believe that this test should be supported and continued to completion. The dissenting member believes that the desired program of investigations could be better carried out in a controlled drift-scale program.

In the opinion of the PRT, the different Single Heater Tests and the Drift Scale Test with Flat Jacks (DSTFJ) can be considered intermediate scale underground tests, because of the similarities in objectives and overall testing plans. They have therefore been reviewed together as intermediate tests. The Single Heater Tests were designed to run for a 12-month heating period, and the DSTFJ was designed to run for an 18-month heating period. As will be discussed below in connection with the LSLD test, there are a number of critical problems facing the YMSCP that need to be addressed by thermally perturbing an appropriate volume of rock under conditions approximating that of the near field environment. The PRT does not believe it will be possible, using either single heater tests or the DSTFJ, to do this. In the opinion of the PRT, the heater tests are not needed. Five of the six members of the PRT recommend dropping the DSTFJ. The same dissenting member believes that, again with reference to the LBT, additonal testing is not warranted on this block and that an accelerated schedule of intermediate-scale underground testing with the DSTFJ would better serve the objectives of the YMSCP.

The PRT strongly supports the need for a large-scale, long-duration (LSLD) test. The process of increasing the temperature of a very large volume of the Topopah Spring Tuff, possibly up to maximum levels of about 200°C, raises some issues about rock system behavior, for which there is little or no field experience to serve as a guide to the expected response of the system. A number of complicated phenomena will occur, some interactively, as this highly fractured rock mass is thermally perturbed. It is the opinion of the PRT that these phenomena are unlikely to be sufficiently clarified by shorter, smaller tests, and that an LSLD test must be given the highest priority in the YM thermohydrologic testing program.

There are a significant number of critical issues that can only be addressed in an LSLD test. These include assessing: (1) whether the magnitude of infiltration will affect the whole thermohydrologic process; (2) whether the countercurrent heat pipe activity will actually develop; (3) whether condensation zones will actually coalesce; (4) whether dry-out zones will develop and coalesce; (5) whether the development of these various processes will be the same above the repository as they are below; (6) whether any of the above factors will be significantly affected by anisotropy of the fractured rock; and (7) whether the permeability of the Topapah Spring Tuff will be changed due to thermochemical and/or thermomechanical reactions.

The PRT believes that important results will be obtained from the LSLD, both from early and later results, and that subsequent analyses of the cumulative data will produce a picture that becomes increasingly more clear as those components of the controlling mechanisms are revealed. Therefore, the

PRT favors a flexible schedule. It could be that, during the heating period, sufficient results will be obtained more quickly than expected and the planned length can be shortened. On the other hand, with a flexible schedule, the planned length might have to be extended to achieve the desired goals.

5. MODELING

This section addresses the problem of the sufficiency of modeling and modeling approaches to predict moisture redistribution and changes in water chemistry in response to heat, which forms Part 3 of the PRT charge (see Table 1.2). To address these issues, we first present a review of past and present modeling efforts and then comment on their sufficiency. It is necessary to discuss several aspects of the process: (1) the modeling of the underlying fundamental physical processes in terms of the relevant equations at the small scale; (2) the modeling used for their representation at the numerical grid scale; (3) the actual numerical schemes used; and (4) various alternative models at other scales. Implicit to many of these exercises are the critical issues of scale-up, incorporation of heterogeneity effects, uncertainty in processes and parameters, and validation and calibration, which were also addressed previously in Section 3. It must be kept in mind that the accurate modeling of the THC response is constrained by: (1) the lack of physical understanding of some processes, as discussed above; (2) the uncertainty in site-characterization, as a result of the complex geology; and (3) computational limitations.

As emphasized in this report, predictions of thermohydrologic conditions during repository heating will have to be based on an analysis that includes consideration of irregular infiltration fluxes, development of time-dependent zones of saturation, the possibility of lateral flow in specific lithologic units, and the presence of channelized fast paths in discrete interconnected fracture systems. Of these, the "fast-path" issue bears directly on the equivalent-continuum concept, which is treated as a separate issue in Section 5.1.2 below.

It must also be pointed out that an additional modeling effort in the YMSCP includes performance-assessment modeling. Performance assessment models are used in the total system performance assessments (the most recent of which are TSPA-93 and TSPA-95) to determine whether a proposed repository design meets regulatory performance standards. These assessments incorporate simplified representations of the underlying process models in a probabilistic framework. The process models to be discussed below, however, are not directly incorporated into TSPA models. Rather, the results of process models are abstracted as response surfaces. The PRT has examined the TSPA documentation as a peripheral part of its charge, but a detailed assessment of TSPA models and codes is not part of its mandate. Hence, the emphasis in this portion of the report is on the process models used to improve process understanding and optimize repository design.

5.1 Past and Present Activities

5.1.1 Fundamental Physics

The variety of coupled processes in the thermal-hydrologic-mechanical-chemical (THMC) system has been summarized by Tsang (1987). Among these couplings, current emphasis in process-level modeling studies with the YMSCP includes thermal-only (T), thermo-hydrologic (TH), thermo-mechanical (TM), and thermo-hydrologic-chemical (THC) The TM and THC modeling capabilities are still at an early stage of development, and are discussed at the end of this section.

A description of the fundamental physics of the processes can be found in the report of Reeves et al., (1994). The degree of detail presented is considerable and includes state-of-the-art modeling of the various thermal and hydrologic aspects. Examples of the latter include vapor pressure lowering due to Kelvin effects in the tight matrix, and enhanced vapor diffusion. All relevant heat transfer modes are used, namely conduction, advection and natural convection. Hydrology is described in a conventional way, with the use of equilibrium capillary pressures and relative permeabilities for the matrix, while a similar description is possible for individual fractures.

In these models, important assumptions are made for some of the hydrologic processes, including the following:

(1). Little emphasis is placed on the dependence of capillary pressure, relative permeabilities and residual saturations on the direction of displacement (namely, whether it is drainage, imbibition, primary or secondary).

(2). Capillary pressures and relative permeabilities in the very tight TS matrix are assumed to obey a conventional van Genuchten model.

(3). The treatment of the hydrologic properties in faults and fractures places little emphasis on capillary effects and trapped saturations, associated with fracture roughness or with viscous-gravity instabilities.

(4). The flow of steam and water in the heat pipe region, where the two phases co-exist, is modeled with a relative permeability formalism directly borrowed from isothermal drainage displacement.

(5). Attention to the matrix-fracture interaction is limited.

(6). THC effects of the type discussed by Lin and Dailey (1989b) are not considered.

The limitations of these assumptions are discussed in more detail in Section 5.2.1.

5.1.2 Effective Models at the Numerical Grid-Scale: The Effective Continuum Model

Because of the obvious computational limitations, and in view of the highly heterogeneous nature of the site, the scale-up (averaging) of the fundamental equations to larger scales, both in space and time, is necessary. As discussed in Section 3, the typical grid scale of current numerical models is of the order of several tens of meters. Within such large grid blocks, a large number of intersecting fractures would exist, given that the typical linear size of a matrix block is of the order of a third of a meter or less. Hence, one is faced with the formidable problem of developing effective models that adequately capture the TH behavior at this scale. Furthermore, it is required that the degree of detail and resolution is much higher in the NFE, where complex two-phase water-steam flows develop, compared to regions in the far-field.

The main approach taken in solving this problem is based on the so-called Equivalent Continuum Model (ECM). This model has been the key tool for the current design philosophy of the YMSCP (see publications by Buscheck and Nitao). The basic ECM considers thermal and hydrologic coupling only. Chemical effects and THC coupling were recently introduced in a preliminary study of Robinson (1995), also in an ECM context. Mechanical effects and their coupling have not been systematically addressed. Because of the key role it plays, ECM is reviewed in some detail below.

The ECM is a single-continuum effective medium model. Standard conservation and transport laws for a single continuum (such as Darcy's law, Fourier's law and Fick's law) are assumed, but with coefficients (or coefficient functions) that attempt to capture the average behavior of the geological complexity. For their determination, two important approximations are inherently made:

(a). The fracture-matrix system of the TS tuff can be represented as an array of infinitely long vertical "columns" in 3D (or of inifinitely long vertical slabs of equal-size width in 2D) (Figures 5.1a-5.1c, which are idealizations of Figure 2 of Peters and Klavetter, 1988). The assumption implied is that fractures are parallel (and that they may or may not intersect each other, depending on whether the assumed geometry is that of "slabs" or "columns"). Clearly, such a geometric configuration is highly anisotropic.

(b). At each horizontal plane, capillary, thermal and chemical equilibrium exists in the matrix element contained between adjacent fractures (e.g., segment AB in Figure 5.1b) and between the matrix and the fractures. (Each such element in essence represents the individual matrix blocks of the more traditional dual porosity representation, Figure 5.1d). It follows that saturation, pressure, temperature and concentration profiles in each element are flat and that their response to transients is instantaneous. Appropriate coefficient functions can then be derived.

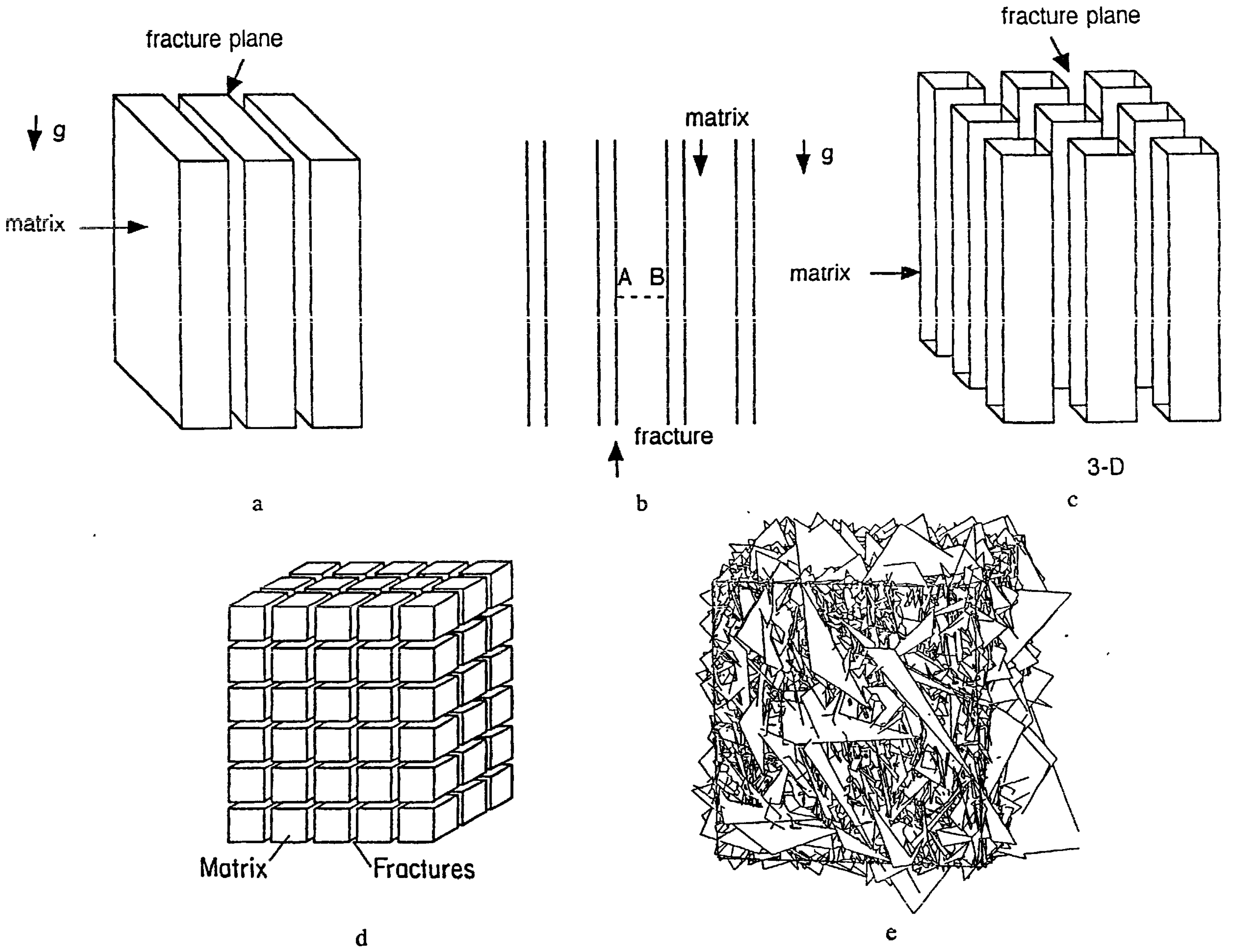


Figure 5.1. Conceptual geometries of the fracture network.

In the following, we briefly elaborate on the approach used for determining hydrologic and transport coefficients.

Hydrologic Coefficients

Because of its single-continuum nature, the ECM requires three hydraulic coefficients (or coefficient functions): (1) an effective single-phase flow permeability, k_{eff}; (2) an effective capillary pressure curve, $P_{c,eff}(S_{eff})$; and (3) an effective water relative permeability curve, $k_{rw}(S_{eff})$. In view of the geometric assumption (a), the effective *vertical* permeability is taken as the volume-fraction weighted arithmetic mean of the permeabilities of the matrix, k_m, and the fracture, k_{fr} ("conductances in parallel" model)

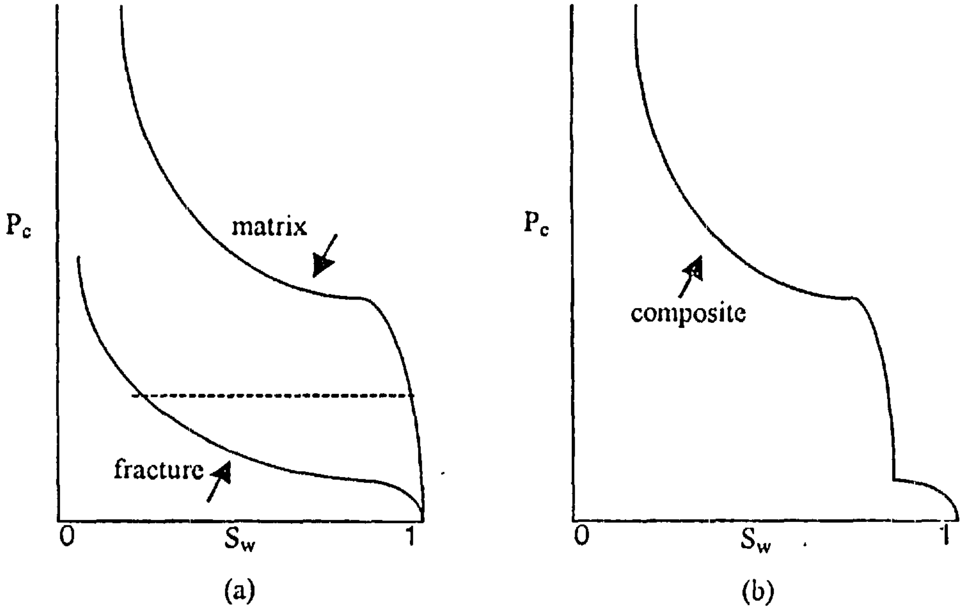
$$k_{eff} = [\phi_m k_m + \phi_{fr} k_{fr}]/[\phi_m + \phi_{fr}] \tag{5.1}$$

From the theory of networks of resistors, it is well known that this represents an upper bound estimate. More importantly, however, the ECM assigns the same value in (5.1) to every direction, even though the underlying geometry may be anisotropic. For example, consider the geometries of Figures 5.1a and 5.1b. In a self-consistent model, one component of the horizontal permeability of this system would be the harmonic average ("conductances-in-series" model). Then, for typical values, the ratio between horizontal and vertical permeability would be approximately equal to k_m/k_{fr}, which is very small $[O(10^{-6})]$, and which would suggest a very strong anisotropy. The implications for the accurate representation of transport in the various directions could be significant.

To calculate the effective capillary pressure, the individual capillary pressure curves of the matrix and fracture, $P_{c,m}$ and $P_{c,fr}$, respectively, are used (Figure 5.2). Because of the equilibrium assumption (b), saturations for the matrix, $S_m(P_{c,m})$, and the fracture, $S_{fr}(P_{c,fr})$ can be read at each level of capillary pressure, $P_{c,eff}=P_{c,m}=P_{c,fr}$. Then, the effective saturation is

$$S_{eff} = [\phi_m S_m(P_{c,eff}) + \phi_{fr} S_{fr}(P_{c,eff})]/[\phi_m + \phi_{fr}] \tag{5.2}$$

and the effective capillary pressure curve is obtained by inverting (5.2). Clearly, for a small volume fraction of fractures, $P_{c,eff}$ will be dominated by the matrix capillary pressure curve. This approach does not recognize possible non-equilibrium effects or the history (and direction) of the displacement process.



(a) (b)

Figure 5.2. Individual capillary pressure curves (a) and effective capillary pressure (b).

For the effective water relative permeabilities, a combination of the individual relative permeability curves in the matrix and the fracture, $k_{r,m}$ and $k_{r,fr}$, respectively, are used. Given a value of $P_{c,eff}$, hence of S_m and S_{fr}, the overall permeabilities $k_m k_{r,m}(S_m)$ and $k_{fr} k_{r,fr}(S_{fr})$, for water flow in the matrix and the fracture, respectively, are calculated. Then, the effective relative permeability curve, $k_{rw}(S_{eff})$, is the volume-fraction weighted arithmetic mean of the two water permeabilities

$$k_{rw}(S_{eff}) = [\phi_m \, k_m k_{r,m}(S_m) + \phi_{fr} \, k_{fr} k_{r,fr}(S_{fr})]/k_{eff} \tag{5.3}$$

using the same approach as in the derivation of (5.1) ("conductances in parallel" model). The resulting curve has a characteristic "double-hump" shape (Figure 5.3). As in single-phase flow, this representation overlooks the anisotropy inherent to the geometry of Figure 5.1. The above ECM approach neglects gravity and viscous effects, and does not allow for, or assume negligible, transport in the vertical direction within each matrix block. Furthermore, it is directly applied to steam-water flows undergoing possible phase changes, thus disregarding possible heat transfer couplings.

Transport Coefficients

In the ECM framework, effective transport (thermal and chemical) coefficients, such as thermal conductivity and mass diffusivity, are calculated as volume-fraction weighted arithmetic means, similar to equation (5.1). This approximation overestimates conduction in the matrix over convection in the fractures. However, this effect may be compensated (perhaps overly so) by the dominant role the fracture permeability plays in the computation of k_{eff}, which will lead to an exaggeration of the effective convective flux.

We should mention that another situation when there is a deviation in behavior occurs between equilibrium and non-equilibrium approaches during heating. For example, Buscheck and Nitao (1995b) compared equilibrium (ECM) versus non-equilibrium (FMM) conceptualizations at the drift-scale. At early times for cases with a relatively large bulk permeability (k_b = 280 millidarcy), the non-equilibrium approach, associated with the fracture-matrix model, indicated relatively rapid downward condensate drainage. These effects were not apparent with the ECM. With smaller bulk permeabilities and buoyant gas-phase conduction dominating the vapor flow, the ECM and the Fracture Matrix Model yield comparable results.

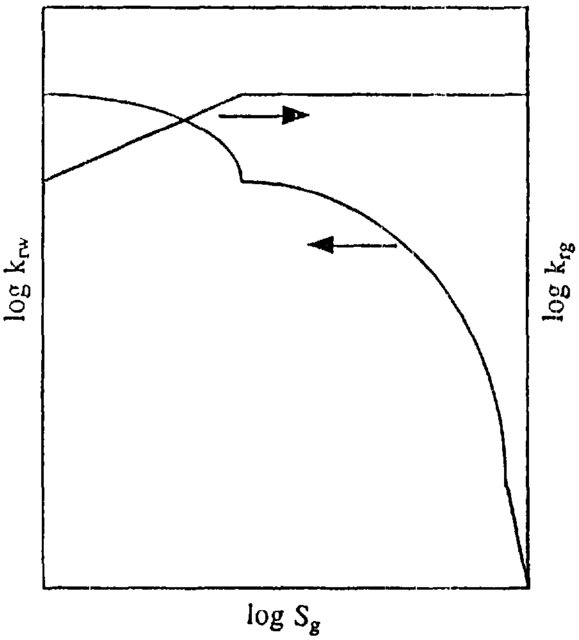


Figure 5.3. Effective relative permeabilities (adapted from Pruess et al., 1990).

The need to improve on the ECM and suggestions for its improvement are discussed in Section 5.2.

5.1.3 Existing Codes

In this section we review the relevant numerical codes that have been used in modeling the THMC response.

The thermal-only modeling, as represented most recently by the work of Ryder (1992) and Bahney and Doering (1994), considers conduction and radiation, but does not incorporate convective heat transport. It provides predictions of a conservative upper bound for temperature fields around the waste packages and in the adjacent host rock. It has little relevance to the expected thermohydrologic complexities that are the focus of this review, and for that reason the thermal-only codes are not reviewed in detail here.

The subsequent emphasis is on thermohydrologic (TH) modeling. The TH codes that are in current use in the program include TOUGH2 (at LBNL), V-TOUGH and NUFT (at LLNL), and FEHM (at LANL). The codes TOUGH2, V-TOUGH and NUFT are integrated finite difference (IFD) codes; FEHM is a finite element code. The code V-TOUGH is a vectorized version of TOUGH2. Applications at LBNL have tended to emphasize process understanding; those at LLNL primarily serve the needs of engineering design; and those at LANL highlight transport issues. Simulations have been carried out at the various labs on many scales, including drift-scale, repository-scale, and mountain- scale.

As noted by Pruess and Tsang (1994) and by Mishra (1995), all these codes have similar TH capabilities. They include two-phase fluid flow in aqueous and gas phases, heat transfer by conduction, and heat transfer by convection in both gas and water phases. Their treatment of capillarity, phase equilibrium, binary gas diffusion, latent-heat effects and vapor-pressure lowering are all similar. All four codes offer a variety of options for representing fracture-matrix interactions, including the equivalent-continuum formulation, the dual-porosity formulation, and the dual- permeability formulation. The three IFD codes also offer a more-generalized dual-porosity formulation known as the multiple-interacting-continua (MINC) approach. None of the codes has a true discrete-fracture option that allows for channelization of "fast-path" flow.

A full description of these codes is included in Reeves et al., (1994), which also recommends their continued use and development. Lingineni et al., (1995) provides a comparative assessment of TOUGH2 and FEHM. The codes have been fully documented, benchmarked against other codes, and verified against available analytical solutions. The benchmarking and verification includes heat-pipe problems, and problems specific to Yucca Mountain. However, it appears that all such tests were carried out with an ECM formulation using composite characteristic curves based on a van Genuchten representation of matrix and fracture properties.

In addition to their TH capabilities, the codes discussed above also have transport capabilities for radionuclides in both gas and liquid phases. Transport processes include advection, diffusion, dispersion, phase partitioning, and radioactive decay. At LANL, Robinson (1995) is in the early stages of adapting FEHM to handle geochemical rock-water interactions. He has coupled FEHM with a precipitation/dissolution module, and intends to use it to investigate fracture-sealing and fracture-opening mechanisms during thermohydrologic events. The enhanced code will require future documentation, benchmarking, verification, and validation against experimental results.

Emphasis in thermomechanical (TM) research is on mechanical impacts to porosity and permeability, especially as affected by changes to fracture apertures and distributions. Time did not permit a full discussion of thermomechanical modeling at the PRT meetings, but it is apparent that TM modeling is still in an early stage. Two codes were mentioned by Blair (1995b): FLAC, which is a 2D code, and ABAQUS, which is a 3D code. The FLAC code treats fractures in an ubiquitous manner, in which the material properties of the rock are adjusted to reflect the mechanical behavior of the combined rock and fracture. The FLAC code has been used in some preliminary studies of the mechanical behavior of the LBT in terms of the effect of the thermal field on stresses and displacements for a simple elastic model with and without fracture zones.

The ABAQUS code has been used in some preliminary studies of the 3D behavior of the LBT but without introducing fractures. The results produced 3D pictures of the thermal field and the effect on stresses and displacements of the LBT as an intact block of rock. The ABAQUS code uses a finite element formulation and can include fractures as discrete elements in 3D, so this code should be useful in modeling investigations of the fractured rock behavior in the LSLD test discussed above in Section 4. Blair has also been investigating rock failure with another thermomechanical code that uses a "field theory" model to analyze fracture of rock in compression, involving a statistical process of handling crack coalescence and fracture formation, and the effects of grain-scale heterogeneities on the macroscopic behavior of rock (Blair, 1994). This code is under development and should be useful in investigations of the nature of rock failure in the various formations at the YMP.

5.1.4 Dimensionality and Boundary Conditions

Modeling of hydrologic and thermohydrologic conditions in the YMSCP has been carried out in one, two, and three dimensions. Early 1D hydrologic analyses used measured borehole saturation profiles to calibrate models with respect to unsaturated formation properties. Early 1D TH formulations (Pruess and Wang, 1984; Tsang and Preuss, 1989) investigated the sensitivity of dryout to uncertainties in formation properties and upper boundary conditions.

The most meaningful 3D modeling at the site is hydrologic, rather than thermohydrologic in nature. LBNL in cooperation with the USGS developed a site-scale, three-dimensional model of the unsaturated zone at Yucca Mountain. The main objective is to investigate the feasibility of constructing a complex hydrologic model and of using that model for interpreting features of the hydrogeologic setting and for defining parameter values. Beyond the proof-of-concept work and scoping calculations that have been completed to date (Wittwer et al., 1995), the three-dimensional model is presently being used for a barometric pressure analysis, and to some extent to examine effects of repository heating (Bodvarsson, 1995). The model uses the TOUGH2 code with the ECM formulation. It has been used to investigate regional hydrologic issues, such as the role of faults and capillary barriers in creating perched zones and lateral flow, and the sensitivity of the moisture field to uniform and non-uniform infiltration.

Most TH modeling, however, has been done in 2D vertical cross-sections, in either radial or Cartesian coordinates (Buscheck and Nitao, 1992, 1993, 1994; Preuss and Tsang, 1993). Three-dimensional TH modeling has not been attempted due to the limitations of the computational grid size. The question is raised in the White Paper (DOE, 1995a) as to whether the lack of 3D TH simulation is a serious limitation for the program. This will be addressed below.

On the question of boundary conditions, issues arise both at the top and bottom of the system. It is necessary to specify both thermal and hydrologic conditions in both cases. At the top, the extent and duration of the condensate buildup will be very sensitive to the conditions specified on the upper boundary. In particular, the system will be sensitive to the spatial and temporal distribution of infiltration (see Section 3). Past simulations almost all use uniform average values rather than episodic patterns of infiltration. At the bottom, past simulations have tended to use an isothermal boundary condition located at the water table, which is assumed to remain in a stationary position. However, Buscheck and Nitao (1993) have shown that the thermal influence of the repository extends into the saturated zone. Furthermore, historical evidence suggests that water-table fluctuations may have exceeded 85 m or more over geologic time.

5.2 Sufficiency of Models

Sufficiency of models must be viewed in the following three contexts: (1) Do they contain an adequate description of the fundamental physical processes? Is the averaging at the numerical grid-scale, implicit to all computationally manageable models, adequate?; (2) Are the models developed validated and calibrated in the sense of Section 3? How do they account for the representation of the various heterogeneities and the reduction of uncertainty?; and (3) What are the effects of the various simplifications made? In this section we provide some answers to these questions and proceed with some recommendations. As in the case of the laboratory program, we comment on the relation of the proposed activities to resolving the Critical Issues of Section 3. The PRT believes that simultaneous efforts in many directions are needed.

5.2.1 Fundamental Physics

From the discussion in Section 5 1.1, the PRT finds that the present models are quite sufficient in the general description of the relevant physical processes. However, additional work is required in modeling some of the key processes identified above, and specifically on the following:

(1). The dependence of hydraulic properties on the direction of displacement, which can significantly impact the estimation of the capillary diffusivities, hence of the re-wetting times. As repeatedly emphasized, this issue is fundamental to the premise of the "extended dry repository", which was identified as a Critical Issue in Section 3.4.

(2). The investigation of relative permeabilities in the very tight TS matrix, where the current use of the van Genuchten model may be questionable. More generally, the project will benefit from an improved understanding of immiscible displacements in very tight porous media, in view of possible force interactions between the fluids and the pore walls in the tight pores of the matrix.

(3). The appropriate representation of the hydraulic properties of fractures and faults, with emphasis on capillary effects, trapped saturations and with viscous-gravity instabilities that can lead to channeling. This issue has significant implications for "fast paths", which appear to play a key role in the TH performance of the system, as discussed in Critical Issues 3.1.2 and 3.1.3.

(4). The modeling of the countercurrent flow of steam and water in the heat pipe region, particularly when the system under consideration is fractured. The current formalism, directly borrowed from isothermal drainage displacement, may be very inadequate in this context.

(5). More generally, the knowledge and modeling of two-phase flows in the matrix-fracture system must be improved. Issues (4)-(5) are of fundamental importance as they relate to the distribution of moisture in the dryout region, and could affect one key premise of the "extended dry repository" concept, criticised by Pruess and Tsang (1994), and also identified as Critical Issue 3.2.

(6) Finally, THMC effects of the type discussed by Lin and Dailey (1989b) should be further investigated and properly incorporated in the model, if found warranted.

We point out that the investigations above are intimately coupled with the laboratory investigations proposed in Section 4.4.2. These two programs should run in parallel and interactively.

5.2.2 Effective Models

Effective models at the numerical grid-scale address the important issue of scale-up, which was identified as Critical Issue 3.1.6. As pointed out above, the only effective model developed for the YMSCP is the ECM, based on two assumptions, one related to the perceived geometry, and the other related to matrix-fracture equilibrium. We discuss below in some detail the validity of these assumptions and their possible consequences if they are violated.

The validity of the geometric assumption is certainly a problem in fracture characterization. The current ECM approach for the evaluation of effective properties is correct regarding the "vertical" direction for either of the geometries of Figures 5.1a-5.1c (although not for those of Figures 5.1d-5.1e). If one were to accept the geometry of long, parallel, unconnected fractures (Figure 5.1a), one component of the "horizontal" permeability should be the harmonic average. As pointed out above, for typical values,this would imply a strong anisotropy, contrary to the assumption of isotropy inherent to the present version of ECM.

If one were to accept the geometry of Fig. 5.1c, in which long vertical fractures regularly intersect one another, the "horizontal" permeability should be calculated from the effective conductance of a two-dimensional (square) lattice of conductors. The resulting anisotropy would be less than in the previous case, but still significant, particularly if the distribution of fracture conductivities is broad. An analogous calculation would apply to the geometry of Figure 5.1d. Current evidence supports the notion of long, vertical fractures. However, analogues with the intensely fractured Stripa site, where the fractures are interconnected with varying angles (Figure 5.1e), have also been mentioned (Pruess et al., 1995). By assuming isotropy, ECM overestimates horizontal flow (and convection) and underestimates focussed flow in vertical fast paths, the importance of which was stressed by Pruess and Tsang (1994).

Capillary effects would also be affected by the assumed network coordination. For example, although at first glance, the derivation of (5.2) appears to be independent of assumption (a), a more careful analysis, reveals that the limited connectivity between the various blocks may lead to large-scale trapping and large-scale residual saturations, even under the assumption of capillary equilibrium. Such features are lost in the ECM, where connectivity is perfect (elements arranged in parallel). An analogous result would occur with the effective relative permeabilities.

The other key premise of ECM is capillary equilibrium, implying flat pressure profiles in the matrix and the fracture and their instantaneous response to applied transients. The first condition is satisfied when viscous or gravity forces are sufficiently small, compared to capillarity. In dimensionless terms, this is equivalent to requiring sufficiently small values of the capillary number, $Ca=u\mu/\gamma$, and the gravity number, $B=g\Delta\rho\ k/\gamma$. A satisfactory estimate of an upper limit of Ca is obtained by using the critical velocity q^*, of Chapter 3, above which liquid water infiltrates the fracture faster than the matrix. The condition should be implemented as a check in future ECM models.

Likewise the constraint of a small gravity number would be readily satisfied for the matrix (where the permeability is very small). On the other hand, viscous and gravity forces could dominate over capillarity in the (vertical) fractures, leading to channeling and a violation of the ECM premise of capillary equilibrium. This possible problem could be of great concern regarding the applicability of ECM in modeling infiltration or the countercurrent flow in heat pipes. Finally, the requirement of an "instantaneous" response to applied transients would be satisfied when the ratio of the characteristic time for capillary diffusion in the matrix, L^2/D_m, to that of the applied disturbance is small. In the opposite case, important transient effects will be misrepresented, particularly if the numerical time increment exceeds their characteristic time. This could be of potential significance in the context of episodic infiltration events.

Regarding effective transport (thermal and chemical) coefficients, such as thermal conductivity and mass diffusivity, in the ECM framework, we recall that these are also volume-fraction weighted arithmetic means, similar to (5.1). The approximation overestimates conduction in the matrix over convection in the fractures, although as mentioned above, there is the countereffect from the dominant role of the fracture permeability in the computation of k_{eff}, which exaggerates the effective convective flux. Flow anisotropy will also affect the thermal convection, which controls heat transfer in the vapor-liquid zone. Consideration of a fracture network of finite connectivity is perhaps necessary for a more accurate assesment of all these approximations.

The validity of thermal and chemical equilibrium can be assessed in a fashion similar to capillary equilibrium. For flat temperature or concentration profiles in the matrix to exist, the appropriate Peclet number, $Pe=uL/D_i$, where D_i is diffusivity (thermal or mass), must be sufficiently small. We can derive an upper bound for this, in analogy to the critical velocity q^* of Chapter 2 for capillary equilibrium. In fact, equation (3.1) is directly applicable, if we consider single-phase flow and use D_i in place of D_m. Given that $D_m < D_T$, where D_T is the thermal diffusivity, thermal equilibrium is certain as long as capillary equilibrium exists. On the other hand, this would certainly not be true for chemical equilibrium, where the mass diffusivity can be much smaller than capillary diffusivity. For the same reasons, transient effects are likely to be important in chemical transport. The consequences of this lack of equilibrium in the ECM modeling of the THC coupling can be significant.

The ECM appears to be a reasonable first approach to the complex TH problem of the YMSCP. It certainly gives a first order qualitative picture of the major features expected to develop during the life of the project and provides the "average" response of the system. In fact, in a recent study of infiltration (Bodvarsson, 1995), it was found to compare well with a particular dual-porosity/dual-permeability model. However, it was found less satisfactory in matching the results of the G-tunnel tests, where recourse to discrete fracture modeling was necessary (Nitao and Buscheck, 1995) to explain the experimental findings adequately. Some critics of the ECM (Pruess and Tsang, 1994) have pointed out that the model may severely underpredict the degree of "focusing" of condensed water in fractures, which can greatly increase the probability that the canisters will become wet. To this committee, the ECM quantitative predictions, particularly as they impact the design of the project, should be accepted with a great degree of caution.

To further build confidence in model predictions, the PRT suggests that further studies be conducted to improve the current methods of scale-up implicit in the ECM. Such studies should include the following:

(1). Provision for non-equilibrium matrix-fracture transport, particularly for fluid flow, but also for chemical and thermal transport. Conditions for the existence of this regime should be developed, in conjunction with the investigations in Sections 4.2.2 and 5.2.1. Following the onset of flow and transport in the fractures, an alternative to ECM must be sought (perhaps in the form of a hybrid ECM-double porosity model), that would also recognize the potential of viscous- or gravity-dominated flow in fractures and other fast paths (such as faults).

(2). Even under conditions of equilibrium, the ECM method of evaluating hydraulic and transport coefficients, analyzed in Section 5.1, must be revisited to properly account for possible anisotropic and fracture network connectivity effects. The effect of possible wide distributions and spatial correlations in the hydraulic properties of the fractures must also be carefully incorporated.

(3). Development of novel up-scaling techniques to simulate flow and transport. A possible approach in this direction is the use of small perturbation theory of the type discussed by Gelhar and Axness (1983) for miscible displacements. Other possibilities include the use of homogenization approaches. These are likely to result in dual continuum models.

5.2.3 Existing Codes

The question remains unresolved as to whether the ECM can continue to form the basis for further analyses. Clearly, comparisons between non-equilibrium and ECM conceptualizations are the first step to establish the overall validity of the present modeling approaches. Such an analysis may show that it is appropriate within certain limitations to utilize the ECM-type models. If the ECM method turns out to be inadequate, it will be necessary to undertake dual-porosity or other kinds of simulations to represent the physics of fracture-matrix interactions in a more rigorous manner

It could be argued that none of the models discussed in Section 5.1.3 has been validated for a full thermohydrologic application that includes boiling, dryout, condensation and reflux. The closest attempt is that described by Nitao and Buscheck (1995) in his reassessment of the G-tunnel heater experiments. This exercise and the more general issues associated with validation and calibration were also discussed in Section 3. However, it must be pointed out here, that an implication of the equilibrium model is that virtually all of the codes based on equivalent continuum concepts are calibrated with much lower infiltration rates than those apparently being measured in the field. There appears to be legitimate concerns that some cases of flow may be better represented by a non-equilibrium conceptualization fracture-matrix interactions. Yet, there has not been a major effort to accommodate non-equilibrium assumptions in the large-scale calculational models.

In examining the question of model sufficiency, the PRT has concluded that there is an urgent need to settle on a modeling approach that overcomes or a least can put in some perspective the problems of the ECM discussed above. If the ECM approach turns out not to be appropriate, then analyses conducted with the model will be suspect. The YMSCP has made good progress in eliminating duplication of model effort, yet all of the key computational codes are essentially the same in their treatment of the ECM. Before moving forward on various "applied" fronts (e.g., repository designs, likely performance, test designs etc.), there must be a dedicated effort to resolve the ECM-related issues. It is likely that continued application of these ECM-based computational models in an "applied" mode will not now yield the same kind of important benefits that came from the earlier work.

Future code enhancements that are required would be best made within the framework of the existing computational codes (FEHM, NUFT, TOUGH2). Thus, in most respects, our analysis of how the existing codes should be used and extended are in agreement with the following recommendations made by Reeves et al. (1994):

(1) Current models address program requirements sufficiently well that they should be used as host structures for future development. The development of new stand-alone models should be curtailed, and the limited available resources should be focussed on upgrading existing codes.

(2) Future model development should consider simulation capability for non-equilibrium fracture-matrix flow.

(3) Efforts should be made to substantially improve computational efficiency through software improvements, including those appropriate for massive parallelization.

We have the following remarks on more specific items.

The prediction of large scale geochemical effects on repository behavior requires the coupling of thermal, hydrologic and chemical (THC) processes. Numerical models capable of describing these processes are currently very preliminary. As an initial step, Robinson (1995) utilized the numerical model FEHM, in the effective continuum mode, to explore the effects of silica dissolution and precipitation on the repository rocks. The work is unique in its attempt to account for effects of mineral dissolution and precipitation. However, a number of simplifying assumptions were required to conduct the computations. These involved the mechanisms of dissolution and precipitation, thermal load boundary conditions, the relationship between permeability and porosity, and the hydrologic properties of the rocks (assumed to be equivalent to densely welded Topopah Spring Tuff). The results suggest that there will be an overall redistribution of silica with precipitation occurring near the repository and dissolution occurring at greater distances. According to Robinson (1995), these changes will lead to an increase in the size of the dryout zone over that predicted from only thermal and hydrologic considerations.

At present, major components of the conceptualization of the chemical processes have not been validated by experiments. Hence, the conclusions must be viewed with a great deal of caution as they are likely to be very sensitive to the input conditions. Given the PRT's understanding of the proposed experimental plans and budget limitations, it is likely that the first data appropriate for such a calibration exercise may come from large-scale, long-duration testing in the ESF. Further progress in the area of thermochemical modeling will require complimentary laboratory and field-experimental data.

Given the relatively limited work related to THC processes, the PRT cannot assess how important these processes are to the overall performance of the repository system. However, simply lacking knowledge about the THC processes is not justification for assuming them to be unimportant. The PRT believes that there remain possibilities for significant "surprises" associated with THC processes. In view of the difficulties of developing a rigorous model-based approach, THC problems could be addressed with bounding analyses similar to those of Pruess and Tsang (1994) and field experiments. In particular, the design and implementation of the large underground experiments will provide a strong initiative to sort out issues related to THC coupling.

The status of thermomechanical modeling is similar to that of the thermochemical modeling. Codes like FLAC and ABAQUS are available and have been used to model features of the LBT. However, these codes have largely not been validated for the problems facing the YMSCP. Because of the coupled effect between changes in fracture aperture and fluid flow, codes like ABAQUS would need to be expanded to include the capability of handling hydraulic behavior. Possibilities of coupling ABAQUS to TOUGH2 were mentioned as one approach to providing a full-featured THM code. However, as in the situation with THC processes, it is questionable whether such a code, even if developed, could be validated, given the relatively limited knowledge about the mechanical behavior of the in-place rocks at Yucca Mountain under the influence of a thermal field.

Nevertheless, the PRT is concerned that the limited knowledge about THM processes is not sufficient for the purposes of assessing site suitability, and moving forward with licensing. As is the case with the THC processes, there is, in our opinion, no scientific basis for simply assuming that mechanical effects are unimportant, especially considering the magnitude of the large AMLs. In view of the overall direction and timing of the YMSCP, the most appropriate approach to questions posed by THM coupling will reside with bounding calculations and a detailed examination of results from field studies.

5.2.4 Dimensionality and Boundary Conditions

On the issue of dimensionality, it is obvious that the question involves a tradeoff of dimension versus detail. It is also a matter of scale. It is unlikely that 3D mountain-scale TH modeling will become feasible in the near future. The PRT concurs with Pruess et al. (1995) that at this scale, some of the other shortcomings of TH modeling, primarily those associated with the ECM representation, are of greater concern than dimensionality. His suggestion, wherein 2D vertical sections for TH simulation are taken from the 3D mountain-scale hydrologic model, seems reasonable. However, one should be cautioned that in immiscible flows, the effects of gravity can be misrepresented in x-z vertical cross-sections, compared to r-z cross-sections. The latter allows for an effective 3D connectivity, which is absent from x-z models. In addition, in some of the smaller-scale applications, there are 3D effects that cannot be captured in a 2D formulation. The PRT believes that 3D TH simulations will be required for proper test design of *in situ* experiments, and for meaningful model validation using the data generated from such experiments. In another context, process-level investigations of channelization and the preferential development of "fast paths" in interconnected fracture networks may also require 3D simulation.

We also note that hybrid modeling approaches deserve attention. One example would be the use of quasi-3D rather than full-3D formalizations (i.e. 2D numerical simulations with 1D analytical linkages). A second example might be the carrying out of mass-transport or geochemical calculations in 1D streamtubes identified from higher-dimensional hydrologic simulations. One direction that future work is proceeding is in modeling the barometric response within the mountain as a function of changing conditions at the surface. The PRT believes that the preliminary calibration of the model to observed barometric data has provided an important check on parameter values selected for near-surface units.

The case for representing recharge and other flow conditions in a physically correct manner has been made before. Preuss and Tsang (1994) examine the implications for channelized flow in reducing the benefits of dryout, and causing local flow through the repository. If indeed field studies are able to demonstrate locally high recharge that promotes flow along fractures, they will require that mountain-scale design models accurately reflect the total water fluxes through the mountain. Thus, although uncertainty remains concerning recharge and fast fracture flow, steps can be taken with the modeling to more thoroughly investigate these effects in relation to repository heating.

Future modeling will need to understand the apparent disconnect that exists between the field-based estimates of recharge and those lower estimates that come via model calibration. The need to validate the concept of fast fracture flow that has been discussed at length throughout this report is also pertinent to the effort here. Opportunities exist within the context of the LBL/USGS model to examine this question more fully. The PRT agrees with Bodvarrson's assessment (1995) about the importance of using data like barometric pressure, which have yet to be used explicitly in model calibration. Models provide an ideal way to integrate diverse data of all kinds.

Finally, the PRT recommends that future modeling efforts further investigate the sensitivity of the thermohydrologic response to the upper and lower boundary conditions. The heat source at the repository horizon also represents an imposed boundary condition. Comparisons of repository and mountain-scale simulations, that use a smeared heat source against drift-scale simulations that use a more detailed representation of individual waste packages, indicate that the smeared source may overpredict the temporal persistence of thermal effects. Thus, the PRT also recommends further sensitivity analyses of these alternative heat-source representations.

5.2.5 Calibration and Validation

The PRT expects that it should be possible to enhance the validation of thermohydrologic models in conjunction with the large scale thermal testing projects in the ESF. One of the original objectives of the large block test (LBT) was to perform such model validation. At this stage of the project, these validation exercises are extremely important because they represent the best possible test of our basic understanding of thermohydrologic processes.

Scoping calculations have been conducted with respect to proposed tests in the ESF. These calculations are being used to assure that the tests are of a sufficient size to observe coupled thermohydrologic processes at a scale that is relevant to repository conditions (Buscheck and Nitao, 1995a). The PRT recommends that these calculations be repeated when more detailed pre-test data become available. We believe that it will be important to build into the ESF program a more rigorous test of the validity of current understanding of thermohydrologic processes.

Field tests can also allow calibration against TH parameter values. More important, however, than simply achieving calibration with these tests is the manner in which calibration is achieved. A rigorous comparison of observations with a priori predictions is required. Posterior calibration of the observed test results to various models is helpful but not a sufficient test of predictive capability of thermohydrologic codes.

There are precedents for using rigorous procedures associated with tests to demonstrate modeling capabilities. Examples include:

(1) a test of the ability to predict flow in a fractured system, undertaken during the construction of the shaft at the Underground Research Laboratory (URL) by Atomic Energy of Canada Limited, and

(2) a test of the ability of discrete fracture models to predict the inflow to a drift in the STRIPA mine by the STRIPA International Project.

5.2.6 Uncertainty Analysis

In Section 3.4, we reviewed the different types of uncertainty. Arguments are made there that it will be difficult to quantify the degree of uncertainty reduction that will be acheived for process uncertainties through laboratory and field testing. Further, the argument is made that classical geostatistical analysis of geological and parameter uncertainties will be hindered by the sparseness of the available data base.

An alternative approach to full uncertainty analysis is a hypothesis-testing approach in a decision framework. This is a more pragmatic style that recognizes that uncertainty reduction only has value insofar as it meets the programmatic needs outlined in Chapter 2. In this context, uncertainty need only be reduced to a level that allows regulatory-acceptable decisions to be made with respect to repository thermal loading, waste-package canister composition, and site suitability. Sensitivity analysis is used to determine which uncertainties matter and which do not, and also to identify critical performance measures. These performance measures may relate to processes, parameters, or geological configurations. Results from site-characterization activities, including the exploratory drilling program, ESF studies, and the *in situ* experiments, are then interpreted in a hypothesis-testing mode relative to the performance measures. For example, Buscheck and Nitao (1993) outline a set of hypotheses suitable for testing with an *in situ* thermo-hydrologic experiment. Another example of this approach could be built around the observations of Bodvarsson et al. (1994), based on modeling, that permeable faults lead to significantly different saturation fields adjacent to the faults than do capillary-barrier faults. Hypotheses about fault behaviour could therefore be tested by making saturation measurements nearby.

There is a close relationship between uncertainty reduction and model calibration and validation. Model validation reflects reduction in process uncertainties. Model calibration reflects reduction in parameter uncertainties and geological uncertainties. The process should be viewed as ongoing, iterative, and cyclical, with models used to design experiments, and experimental results used to update models, both in terms of process descriptions and parameter values.

5.3 Summary

The question of whether the models and modeling approaches that have been developed for the YMSCP are sufficient to predict moisture redistribution and changes in water chemistry as a result of the effects of heat are examined in Section 5. The starting point begins with a review of the past and present modeling activities, which focuses on: (1) the fundamental physics that are represented in the models; (2) the use of an effective continuum approach for upscaling basic properties to computational grid sizes of several tens of meters; (3) the implementation of the concepts in a variety of THMC codes; and (4) decisions taken with regard to dimensionality and boundary conditions.

In terms of fundamental physics, most of the effort has been directed toward developing codes to represent thermal-only (T) and thermo-hydrologic (TH) processes. There has been some progress in thermo-mechanical (TM) and thermo-hydrologic-chemical modeling (THC), but essentially no progress on other types of complex coupling (e.g., THM and THMC). Codes developed for TH modeling are detailed and complete in terms of the coverage of the relevant processes. Like all models, however, they depend upon simplifying assumptions to represent the rock system.

One of the difficult steps in any modeling effort is to represent the heterogeneous nature of the hydrogeologic system at the scale of the computational grid. The main approach adopted for scaling up to the grid scale is based on the concept of an equivalent continuum (ECM). The ECM approach utilizes standard conservation and transport laws for a single continuum with coefficients that are designed to capture the geological and hydrogeological complexity. Inherent in this approach are assumptions about geometry of the fracture-matrix system, and the nature of fracture-matrix interactions. These assumptions provide the basis for defining an effective permeability, k_{eff}, an effective capillary pressure curve, $P_{c,eff}(S_{eff})$, an effective water relative permeability curve, $k_{rw}(S_{eff})$, and various transport coefficients.

The processes and scaling models are represented in various TH models (e.g., FEHM, NUFT, TOUGH2) that are used at the drift, repository, and mountain scales. The codes have been reviewed in detail by Reeves et al. (1994) and cross-verified in a variety of tests. However, work to date has not examined the efficacy of the ECM approach. There has been initial developmental work in THC modeling at LANL by Robinson (1995), and in TM modeling at LLNL with the FLAC and ABAQUS codes (Blair, 1995b).

In evaluating the sufficiency of the modeling approach in the area of fundamental physics, the PRT finds the models to be largely comprehensive in their treatment of processes. There are details of the modeling approach such as: the estimation of capillary diffusivities, relative permeabilities in the tight TSw matrix, the treatment of trapping and instabilities, the nature of counter current flow in heat pipes, the general treatment of two-phase flow, and THMC effects, which need to be studied in more detail. The PRT finds that the ECM model could be applied under some restrictive conditions at Yucca Mountain, and provides a useful qualitative approach to complex TH problems. The ECM is not, however, general and is likely to be inadequate for many types of fracture-rock geometries, as well as conditions where non-equilibrium fracture-matrix interactions develop. In the opinion of the PRT, the ECM quantitative predictions, particularly where they impact the design of underground projects, should be accepted with a great deal of caution.

The main computational codes (FEHM, NUFT and TOUGH2) have undergone extensive development and verification. The next step in their use, however, should involve investigations, primarily in underground tests, where the efficacy of ECM can be carefully examined. Given the apparent limitations of the ECM, further applications of these models would appear to be inappropriatewithout such confirmation. The THC and TM modeling is not sufficiently advanced, and the PRT believes it will be difficult to validate these codes in a timely manner. This situation, however, does not imply that THC and TM issues are not important, but that other alternatives (e.g., bounding calculations or field experiments) may simultaneously be required to meet program needs.

The PRT finds that the present use of 2D and 3D models is generally appropriate. Specific issues of experimental design and fast-fracture pathways will likely involve a more rigorous 3D treatment. Additional work in representing features of the upper and lower boundaries of the global system appears to be warranted.

6. RECOMMENDATIONS

This section summarizes the PRT recommendations with respect to the laboratory and field testing program, and with respect to modeling activities. The recommendations derive from the detailed discussions contained in Sections 3,4 and 5. Following the recommendations on strictly technical issues, we comment briefly on some programmatic issues.

On the technical front, the PRT believes that activities in all three facets of the laboratory and field program, namely site characterization, laboratory-scale processes, and field tests must continue. There is a need for a balanced approach in all these three elements. The next three subsections summarize our recommendations under these headings.

6.1 Site Characterization

The PRT believes that the following four programs, currently underway, must be continued without any significant reduction in effort:

(1). Measurement and interpretation of infiltration rates at the ground surface and in the shallow subsurface formations over Yucca Mountain.

(2). Analysis and interpretation of water samples using geochemical age dating techniques based on ^{36}Cl and ^{14}C.

(3). Air injection and pneumatic testing program to determine large-scale permeability distributions in the various lithographic units and fault zones in the mountain.

(4). Geological mapping, and borehole drilling program in the ESF, with special emphasis on assessing fracture and fault heterogeneity and connectivity.

In addition, the PRT has identified an additional site characterization program that we believe would have significant merit. We recommend initiation of the following program:

(5). Tracer tests, using vapor-phase tracers in ESF boreholes, to identify and asssess "fast paths", in the fractured repository host rocks.

Lastly, the PRT recognizes the value of the following program to site-characterization efforts, and recommends its continuation:

(6). Natural analogue studies of geothermal sites such as the Geysers, or those under study in New Zealand.

The rationale for the first five recommendations is given in Sections 4.1 and 4.4.1. The PRT gives these activities a high priority, more or less equal to that of the LSLD *in situ* field test (see Section 6.3). The sixth activity recommended above has a somewhat lower priority than the other five. Site characterization activities should be carefully integrated with laboratory and field experiments, with emphasis on a hypothesis-testing approach designed to lead to a better understanding of fracture-matrix interactions, fast paths, and infiltration under the impact of thermal loads

6.2 Laboratory Tests

The laboratory-testing effort within the YMSCP has two facets: (a) the testing of rock properties, and (b) the testing of processes related to TH, THC or TM coupling. The PRT believes that significant reductions have been achieved at this stage of the program with respect to property measurements. In particular, thermal and mechanical bulk-rock properties are now sufficiently well known to allow curtailments in these areas. Hydrologic properties, on the other hand, are still highly uncertain for the various rock types. We therefore recommend continuation and enhancement of the following program:

(7). Measurement and interpretation of hydrologic rock-matrix properties, including relative-permeability functions and capillary-pressure vs. saturation curves, with emphasis on differences between wetting and drying, and between primary and secondary imbibition, and on the appropriateness of the van Genuchten representation of the characteristic curves.

Process-oriented laboratory investigations should continue. They provide fundamental understanding of the THMC processes and the testing of various hypotheses and new models. Furthermore, they constitute the least expensive aspect of the program, while having a signifigant impact on the overall project. In addition, they indirectly provide for the continuing support of a scientific base, which must be maintained, despite temporary budgetary problems.

Of the four laboratory experiments proposed in the White Paper, the PRT believes that two have particular merit. These are described as experiments (1) and (2) in Section 4.2.2 of this report. We therefore recommend that these experiments proceed:

(8). Thermally-driven fracture flow test (Figure 4.1a).

(9). Laboratory evaluation of heat pipes in fractured rock (Figures 4.1b and 4.1c).

We do not recommend that experiments (3) and (4) from Section 4.2.2 proceed These experiments, on bouyant-phase gas flow, and enhanced vapor diffusion, have much lower priority in our opinion. Experiment (3) has a radionuclide-transport component that may have relevance to other parties within the YMSCP, but it is not directly related to the TH issues that are the focus of this PRT.

The PRT recommends the following new process-oriented laboratory experiment:

(10). Experimental verification of the concept of a critical rate, q*, during infiltration of a fracture-matrix system.

The rationale for these recommendations, and more detailed descriptions of the tests, can be found in Sections 4.2 and 4.4.2. The PRT gives these activities a high priority.

The above process-oriented laboratory activities relate to TH coupling. There is also the question of THC and TM coupling. On the THC front, the PRT was impressed with the experimental work of Lin et al. (DOE,1995a) and recommends the following enhanced experimental program:

(11). Continuation of laboratory fracture-healing experiments, but with a stronger attempt to show relevance to Yucca Mountain conditions, and particularly the chemical processes associated with a heat pipe. In addition, the effects of mineral deposition at the fracture-matrix boundary should be investigated in the same experimental framework.

On the TM front, it is the opinion of the PRT that experimental studies of the effects of TM coupling on permeability are ongoing at many research centers elsewhere, and that there is little need for process-level thermomechanical laboratory experiments within the YMSCP. The TM component of the LSLD (section 6.3) should meet project needs.

6.3 Field Tests

The five field experiments proposed in the White Paper are listed in Section 4.3.2 of this report and are further assessed in section 4.4.3. The PRT is unanimous in its primary recommendation, which gives the highest priority, in terms of all TH activities, to the following *in situ* field test:

(12). Carry out the large-scale, long-duration (LSLD) *in situ* field test in the ESF.

Our reasons are straightforward. There are a significant number of critical issues that can only be addressed in an LSLD test. These include assessing: (1) whether the magnitude of infiltration will affect the whole thermohydrologic process; (2) whether the countercurrent heat pipe activity will actually develop; (3) whether condensation zones will actually coalesce; (4) whether dry-out zones will develop and coalesce; (5) whether the development of these various processes will be the same above the repository as they are below; (6) whether any of the above factors will be significantly affected by anisotropy of the fractured rock; and (7) whether the permeability of the TS fractured tuff will change due to thermochemical and/or thermomechanical reactions.

Assuming the results of the large scale test portrayed in Figure 4.3 are a reasonable approximation, it is clear that the effects listed above take place over a cross-sectional area about 30 m in diameter. (The thermal field, of course, would be far larger.) We believe the key to an understanding of the controlling physics of repository response will be learned from the data and observations that can be collected in a region of this scale, or even larger. The response should enable DOE to decide how to proceed with the YMSCP. We do not see how critical design decisions can be made using smaller tests, because the volume of rock being thermally perturbed is too small to develop the effects that reveal the "global" picture.

The costs and time required to carry out the LSLD will be substantial, and the PRT realizes that this will be a major problem for management. It must be clearly understood, however, that DOE is involved in a major undertaking involving the thermohydrologic behavior of a fractured rock mass for which there is no precedent experience. As such, one cannot expect to be able to anticipate all aspects of this behavior; there are bound to be surprises. By setting up a long-term experiment, a substantial data base can be acquired. The analysis of this data can begin almost immediately after the experiment begins, because experience with underground thermal tests on rocks indicates that changes in behavior occur rapidly at the beginning of such a test. However the long-term data is equally important, and the PRT encourages a flexibly-scheduled test of sufficient length to insure that all TH processes are fully measured and understood.

It is the opinion of the PRT that a very wide use will be made of the data collected from the LSLD test in repository design, canister design, and the determination of thermal loading strategies. There is the potential to realize significant economies depending on results obtained from this test.

The PRT was also unanimous in favoring a "walk-before-you-run" test, prior to the LSLD test, at a scale intermediate between the process-oriented laboratory tests and the LSLD test. Firstly, there is a need to test and prove out instrumentation. Second, such a test would provide an opportunity to further validate TH numerical models before using such models to design the LSLD test. And lastly, an intermediate scale test would provide preliminary indications of the size and timing of the TH phenomena to be expected in the LSLD test, thus allowing for an improved design, and an enhanced probability of success for this major experiment on which so much rests.

The possibilities for this intermediate-scale test include: (1) Single-heater test; (2) Two spatially-distributed single-heater tests; (3) Large-block test; and (4) Drift-scale test with flatjacks. The PRT discards the first two of these as being of insufficient size to insure the full development of all the relevant TH processes cited above. Of the two remaining, five of us prefer the large-block test, and one of us, the drift-scale test. On this basis, then, we recommend:

(13). Reinstatement of the large-block test into the TH program at Yucca Mountain.

The LBT has the advantage that it is almost ready to go and would provide timely results. It is suitable for equipment and model testing. The LBT suffers in comparison with the drift-scale test, in terms of representativeness. The minority opinion is that the lack of representativeness is sufficiently severe to disqualify the worth of the test. The majority are not particularly strong in their preference of the LBT over the drift scale experiment. The LBT is not held to be indispensible, but it is held to be valuable, and given the investment already made, cost effective.

The PRT is firm in their position that in no way can either the large-block test or the drift-scale test be considered as a suitable substitute for the LSLD test.

6.4 Modeling

The rationale for the recommendations in this section can be found in Section 5 of the report, and particularly in Section 5.2. We first state our recommendations and then discuss some of them in greater detail below.

(14). The PRT concurs with the findings of Reeves et al., (1994) that current TH computer codes address program requirements sufficiently well that they should be used as host structures for future development. Available resources should be focussed on enhancing existing codes, rather than developing new stand-alone codes. (See Section 5.2.3.).

(15). Enhancements are needed in existing TH codes to improve their representation of the fundamental physics, with respect to: (a) anisotropy of flow processes in matrix-fracture systems; (b) two-phase steam-water flow in matrix-fracture systems, with special emphasis on capillary effects and two-phase flow instabilities; and (c) representation of channeling and fast-path flow due to heterogeneities in the fracture network. (see Section 5.2.1.)

(16). The conditions under which the ECM approximation is valid must be investigated and identified. Under those conditions where it is not valid, alternative modeling approaches must be developed that do not rely on the ECM assumptions with respect to geometry, averaging of coefficients across grid blocks, and equilibrium between fractures and matrix. (See Section 5.2.2.)

(17). The PRT encourages continued TH modeling both at mountain scale (Bodvarsson, 1995), for support of performance assessment, and at repository scale (Buscheck and Nitao, 1995b), for design support.

(18). Improvements may be needed in the representation of infiltration on the upper boundary of TH models to properly reflect the spatial and temporal distribution of infiltration rates. Similarily, the appropriateness of using the water table as the lower boundary condition on TH simulations needs further investigation. (See Section 5.2.4.)

(19). Three dimensional TH simulations will be needed at the in-situ testing scale, but will not be feasible at mountain scale, where 2D simulations should suffice. Quasi-3D, and other hybrid modeling approaches, deserve attention. (See Section 5.2.4).

(20) Improved validation of TH models is required in connection with the next round of laboratory and field testing. A convincing demonstration is needed, using rigorous comparison of observations with prior predictions, rather than retroactive calibration and fitting. (See Sections 3.3 and 5.2.5)

(21). Uncertainty analysis of TH behaviour using traditional geostatistical analysis to analyse parameter uncertainty is neither feasible nor warranted. The PRT espouses an alternative approach involving hypothesis testing in a decision framework. Reductions in process uncertainty should have highest priority, followed by geological uncertainty, and then parameter uncertainty. (See Sections 3.4 and 5.2.6).

(22). THC modeling should move forward, but at a lower priority, and at a different scale than the current mountain-scale studies. The PRT would prefer to see simple scoping calculations first (the geochemical equivalent of Preuss and Tsang's TH scoping calculations), followed by numerical simulations at a scale that can be validated and calibrated by proposed laboratory and field tests. Another possible approach would be to try to apply thermochemical models, such as EQ3/EQ6, to conditions anticipated to occur at the boiling front, rather than trying to fully couple TH flow models and HC transport models. (See Section 5.2.3).

(23). THM modeling should also move forward, but at a lower priority, and at a scale suitable to validation and calibration testing with the LBT and LSLD tests. (See Section 5.2.3).

The most important of the above recommendations is the one associated with the ECM (16). The question remains unresolved as to whether the ECM can continue to form the basis for ongoing analyses. Clearly, comparisons between dual-porosity/dual-permeability and ECM conceptualizations are needed to establish the potential importance for non-equilibrium effects in relation to various energy-transport mechanisms. Such knowledge should make it possible to bound mountain-scale calculations where it is not now feasible to model non-equilibrium flow conditions. The obvious further step in code enhancement would be to utilize more fully the double porosity formulations of the available codes. However, given other uncertainties, such as the role of channeling on fracture planes, such an effort may not be warranted. Possibilities may exist in extending the present equivalent continuum approaches, but with pseudo-functions to account for nonequilbrium coupling.

A significant concern related to the ECM is the possibility for mismatches between the style of fracturing that is observed at YM and that represented implicitly in the codes through an isotropic formulation of k_{eff}. As indicated in Chapter 5, the averaging scheme in a situation with dominant vertical fracturing would overestimate horizontal flow (and convection) and underestimate the possibilities for focused vertical flow. As a preliminary step, there is a need to assess the extent of anisotropy produced within the key stratigraphic units by fracturing, and whether such effects explicitly need to be accounted for in the modeling.

In examining the question of model sufficiency, the PRT has concluded that there is an urgent need to settle on a modeling approach that overcomes, or a least can put in some perspective, the problems of the ECM discussed in this report. If the ECM approach turns out not to be appropriate, then analyses conducted with the model will be suspect. The YMSCP has made good progress in eliminating duplication of model effort, yet all of the key computational codes are essentially the same in their treatment of the ECM. Before moving forward on various "applied" fronts (e.g., repository designs, likely performance, test designs etc.), there must be a dedicated effort to resolve the ECM-related issues. It is likely that continued application of these ECM-based computational models in an "applied" mode will not continue to yield the same kind of important benefits that came from the earlier work.

Recommendation (22) also deserves further discussion. There has been an initial effort through Robinson's (1995) work to develop an understanding of how chemical processes may operate while the repository is being heated. The modeling approach remains in a developmental stage, and possible experiments to validate the theoretical underpinnings of the chemical interactions rest somewhere in the future. It is unlikely in the present fiscal environment that this modeling initiative can be moved forward fast enough to address key unknowns about the importance of THC coupling. The PRT believes, however, that the significant uncertainty associated with THC processes in general suggests that a potential for significant "surprises" remains a possibility. There remains an urgent need to address THC problems with alternative approaches including bounding analyses, analogue systems, and experiments. The design of the large underground experiment, in particular, must accommodate a strong initiative to sort out issues of THC coupling.

6.5 Programmatic Issues

Implicit in the Program Approach is a phased design to testing that assures that critical information is available when it is needed. In most cases, it is likely that testing programs will provide information in a timely manner. However, the thermohydrologic field tests require an intensive long-term effort to design the tests, set them up, and run them for an appropriately long period of time. In our deliberations, the PRT identified and discussed at length a major concern as to whether or not critical thermal testing could be accelerated to meet the needs of the YMSCP.

For the schedule implied by the Program Approach, the most significant field-based thermal-testing data that might be available for the determination of technical site suitability in 1998 would have been the Large Block Test. With this test apparently canceled, the next potential test will take place in the ESF. A minimum-scale test (the winged heater test) has been proposed that attempts to optimize the acquisition of thermohydrologic data in relation to the fast-track schedule implied by the Program Approach. The winged heater test will probably yield results that could provide input to licensing activities. However, the PRT is concerned that the test may not yield sufficient technical data required to resolve fully uncertainties about post-closure performance The technically more superior test (the LSLD test) likely cannot be executed and interpreted on a schedule that is appropriate to the Program Approach.

Beyond the issues of the technical merits of the tests are concerns about "style" in conducting scientific research. Some PRT members are uncomfortable with the notion of "one grand experiment" that is implied if the LSLD test is run without a shorter and perhaps technically less satisfying experiment as a precursor. If technical issues emerge from a long-term test, and that test is the only test, the project may not be in a position to deal with them adequately. In another context, some of us are concerned about the viability of a long-term program within the Yucca Mountain Project, given the conflicting priorities within such a large science and engineering project. In this light, our recommendation for reinstatement of the LBT, followed by the LSLD test, may strain management's ability to accept our recommendations.

Discussion that presents our evaluation of field-testing priorities reflects the difficulty the PRT has had in resolving these concerns. Inherently, all three of the experiments (LBT, drift-scale, and LSLD) involve various risks, especially if any one of them (and only one of them), is to represent the total field program for thermal testing at Yucca Mountain. All of the PRT are convinced that with any experiment alone, the project will fall below, or be very close to falling below, the minimum viable field program necessary to demonstrate understanding of thermally-driven processes.

If forced to choose one test, and one test only, the PRT comes down in favor of the LSLD test. In other words, scientific defensibility must overrule management-mandated scheduling and cost constraints.

6.6 Changing Regulations: A Moving Target

The U.S. Environmental Protection Agency is being directed to promulgate new standards to govern the performance of a repository at Yucca Mountain. As part of this process, Congress asked the National Academy of Science (NAS) to advise the agency in relation to the technical bases for the new standard. The recommendations of the NAS committee differ considerably from the present standards in three ways (NRC, 1995):

(1). The committee advocates replacing the 10,000-year release limits to the accessible environment by an individual-dose standard,

(2). The compliance with the dose-based standard must be measured at the time of peak risk, whenever it occurs; such times are likely to be tens or hundreds of thousands of years into the future, and

(3). The consequences of human intrusion, rather than the probability of human intrusion, should be determined.

If there is a change in the regulations that extends the period of compliance to very long times into the future and emphasizes peak doses, then there is much less performance benefit to be achieved with container or repository designs that simply delay the release of contaminants from the repository. In particular, the performance benefits of the extended dryout concept would become less obvious over the total compliance time. A case for performance would need to be made on the ability of repository heating to reduce peak doses, or possibly the geochemical immobilization of particular radionuclides.

Under revised regulations, there may be in fact little performance incentive to design the repository with high areal mass loadings. Without the final regulation in place, however, there is an implicit requirement for the program to remain flexible.

The possibility of a change in regulations does not relieve the program of the requirement to understand thermohydrologic processes. The theoretical and testing work must continue to understand the impacts of heating in the near and far field. Practical issues relating to limits on repository size and to the use of the MPC containers dictate that the repository will be strongly affected by thermal processes.

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Appendix A

PEER REVIEW PLAN FOR PEER REVIEW OF THE THERMOHYDROLOGIC MODELING AND TESTING PROGRAM

Purpose

The objective of the peer review is to evaluate the Yucca Mountain Site Characterization Project approach to understanding hydrothermal conditions at Yucca Mountain, Nevada that would be generated by repository heating. Questions that should be considered in developing this understanding are listed in Table A1. The approach is to be evaluated with the understanding that the information obtained from thermohydrologic tests and models will be used by performance assessment and design to assess behavior of the mountain under a thermal load. The evaluation is to include consideration of laboratory and in situ test design and sufficiency, and model sufficiency.

Scope

The scope of the Peer Review is to:

1. Evaluate a White Paper on Thermohydrologic Modeling and Testing including key references cited within.

2. Evaluate adequacy of laboratory and field experimental program to build confidence in understanding and predicting thermohydrologic processes and development of models.

3. Evaluate sufficiency of models and modeling approaches to predict moisture redistribution and changes in water chemistry in response to heat.

Criteria

The criteria to be applied in carrying out the Peer Review include:

1. validity of basic assumptions,
2. alternate interpretations,
3. adequacy of requirements,
4. appropriateness and limitations of methods and implementing documents,
5. adequacy of application,
6. accuracy of calculations,
7. validity of conclusions, and
8. uncertainty of results of impact if incorrect.

Quality Assurance

This peer review is in accordance with existing project requirements for quality assurance and with the YMP Office Quality Management Procedure, QAP 2.5, Peer Review.

TABLE A1

GENERAL QUESTIONS REGARDING THERMOHYDROLOGIC MODELING AND TESTING PROGRAM

1. Is the framework presented in the White Paper adequate for understanding thermohydrologic processes and conditions that may be present in a potential repository at Yucca Mountain?

2. Will testing described in the White Paper be adequate to support the development of conceptual models for thermohydrologic behavior of the site?

3. Does the White Paper cover the range of alternate conceptual models that must be considered for understanding the thermohydrologic behavior of the site?

   a. Are there parameters that have not been addressed that have greater sensitivity and should be addressed?

   b. What is the impact of not considering these process interactions?

4. Do the number, types, and spatial and temporal scales of proposed tests represent the range of conditions needed to build confidence in the thermohydrologic behavior of the site?

5. Do the coupled processes described in the White Paper reasonably encompass the range of effects associated with the influence of repository heat on the mountain?

6. Are there additional tests or analyses that would feasibly build additional confidence into understanding thermohydrologic behavior of the mountain?

7a. Is it reasonable to decouple thermohydrologic processes from thermomechanical and thermochemical processes in modeling behavior at the site?

7b. If it is not reasonable to decouple these processes, how might the coupling best be accomplished?

Peer Review Chairperson, Director's Representative, and Technical Secretary

The DOE Assistant Manager for Scientific Programs, Susan B. Jones, has appointed Dr. Paul A. Witherspoon, President of Witherspoon, Inc., as Chairperson. The Chairperson is responsible for conducting the peer review. The Assistant Manager's representative is Ardyth M. Simmons. Ms. Kathryn Mrotek has been appointed Technical Secretary. The Technical Secretary facilitates the peer review process and assures that a peer review record is compiled.

Peer Reviewers

The peer reviewers were selected according to QAP 2.5 and are listed in Appendix B.

Background Reading

The Peer Review Team will receive, approximately by June 23, 1995, a copy of "White Paper on Thermohydrologic Modeling and Testing at Yucca Mountain," which contains background information on the thermohydrologic program of modeling and testing at the Yucca Mountain Project plus selected key references. This background reading is required before the first meeting.

The team members will also receive a copy of QAP 2.5; prior to the first meeting the team members will read and acknowledge the requirements set forth in this document.

First Meeting

The Peer Review Team will be convened in Las Vegas on July 13, 1995. The purpose of the first meeting is to acquaint DOE with the peer review members and to develop a set of questions that will be addressed at the second meeting. The Peer Review Chairperson has prepared an agenda for this meeting, which will include an introduction and overview by the Assistant Manager for Scientific Programs, or her representative, technical presentations by the peer reviewers, a presentation on the Thermohydrologic Modeling and Testing Program, discussion of the issues on Table 1, and the preparation of a list of questions and topics for the Principal Investigators to address in the second meeting.

Reference Package

The Peer Review Team will be provided a selected package of representative publications that supplement the key references given in the White Paper and address the issues raised in the first meeting on the Thermohydrologic Modeling and Testing Program. The reference package is to be read before the second meeting.

Second Meeting

The second meeting of the Peer Review Team will be held in Las Vegas August 21-24, 1995. During this meeting the Principal Investigators will make presentations and answer further questions from the reviewers. Discussions of the presentations will follow, and the Thermo-hydrologic Modeling and Testing Program will be evaluated in the light of material presented to address the questions developed at the first meeting. A field trip to Yucca Mountain will take place on August 25, 1995.

Peer Review Record Memorandum

The Peer Review Team will prepare a summary report of their evaluations and findings that includes peer review agreements, any minority reports, conclusions and recommendations. Members of the Peer Review Team will provide results of their reviews and investigations to the Chairperson on October 25, 1995, and the Peer Review Report will be submitted to the YMSCO by the Chairperson by January 2, 1996. YMSCO will provide comments by the PIs on the Peer Review Report to the Chairperson by February 9, 1996. The Chairperson will provide the YMSCO with responses to these comments on March 8, 1996, and the Technical Secretary will submit the Peer Review Record Memorandum to YMSCO on March 29, 1996.

Records

The Technical Secretary will assure that a complete record is maintained of the Peer Review Team's actions. At the conclusion of the review, she will, with the assistance of the Chairperson, review all records for completeness, and assure that they are placed in the Project records system, in accordance with YAP17.1Q.

Appendix B

PEER REVIEW TEAM FOR THERMOHYDROLOGIC MODELING AND TESTING PROGRAM

	Expertise
1. Dr. Paul A. Witherspoon, Chairperson President, Witherspoon, Inc. 1824 Monterey Avenue Berkeley, CA 94707-2544 510-527-1680, FAX: 510-527-1336	Fluid flow in fractured and porous media. Large scale, underground hydraulic and thermal testing of fractured rocks. Multi-phase fluid flow modeling. Petroleum and geothermal reservoir behavior. Underground storage of liquids and gases. Underground radioactive waste isolation.
2. Dr. R. Allan Freeze, President R. Allan Freeze Engineering, Inc. 3755 Nico Wynd Drive White Rock British Columbia, Canada V4P1J1 604-538-8210, FAX: 604-538-8061	Applications of hydrogeological analysis in geotechnical projects, siting of nuclear and hazardous waste-management facilities, and remediation of contaminated sites. Numerical modeling of saturated, unsaturated, multiphase, and coupled flow. Decision analysis in engineering design of projects with a hydrogeological component. Analysis of worth of data in site characterization studies.
3. Dr. Francis A. Kulacki Department of Mechanical Engineering 125 Mechanical Engineering University of Minnesota Minneapolis, MN 55455 612-625-3807 FAX: 612-624-1398	Heat transfer, thermodynamics and fluid flow. Laboratory investigation of convective heat transfer in porous and fractured media. Physical and analytical modeling of near- and far-field thermohydrologic processes in a radioactive waste repository. Heat transfer in radioactive waste canisters.
4. Dr. Joseph N. Moore Research Professor and Senior Geologist Earth Sciences and Resources Institute The University of Utah 1515 East Mineral Square, Suite 109 Salt Lake City, UT 84112 801-584-4428, FAX: 801-584-4453	Geology and hydrogeochemistry of geothermal, epithermal, and contact metamorphic environments. Characterization of hydrothermal alteration of such environments through petrographic analyses, fluid inclusion systematics, and stable isotopes. Applications of tracers to fluid migration. Exploration and characterization of fracture-dominated geothermal resources.
5. Dr. Franklin W. Schwartz Ohio Eminent Scholar Department of Geological Sciences Ohio State University 125 South Oval Columbus, OH 43210 614-292-6196, FAX: 614-292-7688	Geochemistry of natural water systems. Flow and mass transport in fractured and porous media including dispersion. Reactive barrier technologies for metal immobilization. Reactive chemical transport. Convective instabilities in variable-density flow. Nuclear waste management.
6. Dr. Yanis C. Yortsos, Chairman Department of Chemical Engineering University of Southern California, HED216 925 West 37th Street Los Angeles, CA 90089-1211 213-740-0317, FAX: 213-740-8053	Fluid flow, fluid displacement processes, mass and heat transport, and chemical reactions in porous and fractured rocks. Phase change processes in porous media. Reservoir engineering of petroleum and geothermal systems. Application of thermal methods in porous media. Application of percolation and fractal methods. Mathematical and numerical modeling.

Appendix C

DOCUMENTS REVIEWED

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Appendix D

QUESTIONS FROM PEER REVIEW TEAM ON THERMOHYDROLOGIC MODELING AND TESTING PROGRAM

INTRODUCTION

To assist in its assessment of the Thermohydrologic Modeling and Testing Program, the Peer Review Team (PRT) has prepared a series of questions. The purpose of these questions is to provide a topical framework for the upcoming presentations by the Principal Investigators (PIs) during the August 21-24, 1995 meetings in Las Vegas. The questions are developed across five topical areas to solicit information concerned with:

- broad questions as to how the Yucca Mountain Project (YMP) is organized with emphasis on budgets, project schedules, strategies to support a license application, and modes of interaction with other research programs and customers,"

- the overall design of laboratory and field programs with emphasis on explaining project goals and objectives, describing the designs of experiments and interpretive techniques, and explaining how the work is integrated within the YMP as a whole,

- the main directions and approaches to be followed in the modeling effort with emphasis on the particular codes to be used, justification of the processes repre-sented in the mathematical models, expected results, and the relationship of these efforts to the laboratory and field tests, and

- how the program will deal with complex technical issues related to the geologic setting, hydrologic processes, thermo-hydrologic processes, thermo-mechanical processes, and thermo-chemical processes.

The PRT hopes that the August meeting can be structured to address these broad areas of concern. The Team is aware that the many questions that follow are complex, often open-ended, and sometimes unanswerable. We expect that as the PIs provide informational material about their investigations, they may be called upon to address these specific questions. To be most helpful, the briefing should include key members of the core research programs that have involved natural analogs, laboratory testing, field-scale testing, and modeling as well as managers who can address broad programmatic issues. The meetings would also benefit from brief presentations by the customers of the research, such as waste package design, repository design, and preclosure and postclosure performance assessment. Brief presentations by representatives of the site-suitability team and the licencing team would also be informative. Other specialists will be required to answer questions on geology and hydrogeology.

What the PRT will gain from these presentations is an understanding of the broad spectrum of activities being carried out in the thermal program, the details of various experiments and modeling activities, and the programmatic constraints. One specific request relates to the recent White Paper and concerns modeling and testing reports (page 23) with somewhat differing viewpoints on the behavior of the repository under conditions of high thermal loading. Given the importance of this issue, the Team attaches great importance to presentations by Drs. T. A. Buscheck and K. Pruess.

A. STRATEGIC ISSUES

The clients of the Yucca Mountain Site Characterization Project (YMSCP) need information and results for: (1) waste-package design, (2) repository design, (3) preclosure performance assessment, (4) postclosure performance assessment, (5) site suitability, and (6) preparation of licencing applications.

A.1 As currently planned, will the proposed YMSCP meet the needs of its clients?

A.2 What information will you have by 1998 from the ESF, laboratory and field investigations, and the modeling analyses to serve the needs of the site suitability determination? Will this information be sufficient to serve these needs?

A.3 What information will you have by 2001 to serve the needs of the initial licencing phase? Will this information be sufficient to serve these needs?

A.4 Specifically, will it be possible to, "bound our understanding of coupled processes to the degree that defensible calculation of postclosure performance can be made," by these dates?

B. ADEQUACY OF LABORATORY EXPERIMENTAL PROGRAM

B.1 Background Information

B.1.1 What laboratory tests have been undertaken or are planned, and what are their objectives in light of the Thermohydrologic Program?

B.1.2 Is the planned program fully funded?

B.1.3 What is the schedule for this program?

B.1.4 In relation to each of the proposed tests, explain what previous work has been performed and the results.

B.1.5 Are experiments not being conducted that should be conducted?

B.1.6 What evidence has been collected to demonstrate that the core samples are representative of the undisturbed rock mass? If such evidence has not been collected, what limitation does this place on the interpretation of the data?

B.1.7 Can a laboratory experiment be run that will adequately duplicate the two-phase flow and heat transfer behavior of the global repository system? If not, why not?

B.1.8 Can the T-H problem be parameterized so as to permit validation with laboratory experiments? If not, why not?

B.1.9 Provide brief details on the design of each of the experiments including: instrumentation, measurements to be made, interpretive techniques, potential errors and limitations, collection and handling of samples, interpretation of results, and techniques for scaling process parameter/measurements to the repository scale.

B.2 Laboratory Results

B.2.1 Which clients are the major customers for these results?

B.2.2 Summarize the results for each of the completed tests.

B.2.3 What are the major implications of these results in terms of the overall program?

B.2.4 Are these results consistent with the conceptual framework of the YMSCP approach?

B.2.5 Is there any evidence in the results from the testing of core samples that the thermal, mechanical, chemical or hydraulic parameters are temperature sensitive? What is the evidence?

B.2.6 Explain how the laboratory results can be used to address Strategic Issues A.2 and A.3.

C. ADEQUACY OF IN SITU FIELD TESTING

C.1 Background Information

C.1.1 What field tests have been undertaken or are planned and what are their objectives in light of the Thermohydrologic Program?

C.1.2 What is the schedule for the field experiments that are now planned and budgeted?

C.1.3 Are there experiments that might be useful in addressing Strategic Issues A.2 and A.3 that cannot be funded?

C.1.4 If additional funding cuts are required, what are the most critical field tests?

C.1.5 What evidence has been collected to demonstrate that the large and small block samples at have been, or are about to be, tested are representative of the *in situ* undisturbed rock mass?

C.1.6 Provide details on the design of the active experiments including: instrumentation, measurements to be made, interpretive techniques, modeling predictions of expected thermally driven rock behavior, potential errors and limitations, collection and handling of test samples, interpretation of results, techniques for scaling, scoping calculations that have been carried out for design, previous problems with instrumentation, and status of enabling technologies.

C.2 Field Test Results

C.2.1 Summarize the results for the most recent block and heater tests.

C.2.2 What has been learned in terms of overall program concerns?

C.2.3 Explain how results have been used to validate numerical models.

C.2.4 Explain how the results can be used to address Strategic Issues A.2 and A.3.

C.2.5 What is the uncertainty in the results of the completed experiments? Is this uncertainty associated with instrumentation problems or in the understanding of the geologic system?

C.2.6 How will this uncertainty impact modeling strategies and/or assumptions?

C.3 Planned Field Tests

C.3.1 Explain how the reference conditions on state of stress, permeability of the fractured rock mass, and water content at the site of the planned field tests will be determined prior to the application of heat.

C.3.2 Explain how modeling investigations will be used to predict changes in these reference conditions due to T-C and T-M effects.

C.3.3 Explain how changes in these reference conditions due to T-C and T-M effects will be determined.

C.3.4 Describe the magnitude and conditions of the heat pipe activity that will be developed in the planned field tests. How will this be verified?

C.3.5 Explain how this heat pipe activity can be considered as representative of what will develop on the repository scale.

C.3.6 Explain how the results can be used to address Strategic Issues A.2 and A.3.

D. SUFFICIENCY OF MODELING

D.1 Background

D.1.1 Present an overview of the existing and proposed modeling studies that briefly explains what models are being used, and what additional model developments are required.

D.1.2 What are the most important implications of the modeling results in terms of the overall program?

D.2 Dimensionality

Most published simulation studies on the global scale at YMP pertain either to a 2-D vertical cross-section or to an r-z model. The first ignores 3-D effects, while the second is based on an assumed angular symmetry in the properties.

D.2.1 What are the consequences of these idealizations in the prediction of process performance?

D.2.2 Would the introduction of 3-D analyses improve this prediction? What are the constraints preventing 3-D analysis?

D.3 Equivalent Continuum Model

The majority of simulations are based on the ECM version of various codes. To what extent is this adequate? In particular,

D.3.1 Discuss the appropriateness of ECM for describing fluid displacements, such as drainage and imbibition, in a network system of fractures and matrix blocks of variable sizes.

D.3.2 Discuss the appropriateness of ECM in modeling heat pipe activity, viz. heat pipe effects in fractures vs. the combined fracture-matrix.

D.3.3 Discuss the appropriateness of ECM in describing unstable phenomena such as gravity/capillarity driven flow in a fracture.

D.3.4 Discuss the appropriateness of ECM in modeling fluid flow through a network system of fractures whose apertures are a complex function of temperatures that are continually changing.

D.3.5 Discuss the effect of fracture orientation on ECM.

D.3.6 Discuss the implications of ECM to mass and heat transfer modeling, particularly when fluid flow is dominated by convection in fractures.

D.4 Validation and Calibration of Models

D.4.1 Given the complexity of the coupled physical processes, the heterogeneity of the geologic setting, and the uncertainties associated with the interpretation of *in situ* field tests, how will the process aspects of thermohydrologic models be validated?

D.4.2 Assuming process-level validation can be achieved through the field-testing program, how will models be calibrated for their predictive applications in repository design and performance assessment?

D.4.3 What laboratory results serve as a benchmark for validating models used to predict T-H processes?

D.4.4 What simplifications to the geologic setting are permissible that would provide more efficient modeling and appropriate bounds on repository performance?

D.4.5 What separate-effects experiments are planned to validate models?

D.5 Uncertainty

Given the uncertainty in site characterization and rock parameters, performance prediction is also subject to uncertainty.

D.5.1 If the thermohydrologic process is dominated by the uncertainty in some large-scale features, what are these features?

D.5.2 What modeling approach (e.g. Monte-Carlo simulation) would be pursued to incorporate stochastic aspects in performance prediction?

D.5.3 Are there alternatives to ECM modeling approaches that can be used for scale-up that incorporate these geostatistics?

D.5.4 What range of uncertainty in parameter values is acceptable for a robust process design?

D.6 Modeling Strategy

D.6.1 Is there a strategy for simplifying process-based models if and when certain processes are found to be of little importance to design decisions or performance measures?

D.6.2 Are there simpler alternatives to process-based modeling that might provide adequate bounding calculations to serve the needs of repository design and performance assessment?

E. SCIENTIFIC ISSUES

E.1 Geologic Setting

E.1.1 What are the characteristics of the faults and fractures (aperture, spacing, and orientation) and how variable are these characteristics?

E.1.2 What is the evidence for fracture controlled fluid flow (or fast paths) in the geologic record?

E.1.3 What evidence exists for the presence of geologically young water within the near field environment?

E.1.4 What is the variability in rock properties?

E.1.5 What is the orientation and magnitude of the present stress field? What does this imply about the orientation of fast paths?

E.1.6 How will relaxation of stress fields caused by excavation of adits affect long-term behavior of the near field environment?

E.1.7 How will stress fields change in response to heating? What effect will this have on the flow properties of the fractured rock mass?

E.1.8 What is the sensitivity of numerical models to variations in rock properties?

E.2 Hydrologic Processes

E.2.1 Does the concept of overlapping continua correctly represent the physics and hydraulics of fracture/matrix interactions? If not, what are the implications of using the concept as an idealized approach to the actual physics?

E.2.2 What are the ramifications of trying to develop analyses based on dual-porosity, dual-permeability media?

E.2.3 Summarize the conditions under which capillary barriers or other geologic configurations can create perched zones and/or focussed saturated flow in the vicinity of the repository. Have such zones been observed *in situ*?

E.2.4 Summarize the cases for and against fractures and/or fault planes acting as "fast paths" for saturated moisture redistribution. What field data is currently available to document or disprove the existence of fast paths? What is the current conceptualization of channel flow in such planes?

E.2.5 Has there been an improvement in understanding the above hydrologic issues in recent years? Is there the potential for improved understanding from currently proposed *in situ* observations and/or testing programs?

E.2.6 Is it possible that a level of irreducible uncertainty on these hydrologic issues has been reached, and if so, what would be the ramifications of such a realization?

E.2.7 What is the current conceptual model for infiltration at the ground surface? What are the current best estimates of the spatial and temporal distribution of infiltration rates? Is there likely to be episodic addition of meteoric water into the thermohydrologic system?

E.2.8 What estimates are available to determine the impact of discrete, large fractures on thermal and fluid transport in the thermally disturbed zone? Are these estimates supported by laboratory and/or field tests?

E.2 Hydrologic Processes (con't)

E.2.9 What are the characteristic time scales for buoyant convection (vapor/air and liquid) and heat pipe effects?

E.3 Thermal-Hydrologic Processes

E.3.1 What inherent uncertainty is estimated for calculations and measurements of temperature and heat flux?

E.3.2 What are the primary sources of this uncertainty and are they validated by data on thermophysical properties?

E.3.3 What accuracy is claimed for calculations, laboratory measurements, and field measurements in thermal-hydrologic processes?

E.3.4 Can this accuracy be validated either with laboratory or field experiments?

E.3.5 What bounding calculations of the thermal field have been made and on what basis (i.e., assumptions)?

E.3.6 Will 2-D calculations of the thermal field be adequate for licencing? If so, what benchmark provides assurance as well as an estimate of uncertainty?

E.3.7 If it is assumed that the waste packages maintain their integrity for 1,000 years, would the heat-transfer issues be significantly simplified? Could the problem be adequately bounded with either conduction or single-phase buoyant convection models?

E.3.8 What model simplifications for heat transfer and fluid flow can be imposed to provide long-range estimates of repository performance, especially in the thermally disturbed, near-field zone?

E.3.9 Can laboratory studies of key thermofluid processes reduce modeling complexity and uncertainty of results within the time frame available for the determination of site suitability in 1998?

E.4 Thermal-Mechanical Processes

E.4.1 What inherent uncertainty is estimated for mechanical deformations in fractures due to the changing thermal field?

E.4.2 What are the primary sources of this uncertainty?

E.4.3 What accuracy is claimed for calculations of the mechanical deformations of fractures?

E.4.4 How can this accuracy be validated?

E.4.5 To what extent will the thermally induced deformations in the fractured rock mass lead to a significant reduction in the permeability of this rock mass?

E.4.6 Is there the potential for such deformations to cause enough reduction in permeability that an effective barrier to fluid flow can develop either above and/or below the repository level?

E.4.7 If such barriers can develop, will the overall effect result in a significantly different thermohydrologic behavior of the repository system than is predicted by the ECM vestigations?

E.5 Thermal-Chemical Processes

E.5.1 What mineralogical changes will occur in the matrix and fractures of the rock mass in response to heating and the formation of heat pipes?

E.5.2 How will these mineralogical changes affect the mechanical properties of the rock mass (i.e., volume increases due to alteration of glass; dehydration of clays and zeolites; formation of clays, zeolites, quartz, etc.)?

E.5.3 Is there the potential for a coupling of T-M and T-C processes leading to the development of an effective barrier to fluid flow either above and/or below the repository level?

E.5 **Thermal-Chemical Processes (con't)**

E.5.4 If such barriers can develop, will the overall effect result in a significantly different thermohydrologic behavior of the repository system than is predicted by the ECM investigations?

E.5.5 What will the effect of these fluid-rock alterations be on the chemistry of the fluids? What is the importance of these changes?

E.5.6 What measurements will be made in analogue systems to determine the importance and extent of certain fluid-mineral interactions within the heat pipe?

E.5.7 How will these observations be applied to increase confidence in repository performance?

E.5.8 Have you identified other processes in natural systems that are relevant to the repository environment?

E.5.9 To what extent can fluid-vapor behavior in the very small pore spaces of the matrix be modeled using the standard treatment for porous media?

F.6 **Critical Processes**

There appear to be two critical processes associated with the proposed concept of a high temperature repository: (a) the formation of a dryout zone around the drift, and (b) the delayed re-wetting by condensate during the cooling-down period.

F.6.1 What are the critical factors that control these processes?

F.6.2 What is the sensitivity of these processes to external perturbations, such as a sudden and concentrated increase in the infiltration rate?

F.6.3 What is the effect on these processes, and on the corresponding design of the thermal load, of the expected heterogeneity and anisotropy in rock and fracture parameters?

F.6.4 Are there any other processes that can be identified as critical?

F.6.5 What range of uncertainty in the knowledge of these factors is acceptable for a robust design?

F.6.6 What are the implications of a lower-temperature design? Would design and/or performance-assessment issues be mitigated, exacerbated, or remain about the same?

Appendix E

JULY 13, 1995 - LIST OF MEETING ATTENDEES

Name	Organization
Tom Buscheck	LLNL
Victor Dulock	M&O/TRW
Allan Freeze*	RAF Engineering
Dwight Hoxie	USGS
Francis Kulacki*	Univ. of Minnesota
Srikanta Mishra	M&O/Intera
Joseph Moore*	University of Utah
Kathy Mrotek	M&O/WCFS
John Nitao	LLNL
Bruce Robinson	LANL
Franklin Schwartz*	Ohio State Univ.
Ardyth Simmons	DOE
Dale Wilder	LLNL
Dennis Williams	DOE/AMSP
Paul Witherspoon*	Witherspoon, Inc.
Yanis Yortsos*	USC

*Peer Review Team

August 21-24, 1995 - List of Meeting Attendees **

Name	Organization
Pat Auer	YMQAD
Juliana Banks	DOE
H.A. Benton	M&O/BWFC
Kal Bhattacharyya	M&O
David Bish	LANL
Steve Blair	LLNL
Bo Bodvarsson	LBNL
William Boyle	DOE
Stephan Brocoum	DOE
Tom Buscheck	LLNL
Gillies Bussod	LANL
H.Y. Cadoff	DOE
Dwayne Chesnut	LLNL
Bill Clarke	LLNL
Tom Clemo	M&O/Intera
Peter Davies	SNL
Victor Dulock	M&O/TRW
June Fabrynk-Markin	LANL
Jerry Fairley	M&O/WCFS/LBNL
Bill Glassley	LLNL
Chad Glenn	NRC
Steve Hanauer	DOE
Diane Harrison	DOE
John Hevesi	USGS
Dwight Hoxie	USGS
Raymond Keeler	DOE

August 21-24, 1995 - List of Meeting Attendees (con't)**

Name	Organization
John Kessler	EPRI
Wunan Lin	LLNL
Srikanta Mishra	M&O/Intera
Bimal Mukhopakhyay	M&O
Bill Nelson	M&O/Intera
John Nitao	LLNL
N.V. Palciauskus	NWTRB
Russell Patterson,	DOE
Mark Peters	M&O/WCFS
Karsten Pruess	LBNL
Bruce Robinson	LANL
Ralph Rogers	M&O/WCFS
Bill Seddan	AECL
Keith Sheldon	SAIC
Scott Sinnock	TRW
Ken Skipper	DOE
John Stuckless	USGS
Tim Sullivan	DOE
Vincent Tidwell	SNL
Yvonne Tsang	LBNL
Abe Van Luik	DOE
Dale Wilder	LLNL
Dennis Williams	DOE/AMSP
Rob Yasek	DOE

**In addition to the Peer Review Team

Participant MO Prepared - 11/13/95:09:40:52	Yucca Mtn. Site Char. Project-Planning & Control System PACS Participant Work Station (PPWS) Participant Planning Sheet (PSA03)	01-Sep-95 to 30-Sep-95 Page - 1 Inc. Dollars in Thousands

P&S Account No. - 1.2.3.9.10 TR

P&S Account Title - Special Studies: Project Peer Review

WBS No. - 1.2.3.9.10

WBS Title - Special Studies: Project Peer Review

BASELINE Start Date - 10/01/95
BASELINE Finish Date - 09/30/96

Element ID - TR39A

Fiscal Year Distribution

	Prior	FY1996	FY1997	FY1998	FY1999	FY2000	FY2001	FY2002	FY2003	FY2004	FY2005	Future	At Complete
Annual Budget	0	297	0	0	0	0	0	0	0	0	0	0	297

Statement of Work:

The following quality affecting work shall be controlled in accordance with approved implementing procedures identified on the current OCRWM-accepted Requirements Traceability Network Matrix

QARD applies to this effort.

Provide peer review of documents, plans, criteria, data, or models produced by YMP participants. Provide management support to peer reviews as defined in relevant project procedures. Coordinate Project participants in the peer review process. Identify and qualify peer reviewers from within and outside the Project. Participate in peer reviews. Maintain records of peer reviews. Coordinate changes to documents or activities with participants as a result of peer reviews.

DELIVERABLES

Deliv ID	Description/Completion criteria	Due Date
TRWF1	Thermohydrologic Peer Review Report Criteria - This deliverable shall be satisfied by submittal to YMSCO of the Thermohydrologic Peer Review Report. The report shall include the findings and recommendations of the peer review panel in accordance with YMSCO procedure QAP 2.5. ~~The deliverable will be submitted in accordance with procedure YAP 5.1Q~~. 11/13/1995 RAR 11/13/95 11/13/95	15-Dec-95

Participant MO
Prepared - 11/13/95:09:40:52

Yucca Mtn. Site Char. Project-Planning & Control System
PACS Participant Work Station (PPWS)
Participant Planning Sheet (PSA03)

01-Sep-95 to 30-Sep-95
Page - 2
Inc. Dollars in Thousands

P&S Account No. - 1.2.3.9.10 TR -Special Studies: Project Peer Review

DELIVERABLES

Deliv ID	Description/Completion criteria	Due Date
TRWF1		
TRWF2	Rspnses to Comnts Recomnds Made Thrmohydro PRR Criteria - This milestone shall be satisfied by submittal of a letter report to YMSCO that transmits responses to comments and recommendations made in the Thermohydrologic Peer Review Report. The deliverable will be submitted to YMSCO in accordance with procedure ~~YAP-5.10.~~ QAP 2.5. 11/13/1995 11/13/95 RAK 11/13/95	01-Mar-96

P&S Account No. - 1.2.3.9.10 TR -Special Studies: Project Peer Review

DELIVERABLES

Deliv ID	Description/Completion criteria	Due Date
TRWF2		
TRWF3	Peer Review Record Memorandum (PRRM) Criteria - This milestone shall be satisfied by submittal of the PRRM to YMSCO. The PRRM shall include the peer review notice, peer review plan, peer review report, DOE's determination response, responses to comments and recommendations made to the Thermohydrologic Peer Review Report, and other correspondence. This deliverable will be submitted to YMSCO in accordance with procedure YAP 5.1Q.	01-Apr-96

Participant MO
Prepared - 11/13/95:09:40:52

Yucca Mtn. Site Char. Project-Planning & Control System
PACS Participant Work Station (PPWS)
Participant Planning Sheet (PSA03)

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P&S Account No. - 1.2.3.9.10 TR -Special Studies: Project Peer Review

Approvals

THOMAS STATTON 11/13/95
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DENNIS R. WILLIAMS 11/13/1995
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